UNIVERSIDADE DE SÃO PAULO

ESCOLA POLITÉCNICA

PAULO ALENCAR PEREIRA

ESPECIAÇÃO DOS METAIS BÁRIO E CÁDMIO E SUAS IMPLICAÇÕES EM AVALIAÇÕES DE RISCO À SAÚDE HUMANA PARA CONSUMO DE ÁGUAS SUBTERRÂNEAS

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Ao Manequinho por ceder gentilmente suas mesas para as proveitosas discussões sobre tudo na vida...

RESUMO

PEREIRA, Paulo Alencar. Especiação dos metais bário e cádmio e suas implicações em avaliações de risco à saúde humana para consumo de águas subterrâneas. 2020. 66 f. Monografia (MBA em Gestão de Áreas Contaminadas, Desenvolvimento Urbano Sustentável e Revitalização de Brownfields) – Escola Politécnica, Universidade de São Paulo, São Paulo, 2020.

Os metais são encontrados em diferentes concentrações na natureza e, nas águas subterrâneas podem ter origem natural ou antrópica. A especiação dos metais é função, principalmente, das condições de pH e ORP, levando a diferentes estados de valência, complexos metálicos ou precipitados, por exemplo. As espécies de alguns metais, como ferro e cromo, por exemplo, podem ser quantificadas adequadamente a depender das metodologias de coleta e análises químicas laboratoriais de amostras de águas subterrâneas. Isso, no entanto, não é possível para todos os metais. A utilização de modelos hidrogeoquímicos, dessa forma, é fundamental nas avaliações de contaminações por metais em águas subterrâneas e na definição de alternativas de remediação. A toxicidade dos metais pode mudar totalmente a depender da espécie em que é encontrado reforçando, portanto, a importância de um estudo hidrogeoquímico. Várias técnicas de remediação de águas subterrâneas contaminadas por metais têm origem no tratamento de águas residuárias e objetivam a precipitação dos metais, reduzindo as concentrações das formas dissolvidas a valores próximos ou inferiores aos limites de detecção analíticos. Nestes casos, assume-se que os metais precipitados formam espécies estáveis e que não implicam riscos à saúde humana. Os procedimentos de gerenciamento de áreas contaminadas no mundo, contudo, recomendam que as concentrações de metais totais sejam sempre utilizadas nas avaliações de risco, mesmo em casos onde seja possível quantificar as espécies tóxicas. Essa premissa, ainda que conservadora, leva a riscos mais elevados. Tendo em vista a abordagem conservadora recomendada na fase inicial de gerenciamento de uma área contaminada, as concentrações de metais totais são adequadas para a avaliação de risco preliminar. Nos cenários mais detalhados e onde houver compreensão clara das condições hidrogeoquímicas da área contaminada, as concentrações de metais na forma dissolvida ou nas espécies tóxicas aos seres humanos são mais adequadas para o estabelecimento de Metas de Remediação baseadas em risco. No presente estudo, foi avaliada a hidrogeoquímica para os metais bário e cádmio. O primeiro foi escolhido por existir, preferencialmente em sua forma estável e não tóxica de sulfato de bário, em ampla faixa de pH (1-12) e na presença de sulfato. O segundo, por existir preferencialmente na forma iônica (seja em pares de íons com sulfato, cloreto ou outros ânions) que é a mais tóxica aos seres humanos. Os resultados do modelo hidrogeoquímico mostram que a abordagem de adoção de concentrações totais em avaliações de risco à saúde humana para metais é conservadora e pode levar a superestimativas de riscos. A especiação dos metais é fundamental para que se tenha uma avaliação de riscos mais representativa das condições reais em áreas contaminadas.

Palavras-chave: bário; cádmio; águas subterrâneas; hidrogeoquímica; análise de risco.

ABSTRACT

PEREIRA, Paulo Alencar. Barium and cadmium speciation and its implications in human health risk assessment to groundwater human consumption. 2020. 66 f. Monografia (MBA em Gestão de Áreas Contaminadas, Desenvolvimento Urbano Sustentável e Revitalização de Brownfields) – Escola Politécnica, Universidade de São Paulo, São Paulo, 2020.

Metals are found in different concentrations in nature and, in groundwater, they can be from natural or anthropogenic origin. Metals speciation is a function, mainly, of pH and ORP conditions, leading to valence states, metallic complexes or precipitated, for example. Metals species, like iron and chromium ones, for example, can be determined metal depending upon groundwater sampling and analytical methods employed. This is not the case for all metals. Hydrogeochemical models application, this way, is a fundamental tool in groundwater metals contamination evaluation and remedial alternative definition. Metals toxicity may change totally based on its species found, reinforcing, therefore, the importance of hydrogeochemical evaluation. Several remediation techniques to metals contaminated groundwater are based on wastewater treatment technologies and aim metals precipitation, reducing dissolved species concentrations to values close or lower than their analytical detection limits. In these cases, it is assumed that precipitated metals are their most stable condition and do not imply in risks to human health. Contaminated sites management procedures, however, recommend total metals concentration to be used in risk assessment, even in cases where the most toxic species can be quantified. This conservative principle leads to higher risks. Considering the prudent approach recommended on initial steps in contaminated sites management, total metals concentrations are adequate to a preliminary human health risk assessment. In a detailed scenario where the a clear understanding of contaminated site hydrogeochemistry is available, dissolved species or the most toxic forms of metals concentrations are more adequate to establish risk based remediation goals. In this study, barium and cadmium hydrogeochemistry were evaluated. The first one was chosen because of its main species stable and non toxic characteristics, as this metal exists primarily as barium sulfate in a broad pH range (1-12) and in the presence of sulfate. The second, due to its main form being its ionic species (forming ion-pairs with sulfate,chloride or other anions) that is the most toxic to humans. The results of the hydrogeochemical model have shown that using total metals concentrations in human health risk assessment is a conservative approach and can overestimate the real risks. Metals speciation, therefore, is fundamental to a more representative (more realistic conditions) risk assessment in contaminated sites.

Keywords: barium; cadmium; groundwater; hydrogeochemistry; risk assessment.

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LISTA DE ABREVIATURAS E SIGLAS

ABNT	Associação Brasileira de Normas Técnicas
AI	Área Contaminada Sob Investigação
ASTM	American Society for Testing and Materials
ASTDR	Agency for Toxic Substances and Disease Registry
CalEPA	California Environmental Protection Agency
CAS	Chemical Abstracts Service
CETESB	Companhia Ambiental do Estado de São Paulo
CMA	Concentração Máxima Aceitavel
CONAMA	Conselho Nacional do Meio Ambiente
CPF	Carcinogenic Potency Factor
CRS	Congressional Research Service
CTC	Capacidade de Troca Catiônica
DD	Decisão de Diretoria
EUA	Estados Unidos da América
GAC	Gerenciamento de Áreas Contaminadas
HEAST	Health Effects Assessment Summary Tables
I	Dose de Ingresso ou Ingresso
I_C	Dose de Ingresso – crônica média diária
I_V	Dose de Ingresso – integral (vida) média diária
IARC	International Agency for Research on Cancer
ICP-AES	Inductively Coupled Plasma – Atomic Emission Spectroscopy
ICP-MS	Inductively Coupled Plasma – Mass Spectrometry
IP	Índice de Perigo
IPCS	International Programme on Chemical Safety
IRIS	Integrated Risk Information System
IS	Índice de Saturação
K_{sp}	Produto de Solubilidade
LNLL	Lawrence Livermore National Laboratory
MCE	Modelo Conceitual de Exposição
MCL	Maximum Contaminant Level
MS	Ministério da Saúde
NBR	Norma Brasileira

LISTA DE ABREVIATURAS E SIGLAS (conclusão)

NRC	National Research Council
NTP	National Toxicology Program
OMS	Organização Mundial da Saúde
ORP	Oxidation-reduction potential
OSTP	Office of Science and Technology Policy
PAI	Produto de Atividade Iônica
pH	Potencial Hidrogeniônico
phreeqc	pH-REdox-EQuilibrium-C
PVC	Policloreto de Vinila
r_{XY}	Coeficiente de Correlação Linear (ou de Pearson)
RAGS	Risk Assessment Guidance for Superfund
RC	Risco Carcinogênico
RfD	Reference Dose/Dose de Referência
RSL	Regional Screening Level
SF	Slope Factor/Fator de Carcinogenicidade
UFF	Universidade Federal Fluminense
USEPA	United States Environmental Protection Agency
USGS	United States Geological Survey
USP	Universidade de São Paulo
VI	Valor de Investigação
VO	Valor Orientador

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1. INTRODUÇÃO

As águas subterrâneas são utilizadas para diferentes finalidades na sociedade, como consumo humano, processos industriais e agropecuária. Apesar disso, correspondem a uma pequena fração da água disponível no planeta Terra (~4%), sendo a maior parte da água (94%) encontrada em mares e oceanos com elevada salinidade (FREEZE e CHERRY, 1979).

Por conta de sua natureza, as águas subterrâneas contêm substâncias químicas que podem ter origens naturais ou antropogênicas (contaminações). Dentre essas substâncias, os metais são relevantes por conta da essencialidade de alguns deles para os seres vivos (funções nos organismos), bem como pela existência de concentrações limites acima das quais podem levar a problemas na saúde humana. (TCHOUNWOU *et al.*, 2012).

A toxicidade dos metais é função direta das formas/espécies em que se encontram nas águas subterrâneas, seja em sólidos em suspensão (adsorvidos, complexados, precipitados) ou na forma dissolvida. Os efeitos tóxicos são estudados, em geral, com as espécies solúveis e mais biodisponíveis dos metais. Os resultados obtidos nesses estudos servem de base para o estabelecimento de parâmetros toxicológicos que são utilizados em Avaliações de Risco à Saúde Humana visando estabelecer concentrações máximas a que os seres humanos podem ser expostos (seja pela ingestão, seja pelo contato dérmico) sem que efeitos deletérios sejam esperados (USEPA, 1989).

Apesar dessas peculiaridades, os parâmetros toxicológicos são definidos para os metais, em geral, para todas as suas formas sem considerar suas espécies e comportamentos no ambiente (sejam aquelas utilizadas nos estudos toxicológicos, sejam aquelas encontradas nas águas subterrâneas). Isso decorre também das metodologias de análises químicas de águas subterrâneas atualmente disponíveis, que objetivam predominantemente quantificar todas as formas dos metais presentes nas amostras. Algumas exceções para os estados de valência, como ferro e cromo, ou em moléculas orgânicas, como arsênio e chumbo orgânicos (inespecíficos), ou metilmercúrio.

Em face a esse contexto, e tendo em vista a necessidade de melhor compreensão das condições a que estão expostos os seres humanos, a modelagem hidrogeoquímica é uma ferramenta fundamental e útil para a avaliação da especiação

de metais em águas subterrâneas, bem como dos estados de solubilidade (precipitação/dissolução) dos minerais, indicando quais podem existir na forma solúvel (que pode ser também biodisponível) e quais são precipitados e deixam a solução.

Neste trabalho, foi utilizado um modelo hidrogeoquimico para avaliar a distribuição das espécies dos metais bário e cádmio em águas subterrâneas. O primeiro foi escolhido por predominar em águas subterrâneas a forma estável e não tóxica de $BaSO_4$ em ampla faixa de pH na presença de sulfato acima de 0,7 mg/L (DEUTSCH, 1997). O segundo, foi escolhido por predominar a forma iônica (em pares de íons com SO_4^{2-} ou Cl^-) em valores de pH abaixo de 8, que pode ser absorvida no sistema gastrointestinal e é tóxica aos seres humanos.

Estes dois metais foram escolhidos pela disponibilidade de dados hidrogeoquímicos na literatura científica nacional (representativos de regiões no Brasil) e a existência de poucos estudos publicados a respeito de seus comportamentos em casos de contaminações de águas subterrâneas. Para outros metais, alguns mais tóxicos, a exemplo de chumbo e cromo, diversos estudos já existem nas literaturas nacional e internacional.

1.1 Objetivos

O objetivo principal desta monografia é avaliar a influência da especiação dos metais bário e cádmio em águas subterrâneas nos resultados de avaliações de riscos à saúde humana para a via de ingestão de água.

São objetivos específicos deste trabalho:

- Identificar as principais espécies de bário e cádmio em águas subterrâneas.
- Avaliar os estados de solubilidade dos minerais barita e witherita para o bário, do mineral otavita para o cádmio em águas subterrâneas.
- Quantificar os riscos à saúde humana para concentrações dos metais bário e cádmio em águas subterrâneas considerando a precipitação de seus minerais.

2. REVISÃO BIBLIOGRÁFICA

No presente capítulo, são abordados tópicos relacionados ao tema, referentes às diferentes características dos metais bário e cádmio (físico-químicas e toxicológicas), ao tratamento de dados e etapas do gerenciamento de áreas contaminadas, e à avaliação de riscos à saúde humana seguindo protocolos internacionais e nacionais.

2.1 Propriedades Físicas e Químicas e Usos/Aplicações de Bário e Cádmio

Os dados de identificação (número CAS, fórmula química e estrutura química) e de propriedades físicas e químicas (massa atômica/peso molecular, densidade e solubilidade em água) dos metais bário e cádmio, e suas principais espécies, são apresentados na Tabela 1. Resumos dos principais aspectos, bem como dos usos mais relevantes, para ambos os metais, seguem nos subitens 2.1.1 e 2.1.2.

Tabela 1 – Dados de identificação e propriedades físicas e químicas dos metais bário e cádmio e suas principais espécies (Fonte: HSDB, 2020).

Metal/Espécie	Número CAS	Fórmula Química	Estrutura Química	Massa molecular (g/mol)	Densidade (g/cm^3)	Solubilidade em água (mg/L)	
Bário e Principais Espécies							
Bário	7440-39-3	Ba	Ba	137,327	3,62	Reage com a água	
Carbonato de bário	513-77-9	$BaCO_3$	$[Ba^{2+}][CO_3^{2-}]$	197,340	4,31	14,0	(20 ºC)
Cloreto de bário	10361-37-2	$BaCl_2$	$[Ba^{2+}][Cl^-]_2$	208,233	3,90	370.000,0	(25 ºC)
Hidróxido de bário	17194-00-2	$Ba(OH)_2$	$[Ba^{2+}][OH^-]_2$	171,342	4,50	49.100,0	(25 ºC)
Sulfato de bário	7727-43-7	$BaSO_4$	$[Ba^{2+}][SO_4^{2-}]$	233,390	4,49	3,1	(20 ºC)
Sulfeto de bário	21109-95-5	BaS	$[Ba^{2+}][S_{2-}]$	169,393	4,30	89.400,0	(25 ºC)
Cádmio e Principais Espécies							
Cádmio	7440-43-9	Cd	Cd	112,410	8,65	2,3	-
Carbonato de cádmio	513-78-0	$CdCO_3$	$[Cd^{2+}][CO_3^{2-}]$	172,420	4,58	3,2	-
Cloreto de cádmio	10108-64-2	$CdCl_2$	$[Cd^{2+}][Cl^-]_2$	183,320	4,05	457.000,0	(25 ºC)
Sulfato de cádmio	10124-36-4	$CdSO_4$	$[Cd^{2+}][SO_4^{2-}]$	208,470	4,69	540.000,0	(25 ºC)
Sulfeto de cádmio	1306-23-6	CdS	$[Cd^{2+}][S_{2-}]$	144,480	4,82	6,00E-07	(18 ºC)

2.1.1 Bário

O bário é um elemento químico localizado no Grupo 2 (IIA) e no Período 6 da Tabela Periódica, na família dos metais alcalinos-terrosos, com número atômico 56. Seu estado de oxidação é o +2 (Ba^{2+}). Pode ser encontrado muito raramente na forma gasosa em compostos com o flúor no estado de oxidação +1 (LUO *et al.*, 2018).

É bastante reativo e não é encontrado em sua forma pura na natureza. Os principais minerais em que é encontrado na natureza são a barita ($BaSO_4$) e witherita ($BaCO_3$) (McCOMISH e ONG, 1988).

Seus compostos têm diversos usos atualmente, sendo um dos principais a adição da barita (sulfato de bário) à lama de perfuração na indústria de Óleo e Gás para ajustar a densidade em função da pressão hidrostática requerida para a coluna de lama. No Brasil é utilizada apenas a barita (BALTAR e DA SILVA, 2003).

O sulfato de bário é também utilizado na fabricação de tintas, tijolos, vidros e borracha. Outros compostos, como o carbonato de bário, o cloreto de bário e o hidróxido de bário são utilizados na indústria cerâmica, na fabricação de venenos para ratos e insetos, e em aditivos de óleos e combustíveis. O sulfato de bário é utilizado algumas vezes como contraste para execução de testes médicos e raios-X (ATSDR, 2007).

2.1.2 Cádmio

O cádmio é um elemento químico localizado no Grupo 12 e no Período 5 da Tabela Periódica, na família dos metais de transição e seu número atômico é 48. Seu estado de oxidação é o +2 (Cd^{2+}).

Este metal não é abundante da natureza, e obtido principalmente como subproduto do processamento da esfalerita (minério de zinco – ZnS), e em menores quantidades em minérios de cobre e de chumbo. A greenockita (CdS) é o principal mineral do cádmio para a indústria de mineração, quase sempre encontrado em conjunto com a esfalerita. (LLEWELLYN, 1994).

O cádmio e seus compostos são utilizados principalmente para ligas metálicas, revestimentos (*coatings*), baterias de níquel-cádmio (NiCd), pigmentos e, no passado, em estabilizantes para plásticos de PVC (USGS, 2020b). Seu uso já foi predominante

em eletrodos de baterias de NiCd, chegando a 83% do uso total (USGS, 2008). Mais recentemente, seu uso tem sido reduzido com a substituição por baterias de íon lítio.

2.2 Características Hidrogeoquímicas

2.2.1 Bário

A maior parte do bário originado em atividades industriais está em formas que têm pouca dispersão no ambiente (NG e PATTERSON, 1982). No meio aquático, o sulfato de bário ($BaSO_4$) e o carbonato de bário ($BaCO_3$) são as formas que podem limitar as concentrações de bário devido às suas rápidas cinéticas de precipitação, o primeiro independente do pH, enquanto que o último para valores de pH acima de 9,3 (Rai *et al.*, 1984 *apud* McCOMISH e ONG, 1988), mecanismo natural de remoção do bário das águas superficiais e subterrâneas. Pode também adsorver em sólidos suspensos com a formação de pares iônicos com ânions naturais, tais como os bicarbonatos e os sulfatos (USEPA, 1984).

Em ambientes aquáticos, contendo os íons Cl^-, SO_4^{2-}, NO^{3-} e CO_3^{2-}, e pH menor que 9,3, o íon Ba^{2+} é a espécie dominante (McCOMISH e ONG, 1988). A precipitação do bário é acelerada em ambientes aquáticos com elevadas concentrações de sulfatos (>1.000 mg/L) (OMS, 1990).

Verbruggen *et al.* (2020) observaram em estudo realizado com amostras de águas superficiais na Holanda uma forte correlação entre as concentrações de bário e sulfato na fração dissolvida (filtrada com filtro de 0,45 µm), sendo uma indicação de que grande parte do bário na amostra filtrada estava, na realidade, presente como barita ($BaSO_4$) finamente dispersa.

No solo, o bário tem reduzida mobilidade, sobretudo devido à formação de sais insolúveis e pelo íon Ba^{2+} não formar complexos solúveis com os ácidos fúlvicos e húmicos (USEPA, 1984; OMS, 1990).

O transporte do bário do solo para as águas subterrâneas depende, principalmente, da capacidade de troca catiônica (CTC) do solo, da concentração de carbonato de cálcio e de sulfatos, e do pH. Em solos com elevada CTC (e.g., solos de textura fina ou com alto teor de matéria orgânica), a mobilidade do bário será limitada pela adsorção, enquanto concentrações elevadas de $CaCO_3$ ou sulfatos implicarão na precipitação do bário ($BaCO_3$ ou $BaSO_4$) no meio subterrâneo. (HSDB, 2020).

Diagramas de equilíbrio potencial-pH (ou diagramas de Pourbaix) para os sistemas Ba-O-H (bário-água) e Ba-S-O-H-C são apresentados nas Figuras 1 e 2, respectivamente (POURBAIX, 1974; BROOKINS, 1988).

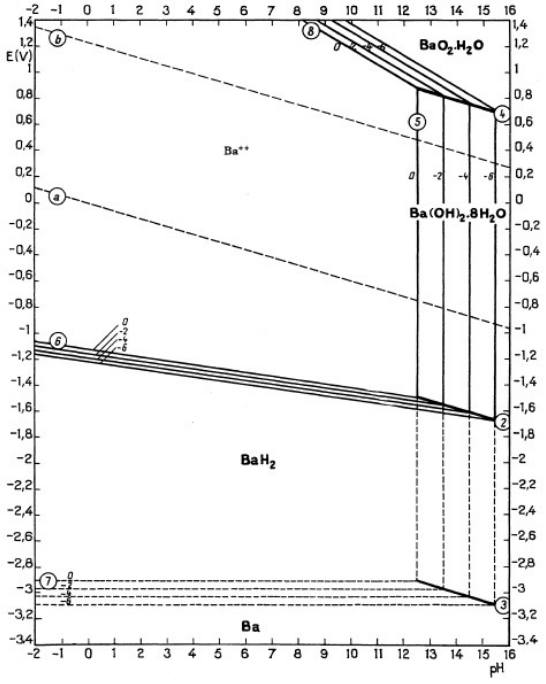
No sistema bário-água, o metal está na forma iônica na maior parte das faixas de pH e potencial redox (*Oxidation-reduction potential – ORP*), mas representam apenas situações teóricas, já que sempre estão presentes outros elementos e íons. O bário, assim como os demais metais alcalinos terrosos, é muito instável em soluções aquosas ao longo de toda a faixa de valores de pH e tenderia a existir na forma catiônica Ba^{2+} (POURBAIX, 1974).

No sistema Ba-S-O-H-C, com maior representatividade para as condições naturais em águas subterrâneas, a espécie predominante é o $BaSO_4$ para quase toda a faixa de valores de pH (entre 1,5 e 12). Apenas em condições bastante alcalinas é indicada a existência do $BaCO_3$. Isso é refletido em seus próprios minerais, com o predomínio da barita (sulfato de bário) em ambientes de estabilidade dos sulfatos e dissolvida em ambientes muito redutores onde o H_2S é estável (USGS, 2017).

2.2.2 Cádmio

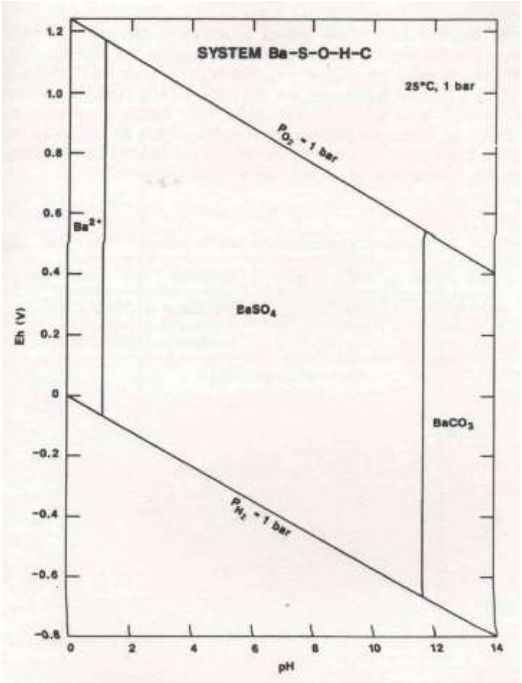
O cádmio é o elemento que apresenta a maior mobilidade dentre aqueles comumente classificados como “metais pesados” (ATSDR, 2012; CALLAHAN *et al.*, 1979). Este metal permanece em solução em valores de pH próximos ao neutro (pH<6,5) ao contrário de outros “metais pesados” (KUBIER *et al.*, 2019a). Sua especiação é similar à do zinco, ainda que seja mais altamente complexado com o íon cloreto em água (McCOMISH e ONG, 1988). Em águas naturais (sem impactos antrópicos), a maior parte do cádmio existirá na forma dissolvida como o íon $Cd(H_2O)_6^{2+}$. (ATSDR, 2012).

Figura 1 – Diagrama de equilíbrio potencial-pH (diagramas de Pourbaix) para o sistema bário-água à 25 °C.



Fonte: Adaptado de Pourbaix (1974).

Figura 2 – Diagrama de equilíbrio potencial-pH (diagramas de Pourbaix) para o sistema Ba-S-O-H-C à 25 °C.



Fonte: Adaptado de Brookins (1988).

Em condições redutoras, o sulfeto de cádmio pode ser formado em uma ampla faixa de pH (1-14) na presença do íon sulfeto (FAUSTY e ALY, 1981). A precipitação na forma de sulfeto é um fator importante na mobilidade do cádmio em ambientes redutores, sendo este metal muito mais móvel em ambientes oxidantes (McCOMISH e ONG, 1988; HOLMES *et al.*, 1974).

Em ambientes oxidantes, o íon carbonato regula a solubilidade do cádmio. Como exemplo, em uma solução com pH 8,3 e sem CO_3^{2-}, o $Cd(OH)_2$ corresponde à fase sólida com solubilidade de 637 mg/L, enquanto que com a presença do carbonato a solubilidade pode reduzir até 0,11 mg/L, em função da reduzida solubilidade do $CdCO_3$ (FERGUSSON, 1982).

Resultados de estudos experimentais de tratamento de água com precipitação por carbonatos realizados por Patterson *et al.* (1975) indicaram que é muito mais eficiente do que os hidróxidos. As concentrações máximas de cádmio nos efluentes foram de 1,7 mg/L com o uso de carbonatos (pH entre 8,4 e 10,8) e de 126 mg/L com os hidróxidos (pH entre 8,6 e 11,9).

Cádmio associado a minerais carbonáticos, precipitado como compostos sólidos estáveis ou co-precipitados como óxidos hidratados de ferro, são menos propensos a serem mobilizados pela ressuspensão de sedimentos ou por atividade biológica. O cádmio adsorvido em superfícies minerais como argilas ou matéria orgânica é mais facilmente liberado para sua forma dissolvida (CALLAHAN *et al.*, 1979) com a perturbação dos sedimentos.

Os principais fatores que regulam a mobilidade do cádmio em solos são pH, reações de oxirredução e a formação de complexos (BERMOND e BOURGEOIS 1992; HERRERO E MARTIN 1993 *apud* ATSDR, 2012). O cádmio pode ser lixiviado do solo para a água, especialmente sob condições ácidas (ELINDER 1985a; EPA 1979).

Kubier *et al.* (2019b) estudaram uma base de dados de mais de 6.300 poços no noroeste da Alemanha para avaliar possíveis níveis naturais (*background levels*) de cádmio em águas subterrâneas. As concentrações elevadas encontradas (de até 0,98 µg/L) foram atribuídas principalmente às características dos depósitos glaciais locais. O metal pode ter sido liberado por indução antropogênica, seja devido à acidificação ligada a denitrificação de fertilizantes nitrogenados ou como impurezas em fertilizantes fosforados nas áreas de agricultura (KUBIER *et al.*, 2019a; KUBIER *et*

al., 2019b) devido à associação com o nitrato encontrada em dados de áreas de agricultura.

Diagramas de equilíbrio potencial-pH (ou diagramas de Pourbaix) para os sistemas Cd-O-H (cádmio-água) e Cd-C- S-O-H são apresentados nas Figuras 3 e 4, respectivamente (POURBAIX, 1974; BROOKINS, 1988).

Em solução aquosa (água e cádmio), o metal existirá na forma iônica Cd^{2+} na maior parte das faixas de pH e ORP. Apenas em valores de pH acima de 10 passaria a existir na forma de $Cd(OH)_2$ e perto do pH de valor 14 como CdO_2^- ou $HCdO_2^-$.

O composto $CdCO_3$ é pouco solúvel, sendo a principal forma em condições alcalinas, na faixa de pH entre 8 e 11, como se observa no gráfico da Figura 4. Ainda assim, pode ocorrer a partir de valores de pH pouco abaixo de 6,5 a depender da configuração/mistura de íons presentes (LONG e ANGINO, 1977).

2.3 Aspectos Toxicológicos

2.3.1 Bário

O fator mais relevante para o desenvolvimento de efeitos à saúde humana é a solubilidade do composto de bário a que se está exposto. O íon Ba^{2+} e os compostos solúveis (principalmente cloreto, nitrato e hidróxido de bário) são tóxicos aos seres humanos. O carbonato de bário tem reduzida solubilidade (ver Tabela 1), mas é solúvel no trato gastrointestinal e, dessa forma, tóxico aos humanos. O sulfato de bário que é pouco solúvel, por sua vez, não é tóxico aos humanos (ATSDR, 2007).

Os estudos toxicológicos publicados na literatura utilizaram, em sua maioria, o cloreto de bário como composto fonte/fornecedor do bário. O carbonato de bário também é utilizado em parte dos estudos.

A reduzida toxicidade do sulfato de bário é evidenciada por sua aplicação na medicina como contraste radiológico do tubo gastrointestinal. O “Caso Celobar®” é o caso mais conhecido de intoxicação por bário no Brasil (CABRAL, 2003; TUBINO e SIMONI, 2007). O sulfato de bário era adquirido junto a um fabricante especializado, mas em um dos lotes do produto o laboratório decidiu sintetizá-lo a partir do carbonato de bário com a adição de ácido sulfúrico. Como resultado, o produto apresentou além do sulfato de bário, o carbonato de bário, com 44,7% de $BaSO_4$ e 13,2% de $BaCO_3$ em massa (TUBINO e SIMONI, 2007).

Figura 3 – Diagrama de equilíbrio potencial-pH (diagramas de Pourbaix) para o sistema cádmio-água à 25 °C.

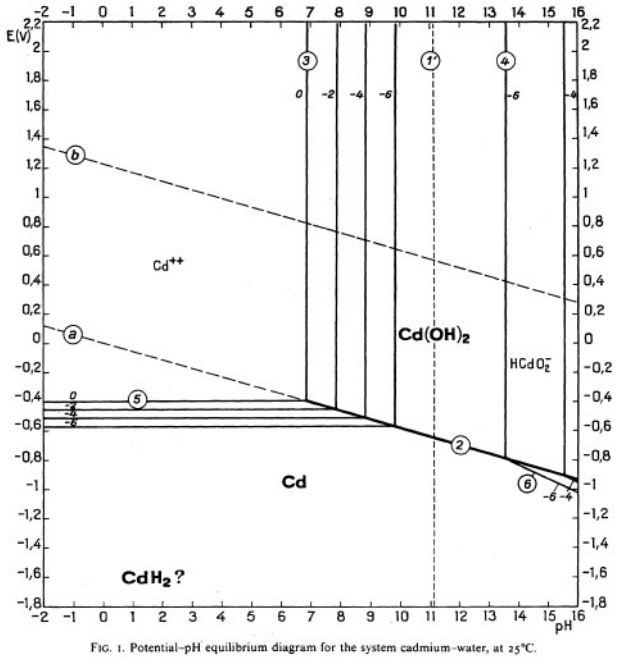


FIG. 1. Potential–pH equilibrium diagram for the system cadmium–water, at 25°C.

Fonte: Adaptado de Pourbaix (1974).

Figura 4 – Diagrama de equilíbrio potencial-pH (diagramas de Pourbaix) para o sistema Cd-C-S-O-H à 25 °C.

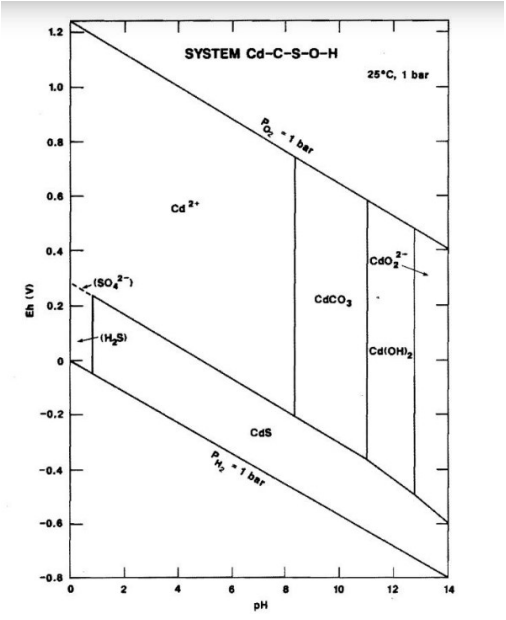


Fig. 25. Eh-pH diagram for part of the system Cd-C-S-O-H.
The assumed activities for dissolved species are: Cd = 10^{-8}, C = 10^{-3}, S = 10^{-3}.
See text for discussion

Fonte: Adaptado de Brookins (1988).

O principal efeito adverso à saúde humana observado nos estudos com os compostos cloreto de bário e carbonato de bário é a hipocalemia, que pode resultar em taquicardia ventricular, hipertensão e/ou hipotensão, fraqueza muscular e paralisia (ATSDR, 2007; USEPA, 2005; OMS, 1990). Isso decorre da ação competitiva do bário no mecanismo de fluxo extracelular/intracelular do potássio (ATSDR, 2007). Segundo ATSDR (2007), apesar de alguns dos estudos não reportarem as doses utilizadas, seus valores devem ter sido elevados, haja vista que estudos com doses reduzidas não encontraram efeitos adversos à saúde humana.

Um estudo com ratos identificou nefropatias como resultado de exposições crônicas e subcrônicas pela ingestão de água com cloreto de bário dihidratado (NTP, 1994). As doses utilizadas nesse estudo foram de até 60 mg/kg-dia para os machos e 75 mg/kg-dia para as fêmeas, por períodos entre 13 semanas e 2 anos.

A carcinogenicidade dos compostos de bário não foi avaliada pela IARC. Eles não são classificáveis quanto à carcinogenicidade aos humanos pela USEPA e estão inseridos no Grupo D (USEPA, 2012).

Os parâmetros toxicológicos para o bário disponíveis nas bases de dados internacionalmente referenciadas são apresentados na Tabela 2.

2.3.2 Cádmio

Uma grande quantidade de estudos toxicológicos sobre os efeitos do cádmio em humanos e em animais de laboratório foi realizada desde o início da década de 1950, quando os perigos da exposição ocupacional ao cádmio foram reconhecidos. As propriedades toxicológicas do cádmio são similares para seus diferentes compostos (sais e óxidos) investigados, e as diferenças nos comportamentos de absorção e distribuição podem levar a efeitos diferentes (ATSDR, 2012).

Para a maior parte da população, a rota de exposição mais provável é pela ingestão na dieta (ATSDR, 2012). A exposição ocupacional e de grupos populacionais sob condições ambientais específicas (ou expostos a contaminações antrópicas) foram os principais focos de estudos toxicológicos.

O caso mais conhecido de contaminação humana por cádmio ocorreu em Toyama no Japão, na bacia do rio Jinzu. O rio foi contaminado pela atividade de extração de zinco na mina de Kamioka. Os efeitos na saúde humana ficaram conhecidos como “Doença de Itai-Itai”. As principais características da doença são

osteomalacia e osteoporose com uma tendência a fraturas acompanhadas de dores severas e disfunção tubular renal (OMS, 1992; AOSHIMA, 2016; NISHIJO *et al.*, 2017).

O órgão crítico para contaminação humana crônica por cádmio é o rim, sendo o córtex o local de ocorrência dos primeiros efeitos adversos, enquanto que o efeito crítico é a disfunção tubular renal (OMS, 1992). Outros sistemas do organismo humano podem ser também afetados, como o sistema gastrointestinal, o sistema hematológico e o sistema hepático (ATSDR, 2012).

Evidências em estudos em laboratório com animais indicam que a inalação de cádmio pode causar câncer de pulmão. A maioria dos estudos para a via oral com animais em laboratório não encontrou aumentos significativos na incidência de câncer (ATSDR, 2012).

A IARC classificou o cádmio como carcinogênico para humanos como parte do Grupo 1 (IARC, 1987b) e a USEPA classificou o metal como provável carcinógeno para humanos por inalação como parte do Grupo B1 (USEPA, 1987). As classificações foram baseadas nas evidências limitadas em humanos e evidências suficientes em ratos de que o cádmio pode causar câncer de pulmão (IARC, 1987a).

Os parâmetros toxicológicos para o cádmio disponíveis nas bases de dados internacionalmente referenciadas são apresentados na Tabela 2.

2.4 Metodologias de Coleta e Análises Químicas de Metais em Amostras de Águas Subterrâneas

Os procedimentos de coleta e de análises químicas para determinação de metais em amostras de águas subterrâneas podem influenciar e até alterar adversamente os resultados analíticos obtidos (PULS e BARCELONA, 1989; PULS e POWELL, 1992).

A adoção de procedimentos de coleta que possibilitem a obtenção de amostras mais representativas possíveis das condições do aquífero, assim como metodologias analíticas que levem em consideração as características hidrogeoquímicas do local de origem da amostra, é fundamental para trabalhos que envolvam concentrações de metais.

Tabela 2 – Parâmetros toxicológicos para os metais bário e cádmio.

Substância	Nº CAS	Clas. USEPA [a]	Grupo IARC [a]	SFO	IUR	RfDo	RfC_i
				$(mg/kg\text{-}dia)^{-1}$	$(\mu g/m^3)^{-1}$	(mg/kg-dia)	(mg/m^3)
Bário	7440-39-3	D	-	-	-	2,0E-01 [d]	5,0E-04 [e]
Cádmio (dieta) [b, c]	7440-43-9	B1	1	-	1,8E-03 [d]	1,0E-03 [d]	1,0E-05 [f]
Cádmio (água) [b, c]	7440-43-9	B1	1	-	1,8E-03 [d]	5,0E-04 [d]	1,0E-05 [f]

Legenda:

- Campos indicados com hífen correspondem às vias de ingresso e substâncias sem parâmetros toxicológicos.

SFO - *Slope Factor Oral* (Fator de Inclinação para Exposição Oral).

IUR - *Inhalation Unit Risk* (Risco Unitário para Exposição por inalação).

RfDo - *Reference Dose for Oral Exposure* (Dose de Referência para Exposição Oral).

RfCi - *Reference Concentration for Inhalation Exposure* (Concentração de Referência para Exposição por Inalação).

Observações:

a - As colunas USEPA e IARC se referem às classificações de carcinogenicidade das substâncias.
USEPA "D": Não classificável quanto à carcinogenicidade em humanos.
USEPA "B1": Provável carcinógeno humano, baseado em evidência limitada de carcinogenicidade em humanos.
IARC "Grupo 1": Carcinogênico para humanos.

b - Doses de Referência para Exposição Oral (RfDo) para ingestão de alimentos (dieta) e ingestão de água (água).

c - Evidências de que o cádmio pela via de inalação pode causar câncer de pulmão em estudos com ratos (ATSDR, 2012). A maioria dos estudos de exposição pela via oral não encontrou aumentos significativos na incidência de câncer.

d - Integrated Risk Assessment Information System (IRIS).

e - Health Effects Assessment Summary Tables (HEAST).

f - Agency for Toxic Substances and Disease Registry (ATSDR).

2.4.1 Metodologias de Coleta de Amostras de Águas Subterrâneas

Os procedimentos de amostragem de águas subterrâneas incluem a purga do poço para retirada de água estagnada em seu interior e a coleta propriamente dita da amostra.

Os dois principais métodos de purga utilizados no Brasil são com uso do *bailer* e com bomba de baixa vazão, que são descritos detalhadamente no Manual de Gerenciamento de Áreas Contaminadas da CETESB (CETESB, 2001) e na norma técnica da ABNT NBT 15847:2010 – Amostragem de Água Subterrânea em Poços de Monitoramento – Métodos de Purga (ABNT, 2010). A purga com *bailer* foi utilizada desde os primeiros trabalhos ambientais na década de 1970, enquanto que a purga por baixa vazão passou a ser utilizada nos EUA em meados da década de 1990 (BARCELONA *et al.*, 2005).

Os métodos de purga por baixa vazão são atualmente os mais adequados para amostragem de águas subterrâneas para determinação de metais, evitando

perturbações no poço e a coleta de materiais em suspensão que não são representativos dos constituintes da formação de interesse (PULS e BARCELONA, 1989). Os procedimentos com purga por *bailer* e outros métodos que possam suspender sedimentos (induzir turbidez) na coluna d'água devem ser evitados sempre que possível (PULS e POWELL, 1992).

Após as coletas, as amostras podem ser enviadas ao laboratório como coletadas (correspondendo aos "metais totais") ou serem filtradas em campo com filtro com diâmetro de poros de 0,45 µm antes do envio ao laboratório (correspondendo aos "metais dissolvidos"). Os valores de "metais dissolvidos" são aqueles utilizados nas modelagens hidrogeoquímicas, pois correspondem às frações dissolvidas/em solução nas águas subterrâneas.

2.4.2 Metodologias de Análises Químicas de Metais em Amostras de Águas Subterrâneas

Diferentes técnicas analíticas laboratoriais foram desenvolvidas ao longo das últimas décadas para determinação de metais em amostras de água, incluindo o bário e o cádmio. Uma lista dos principais métodos analíticos e respectivas técnicas disponíveis na literatura atualmente é apresentada na Tabela 3. Esses métodos são também recomendados para análises de metais em amostras de águas potáveis nos EUA e no Canadá (USEPA, 2019; Health Canada, 2020).

As principais técnicas utilizadas em laboratórios comerciais no Brasil para detecção de bário e cádmio em água atualmente são:

- Espectrometria de massa com plasma acoplado indutivamente (*Inductively coupled plasma - mass spectrometry – ICP-MS*).
- Espectrometria de Emissão Atômica com plasma acoplado indutivamente (*Inductively coupled plasma - atomic emission spectroscopy – ICP-AES*).

Os métodos podem ser utilizados para determinação de metais totais e metais dissolvidos, diferenciando na fase de preparação das amostras. Os metais dissolvidos são analisados na amostra de água filtrada com filtro de 0,45 µm.

Nas análises para determinação de bário, a digestão ácida com ácido nítrico é o método mais comum de preparação das amostras (ATSDR, 2007). Tendo em vista suas características hidrogeoquímicas, predomina o composto $BaSO_4$ para valores de pH entre 1 e 12 independentemente do valor de ORP (ver diagrama potencial-pH na

Figura 2). Assim, esse método de digestão pode levar a maiores concentrações do íon Ba^{2+} pela separação do $BaSO_4$ presente (que pode estar precipitado em partículas finas, mesmo nas amostras filtradas). Esse é o principal fator de interferência nos resultados analíticos, haja vista que o bário não adsorve em material suspenso em quantidades significativas na água (VERBRUGGEN *et al.*, 2020).

Tabela 3 – Principais métodos e técnicas analíticas laboratoriais para determinação dos metais bário e cádmio em amostras de água.

Método Analítico	Técnica Laboratorial
EPA 200.5 – Rev 4.2	Axially viewed inductively coupled atomic emission spectrometry (AVICP-AES)
EPA 200.7 – Rev 4.4	Inductively coupled plasma-atomic emission spectrometry (ICP-AES)
EPA 200.8 – Rev 5.4	Inductively coupled plasma-mass spectrometry (ICP-MS)
EPA 200.9 – Rev 2.2 (específico para cádmio)	Stabilized Temperature Graphic Furnace Atomic Absorption
SMWW 3111 D (específico para bário)	Flame atomic absorption spectrometry
SMWW 3113 B	Electrothermal atomic absorption spectrometry
SMWW 3120 B	Inductively Coupled Plasma (ICP)
SMWW 3125 B	Inductively Coupled Plasma/Mass Spectrometry (ICP-MS)
ASTM D4382-18 (específico para bário)	Atomic Absorption Spectrophotometry, Graphite Furnace
ASTM D3557-17 (específico para cádmio)	Atomic Absorption Spectrophotometry and Differential Pulse Anodic Stripping Voltammetry

O cádmio é encontrado em sua forma dissociada (Cd^{2+}) na maior parte das condições de pH-ORP das águas subterrâneas. Apenas para valores acima de 8 tende a existir no composto $CdCO_3$, ou como CdS para condições redutoras na presença de sulfeto (ver diagrama potencial-pH na Figura 4). As principais interferências nos métodos analíticos para determinação de cádmio estão relacionadas com a presença de constituintes orgânicos na amostra (ácidos húmicos ou surfactantes que podem adsorver nos eletrodos) e de outros metais, como zinco, cálcio e magnésio (SASAKI *et al.*, 2015; ADAMCYK e GRABARCZYK, 2019).

2.5 Padrões de Referência Ambiental para Águas Subterrâneas

O Gerenciamento de Áreas Contaminadas (GAC) no Brasil é realizado com base na Resolução do Conselho Nacional do Meio Ambiente (CONAMA) nº 420 de 28/dezembro/2009. Nesta resolução, foram estabelecidas as diretrizes que devem nortear essa atividade, bem como os padrões de referência, denominados Valores Orientadores (VOs) para a presença de substâncias químicas em solo e águas subterrâneas a serem utilizados.

Os VOs para as águas subterrâneas foram designados como Valores de Investigação (VIs) e correspondem "*a concentração de determinada substância no solo ou na água subterrânea acima da qual existem riscos potenciais, diretos ou indiretos, à saúde humana, considerando um cenário de exposição padronizado*".

Os procedimentos para GAC da Resolução CONAMA nº 420/2009 foram baseados na experiência do órgão ambiental do estado de São Paulo (CETESB) e a legislação em vigor naquele estado. Em 2009, vigorava a Decisão de Diretoria (DD) nº 103/2007/C/E de 22/junho/2007, que foi revogada pela DD nº 038/2017/C de 07/fevereiro/2017.

Os padrões de referência da Resolução CONAMA nº 420/2009 foram os mesmos adotados na época pela CETESB no estado de São Paulo e estabelecidos na DD nº 195-2005-E de 23/novembro/2005. Foi utilizada a mesma nomenclatura de VOs, mas modificada para VIs, que naquele estado corresponde a Valores de Intervenção. A definição é similar, com mudança apenas no termo de definição do cenário de exposição, como segue: "a concentração de determinada substância no solo ou na água subterrânea acima da qual existem riscos potenciais, diretos ou indiretos, à saúde humana, considerado um cenário de exposição **genérico** (grifo nosso)".

Para as substâncias não listadas na Resolução CONAMA 420/209, recomendou-se, em seu Art. 31, § 1º, que o órgão ambiental competente e o órgão gestor de recursos hídricos definisse ações específicas para cada caso.

A CETESB, dessa forma, definiu em sua DD nº 038/2017:

> "Para substâncias químicas de interesse ou meios não contemplados na referida Decisão de Diretoria, deverão ser utilizados os valores definidos na última atualização dos *Regional Screening Levels* (RSLs), desenvolvidos pela *United States Environmental Protection Agency* (US EPA) ou calculados a partir da Planilha de Avaliação de Risco da CETESB. Para as substâncias

> que não constarem nessas listas, poderão ser utilizadas listas de valores orientadores produzidas por outras entidades reconhecidas".

Em relação aos metais, as duas principais normas existentes no Brasil, Resolução CONAMA nº 420/2009 e DD nº 256/2016/E da CETESB para o Estado de São Paulo, estabelecem VOs inespecíficos, ou seja, sem indicar a condição de amostragem/análise (totais ou dissolvidos) e/ou as formas/espécies em que podem ser encontrados nas águas subterrâneas. Para os VOs para bário e cádmio, objetos do estudo deste trabalho, foram adotados os valores constantes no padrão de potabilidade nacional estabelecido pelo Ministério da Saúde (Portaria MS nº 518 de 25/março/2004, revogada pela Portaria MS nº 2.914 de 12/dezembro/2011, mas com os mesmos valores para bário e cádmio). Atualmente, está em vigor a Portaria de Consolidação nº 5 de 28/setembro/2017 do MS, que mantém os mesmos valores da portaria de 2011.

Diferentemente, na Resolução CONAMA nº 357/2005 (incluindo suas alterações posteriores), que dispõe sobre a classificação e diretrizes ambientais para corpos de água superficiais, os valores máximos para alguns metais são especificados para concentrações totais e fração dissolvida. Para os metais bário e cádmio, os valores máximos para águas superficiais foram estabelecidos para suas concentrações totais (bário total e cádmio total).

Os padrões de referência estadunidenses elaborados pela USEPA para águas subterrâneas são denominados *Regional Screening Levels (RSL)* e são utilizados como base de comparação para definir a necessidade de ações de investigação e/ou remediação em áreas contaminadas. Os RSLs apresentam um avanço em relação àquelas normas em vigor no Brasil, pois para vários metais são consideradas as principais formas/espécies que podem ser encontradas em águas subterrâneas.

Como exemplo, os RSLs para chumbo foram calculados para quatro formas (fosfato de chumbo; acetato de chumbo; sub-acetato de chumbo básico ou básico; e chumbo tetraetila) além do valor inespecífico para chumbo, que é oriundo do padrão de potabilidade estadunidense (*Maximum Contaminant Level – MCL*). Já para os metais bário e cádmio, contudo, os RSLs abordam da mesma forma que no Brasil, sendo indicados apenas os padrões de referência sem especificar condições amostrais (total/dissolvido) ou formas/espécies.

Tendo em vista a hidrogeoquímica do bário e do cádmio, e suas toxicidades, as diferentes formas/espécies em que estes metais podem ser encontrados em águas

subterrâneas devem ser consideradas seja na identificação, seja na gestão de áreas contaminadas. Os VOs em vigor no Brasil são úteis para a classificação como Área Contaminada sob Investigação (AI), como previsto na Resolução CONAMA nº 420/2009.

A necessidade de ações de intervenção em função do uso do solo (atual e possíveis usos futuros) para uma determinada área, no entanto, deve ser baseada nos resultados de uma avaliação de riscos à saúde humana. Esta avaliação deve, essencialmente, considerar as formas como os metais estão presentes dadas as condições hidrogeoquímicas das águas subterrâneas na área. Isto, no entanto, não está previsto na Resolução CONAMA nº 420/2009 tampouco na DD nº 038/2017 da CETESB.

Os padrões de referência para concentrações de bário e cádmio em águas subterrâneas nas diferentes normas supracitadas são apresentados na Tabela 4.

Tabela 4 – Padrões de Referência ambientais para águas subterrâneas no Brasil, nos EUA e na Holanda.

Metal	Nº CAS	Unidade	CONAMA 420/2009	CETESB DD 256/2016/E	MS-BRASIL PC 5/2017	USEPA RSL (maio/2020)	VROM/Holanda (2013)
Bário	7440-39-3	µg/L	700	700	700	2.000	625
Cádmio	7440-43-9	µg/L	5	5	5	5	6

2.6 Metodologias de Avaliação de Risco à Saúde Humana

A Avaliação de Risco à Saúde Humana é um processo analítico sistemático para avaliar, gerenciar e comunicar riscos à saúde humana decorrentes de contaminantes liberados e/ou contidos naturalmente no ambiente em que os seres humanos vivem. Uma avaliação de risco abrange uma grande variedade de disciplinas, incluindo geologia, hidrologia, ecologia, toxicologia, biologia, química, física, dentre outras (FJELD et al., 2007).

A avaliação de questões envolvendo os riscos à saúde humana devido à exposição a substâncias é bastante antiga. O questionamento dos cientistas sobre a possibilidade de risco de desenvolvimento de câncer por pessoas expostas a baixas concentrações de substâncias reconhecidamente carcinogênicas em altas concentrações foi muito grande durante a década de 1950 e guiou várias legislações

da época. Como exemplo, pode-se citar a “Cláusula Delaney” (*Delaney clause*) da emenda de 1958 à Lei de Aditivos Alimentícios estadunidense (*Public Law 85-929*) que em sua Seção 409(c)(3)(A) estabeleceu que nenhum aditivo que reconhecidamente fosse carcinogênico a seres humanos ou animais fosse permitido nos alimentos por não ser possível estabelecer um nível seguro de exposição humana (NRC, 1994).

Na década de 1980, o Congresso dos EUA solicitou diversos estudos para avaliar os procedimentos e metodologias de avaliação de risco existentes na época para diferentes tipos de exposição, como a medicamentos, a alimentos, a contaminações ambientais, etc. Os principais documentos públicos consolidando os resultados dos estudos são: *Risk Management in the Federal Government: Managing the Process* (NRC, 1983); *A Review of Risk Assessment Methodologies* (CRS, 1983); *Chemical Carcinogens: A Review of the Science and Its Associated Principles* (OSTP, 1985).

Os procedimentos para realização de Avaliação de Risco à Saúde Humana mais utilizados atualmente são:

- *Risk Assessment Guidance for Superfund (RAGS), Volume I, Human Health Evaluation Manual (Part A)* da Agência Ambiental Estadunidense (USEPA, 1989).
- *Standard Guide for Risk-Based Corrective Action Applied at Petroleum Release Sites ASTM E1739 – 95(2015)* da Sociedade Americana de Testes e Materiais (ASTM, 2015a).
- *Standard Guide for Risk-Based Corrective Action ASTM E2081 – 00(2015)* da Sociedade Americana de Testes e Materiais (ASTM, 2015b).
- *Public Health Assessment Guidance Manual* da Agência para Registro de Substâncias Tóxicas e Doenças dos EUA (ATSDR, 2005).

Esses quatro procedimentos foram publicados por instituições estadunidenses e possibilitam a avaliação quantitativa de riscos à saúde humana, cujos valores numéricos são comparados com as legislações em vigor para definição de condições adequadas, ou não, para exposição de seres humanos.

Os três primeiros procedimentos são voltados para casos de contaminações ambientais em que os seres humanos podem estar expostos, enquanto que o quarto aborda a questão do ponto de vista da saúde pública.

Todos esses procedimentos estão estruturados em quatro etapas principais, a saber (NRC, 1983):

- Identificação do Perigo.
- Avaliação da Relação Dose-Resposta (Toxicologia).
- Avaliação da Exposição.
- Caracterização do Risco.

No Brasil, o primeiro procedimento para análise de risco à saúde humana foi publicado pela CETESB em seu Manual de Gerenciamento de Áreas Contaminadas (CETESB, 2001), incluído no Capítulo 9 da segunda edição do manual.

Em outubro/2009 a CETESB disponibilizou, em seu endereço eletrônico, planilhas em formato Excel® padronizando esse procedimento que foram posteriormente atualizadas em maio/2013. De forma a possibilitar seu uso nas diferentes condições hidrogeológicas e distintos contaminantes, a CETESB estabeleceu valores padrões para os parâmetros de exposição dos receptores, propriedades físicas, químicas e toxicológicas dos contaminantes. Em relação ao meio físico, é possível editar os parâmetros intrínsecos à cada área contaminada. Essas planilhas da CETESB foram elaboradas para os seguintes receptores:

- Residente Rural (criança/adulto).
- Residente Urbano (criança/adulto).
- Trabalhador Comercial/Industrial (adulto).
- Trabalhador de Obra Civil (adulto).

Mais recentemente, com a publicação da DD n° 038/2017/C, a CETESB esclareceu uma dúvida comum a respeito das concentrações utilizadas como dado de entrada. De forma conservadora, aquele órgão demandava a utilização das concentrações máximas detectadas na área contaminada para o cálculo dos riscos. No item 4.1.6.1 da DD n° 038/2017/C, foi apresentada a possibilidade de realização de tratamento estatístico, o que torna a avaliação de risco mais próxima das condições locais em vários casos.

A Associação Brasileira de Normas Técnicas (ABNT) publicou em 2013 a norma brasileira (NBR) 16209 intitulada “Avaliação de risco a saúde humana para fins de gerenciamento de áreas contaminadas” estabelecendo um roteiro para esses tipos de trabalho. Todas as metodologias de avaliação de risco em uso no Brasil foram baseadas no procedimento RAGS da USEPA (USEPA, 1989).

As características intrínsecas dos diferentes grupos de compostos existentes na natureza devem ser consideradas em uma avaliação de risco à saúde humana. Para os metais, estudados neste trabalho, os processos de absorção, distribuição, transformação e excreção dependem do metal e forma ou composto em que se encontra (USEPA, 2007; OMS, 2006).

Tendo em vista a estrutura e as etapas dessas metodologias que utilizam como dado de entrada as concentrações do metal em águas subterrâneas, um estudo hidrogeoquímico considera-se fundamental para que as espécies a que estarão efetivamente expostos os receptores, e suas características toxicológicas, sejam avaliadas.

3. METODOLOGIA

Neste trabalho, foi realizado um estudo de caso com dados publicados na literatura científica de concentrações dos metais bário e cádmio em águas subterrâneas. Os dados levantados foram utilizados em um modelo numérico hidrogeoquímico e posteriormente calculados os riscos à saúde humana associados às concentrações destes dois metais, bário e cádmio.

Os dados obtidos na literatura são descritos na seção 3.1. O modelo hidrogeoquímico utilizado é apresentado na seção 3.2, enquanto que a metodologia de avaliação de risco à saúde humana é abordada na seção 3.3.

3.1 Levantamento de Dados Hidrogeoquímicos

Os dados hidrogeoquímicos utilizados neste trabalho foram obtidos em estudos da Universidade de São Paulo (USP) e da Universidade Federal Fluminense (UFF). São relativos a amostras de águas subterrâneas coletadas em poços tubulares de quatro municípios brasileiros, sendo três no estado de São Paulo (Urânia, Gália e Salto de Pirapora) e um no estado do Rio de Janeiro (Itaboraí). Optou-se pela utilização de dados brasileiros neste trabalho. Os dados de metais correspondem às concentrações “dissolvidas” obtidas pelos procedimentos de coleta e análises químicas

Apesar de terem sido obtidos em áreas sem contaminações antropogênicas, apresentam a maior quantidade de parâmetros analisados dentre aqueles necessários em uma modelagem hidrogeoquímica (parâmetros físico-químicos, cátions e ânions). As publicações de estudos em áreas contaminadas focam apenas os contaminantes, em geral, sem dados suficientes para uma adequada modelagem hidrogeoquímica.

A modelagem hidrogeoquímica é fundamental em casos de contaminações de águas subterrâneas por metais e íons inorgânicos, pois possibilita a compreensão das condições que podem ser encontrados no local de interesse (como principais compostos iônicos esperados e estados de valência para os metais onde isso não [e possível identificar nas análises laboratoriais). As soluções de remediação sempre são melhor definidas e otimizadas com esse conhecimento.

Nas Tabelas 5 e 6, estão apresentados os principais dados utilizados na modelagem, que são os parâmetros físico-químicos (pH e ORP), os íons principais (sódio, cálcio, magnésio, potássio, sulfato, cloreto e alcalinidade por bicarbonatos), os metais bário e cádmio, e os balanços iônicos calculados pelos autores. Os dados completos estão apresentados em tabelas no Anexo A.

Os estudos foram publicados por: Marcolan (2009) para o município de Urânia/SP (Tabela 5); Tavares (2013) para os municípios de Gália/SP e Salto de Pirapora/SP (Tabela 5); Gomes (2012) e Sanches (2015) para Itaboraí/RJ (Tabela 6).

3.2 Modelagem Hidrogeoquímica

Um modelo hidrogeoquímico conceitual envolve um conjunto de equações matemáticas subordinadas aos princípios das reações químicas que são utilizadas na predição de processos geoquímicos que acontecem, por exemplo, num sistema aquífero (GOMES, 2012). Em geral, os modelos hidrogeoquímicos são divididos de acordo com seu nível de complexidade. Neste trabalho, foi utilizado um modelo de especiação-solubilidade, também chamados de modelos de dimensão zero (sem uso de dados espaciais ou temporais), que lidam com um sistema “fechado” ou “estático”. Esse tipo de modelo visa responder três questões, dados resultados analíticos dos constituintes da amostra de água, em um sistema com temperatura e pressão definidos (ZHU and ANDERSON, 2002), a saber:

1. Quais são as concentrações e atividades iônicas e moleculares das espécies em uma solução aquosa?
2. Quais os estados de solubilidade/saturação a respeito dos vários minerais em um sistema e, assim, quais as direções das reações que podem ocorrer para alcançar o equilíbrio?
3. Qual é a distribuição de espécies nas superfícies ou trocadores de íons (*ion-exchangers*) que estão em equilíbrio em uma solução aquosa?

O modelo numérico adotado foi o phreeqc, desenvolvido pela USGS (*United States Geological Survey*) em sua versão escrita em linguagem de programação C (*pH-REdox-EQuilibrium-C*). Foi utilizada a atualização mais recente de 28/janeiro/2020 (3.6.2-15100) da Versão 3 (USGS, 2020a).

Tabela 5 – Dados hidrogeoquímicos obtidos em amostras de águas subterrâneas coletadas em poços de municípios no estado de São Paulo (Urânia, Gália e Salto de Pirapora).

Poço	pH	ORP	Na^{2+}	Ca^{2+}	Mg^{2+}	K^{+}	SO_4^{2-}	Cl^{-}	Alc. HCO_3^{-}	Ba^{2+}	Cd^{2+}	Balanço Iônico
	-	mV	mg/L	mg/L	mg/L	mg/L	mg/L	mg/L	mg/L	mg/L	mg/L	%
Marcolan (2009) - Poços em Urânia/SP												
PM-1	7,47	418,0	8,40	44,00	21,00	6,40	0,27	8,20	201,36	0,419	-	3,0%
PM-2	9,17	386,0	45,00	1,90	0,20	3,60	1,70	1,20	117,97	0,017	-	2,2%
PM-3A	6,33	491,0	9,20	15,00	5,70	4,30	0,28	3,00	79,53	0,217	-	4,6%
PM-3B	7,77	461,0	8,40	23,00	13,00	4,30	0,11	0,25	148,46	0,116	-	5,1%
PM-3C	11,13	260,0	23,00	39,00	<0,1	10,70	14,00	3,30	18,16	0,055	-	-0,3%
Tavares (2013) - Poços em Gália/SP e em Salto de Pirapora/SP												
G PM-03	7,04	287,7	2,70	63,09	16,16	2,30	4,43	4,58	219,56	0,280	-	6,7%
G PM-02	8,86	266,4	4,70	21,08	18,48	5,70	1,29	2,85	159,38	1,540	-	3,5%
G PM-01	9,37	386,5	21,60	7,42	7,29	16,80	7,78	13,45	93,94	0,340	-	-0,5%
PM01	5,58	316,0	0,50	0,56	0,05	0,20	0,08	0,23	18,32	0,070	-	-66,4%
PM07	5,32	93,7	17,00	1,20	1,06	2,10	0,31	24,62	12,21	0,220	-	2,5%
PM03	5,21	101,2	26,00	4,94	6,40	5,60	3,26	81,53	9,16	0,740	-	-10,6%
PM04	7,07	-85,9	10,10	67,37	56,38	3,30	0,24	4,51	457,39	1,480	-	5,7%
PM19	5,65	185,5	128,00	81,11	160,83	5,90	15,58	783,49	48,84	1,900	-	-1,6%
PM24/45	5,36	193,8	3,50	12,10	28,19	3,10	0,49	92,35	30,53	0,610	-	0,0%
PM25	5,52	73,1	15,00	1,05	0,97	1,10	1,99	20,36	42,74	0,900	-	-16,2%
PM27	6,52	-77,2	23,00	7,23	5,20	15,00	0,06	57,79	347,90	8,110	-	-47,3%

Tabela 6 – Dados hidrogeoquímicos obtidos em amostras de águas subterrâneas coletadas em poços de município no estado do Rio de Janeiro (Itaboraí). continua

Poço	pH	ORP	Na^{2+}	Ca^{2+}	Mg^{2+}	K^{+}	SO_4^{2-}	Cl^{-}	Alc. HCO_3^{-}	Ba^{2+}	Cd^{2+}	Balanço Iônico
	-	mV	mg/L	mg/L	mg/L	mg/L	mg/L	mg/L	mg/L	mg/L	mg/L	%
Gomes (2012) - Poços em Itaboraí/RJ												
P-01A (08/09)	8,00	-118,0	76,40	6,40	0,87	2,40	0,80	3,70	229,00	1,050	0,00073	-
P-01B (08/09)	6,00	-137,0	48,40	5,60	1,22	4,20	20,00	-	157,00	0,370	0,00066	-
P-01C (08/09)	7,00	-121,0	144,00	181,00	19,03	18,80	-	626,00	176,00	1,760	0,00069	-
P-02A (08/09)	7,20	66,0	9,10	38,10	3,72	5,90	4,00	5,70	182,00	0,580	0,00068	-
P-02B (08/09)	6,00	107,0	4,20	5,20	1,35	2,20	0,00	6,80	30,00	0,080	0,00079	-
P-02C (08/09)	6,70	88,0	18,40	7,30	2,08	5,20	0,00	3,80	80,00	0,170	0,00099	-
P-03A (08/09)	8,80	-119,0	3,20	4,90	0,79	1,60	-	-	328,00	0,430	0,00094	-
P-03B (08/09)	8,60	-25,0	90,20	4,10	0,88	1,10	5,20	7,80	240,00	0,190	0,00088	-
P-04A (08/09)	7,70	-159,0	33,60	16,10	6,65	8,00	22,50	122,00	50,00	0,260	0,00069	-
P-04B (08/09)	6,80	-109,0	97,00	19,00	8,00	6,00	15,00	158,00	68,00	0,220	0,00068	-
P-05 (08/09)	-	-	-	-	-	-	-	-	-	0,070	0,00067	-

Tabela 6 – Dados hidrogeoquímicos obtidos em amostras de águas subterrâneas coletadas em poços de município no estado do Rio de Janeiro (Itaboraí). conclusão

Poço	pH	ORP	Na^{2+}	Ca^{2+}	Mg^{2+}	K^{+}	SO_4^{2-}	Cl^{-}	Alc. HCO_3^{-}	Ba^{2+}	Cd^{2+}	Balanço Iônico
	-	mV	mg/L	mg/L	mg/L	mg/L	mg/L	mg/L	mg/L	mg/L	mg/L	%
Sanches (2015) - Poços em Itaboraí/RJ												
P-01 (06/13)	5,50	40,0	52,30	18,50	4,26	7,00	73,10	66,80	30,00	<0,002	-	-
P-02 (06/13)	6,50	6,0	65,10	71,00	5,41	5,30	18,20	73,80	291,00	1,170	-	-
P-03 (06/13)	7,20	38,0	141,00	49,00	5,14	4,30	52,10	174,00	183,00	0,620	-	-
P-04 (06/13)	5,90	14,0	193,50	337,90	85,95	16,20	55,60	950,00	269,00	1,370	-	-
P-05 (10/13)	5,20	175,0	13,40	9,10	2,34	2,50	4,30	9,60	58,00	2,810	0,00092	-
P-06 (10/13)	4,20	576,0	20,50	13,30	7,55	8,20	2,70	63,00	34,00	1,800	0,0013	-
P-07 (10/13)	6,50	211,0	62,30	29,80	6,74	3,20	2,90	17,90	263,00	1,510	0,00083	-
P-08 (10/13)	4,40	310,0	13,30	8,60	2,81	2,50	13,00	9,20	47,00	0,800	0,00088	-
P-09 (10/13)	6,10	163,0	15,30	14,50	3,73	2,80	12,10	9,00	80,00	1,200	0,00102	-
P-10 (10/13)	6,40	135,0	18,00	14,00	4,00	2,00	2,00	4,00	100,00	1,790	0,00061	-
P-11 (10/13)	6,90	13,0	58,00	36,30	7,42	4,60	3,60	16,00	300,00	0,750	0,00091	-
P-12 (10/13)	5,80	35,0	21,30	17,60	9,18	4,00	4,80	18,00	114,00	2,520	0,00065	-
P-13 (10/13)	8,40	60,0	239,20	20,00	13,54	3,30	3,60	37,00	743,00	1,980	0,00083	-
P-14 (10/13)	7,50	12,0	50,80	54,10	14,24	5,40	17,20	60,40	247,00	0,980	0,00077	-
P-15 (10/13)	7,20	102,0	29,60	42,80	27,40	3,10	6,90	33,20	288,00	<0,002	0,00071	-
P-16 (10/13)	4,60	283,0	24,10	14,10	16,74	7,50	4,90	29,70	145,00	1,610	0,00098	-
P-17 (10/13)	5,00	227,0	16,50	20,30	12,12	4,50	3,50	16,60	126,00	2,310	0,00103	-

O phreeqc é um modelo que possibilita a simulação de reações químicas, condições de precipitação/solução de minerais e processos de transporte em águas naturais ou contaminadas, em experimentos laboratoriais ou processos industriais (PARKHURST and APPELO, 2013).

Ele consiste em um modelo de associação de íons (*ion-association model*) que estabelece pares de íons e complexos (multi-iônicos e agregados iônicos) em uma solução aquosa em função dos dados de entrada inseridos (concentrações e base de dados hidrogeoquímicos). O objetivo final é avaliar os estados de solubilidade dos minerais, precipitados ou dissolvidos (PARKHURST, 2020).

O modelo calcula o balanço de cátions e ânions de um sistema com características informadas pelo usuário (dados de entrada) e resolve um sistema de equações hidrogeoquímicas para estabelecer um conjunto de condições de equilíbrio. O modelo utiliza o método de Newton-Raphson para a solução do sistema de equações.

As espécies em solução e as fases puras são obtidas a partir de bases de dados hidrogeoquímicas incorporados ao programa. Para este trabalho, foi utilizada a base de dados padrão “phreeqc” que é aplicável para águas naturais com baixa a média salinidade dentro da faixa de aplicação da teoria de Debye-Hückel (PARKHURST and APPELO, 2013).

A essa base de dados, foram incorporadas as espécies $BaCl^+$ e $BaNO_3^+$, e as fases puras (minerais) $BaCl_2$ e BaS, oriundas da base de dados “lnll”; e a fase pura greenockita (CdS) oriunda da base de dados “wateq4f”. Ainda assim, o sulfeto é instável e reage ao entrar em contato com a água para formação de H_2S (rapidamente liberado para a atmosfera) e alcalinizando a água. Esse ânion não foi determinado nas amostras utilizadas neste trabalho (descritas na seção 3.2).

3.3 Procedimentos para Avaliação de Risco à Saúde Humana

O procedimento de análise de risco adotado neste trabalho foi o RAGS da USEPA (USEPA, 1989). Este procedimento é estruturado em quatro etapas para a caracterização qualitativa e quantitativa do risco à saúde humana que estão ilustradas na Figura 5 e incluem:

- Identificação do Perigo (Levantamento e avaliação de dados).
- Avaliação da Relação Dose-Resposta (Toxicologia).

- Avaliação da Exposição.
- Caracterização do Risco.

O Modelo Conceitual de Exposição (MCE) é estabelecido com base nas três primeiras etapas da análise de risco e é utilizado como referência para os cálculos dos riscos. O MCE é formado por três partes, sendo: fontes de contaminação, caminhos de transporte da contaminação e receptores potenciais. Os caminhos de transporte correspondem aos compartimentos ambientais onde ocorre a migração das substâncias desde a fonte até o receptor, como solo, águas superficiais, águas subterrâneas, ar atmosférico, alimentos etc.

Como já discutido, a CETESB elaborou planilhas para a realização de análises de risco à saúde humana em áreas contaminadas no estado de São Paulo, tendo como base o procedimento RAGS da USEPA. O objetivo foi padronizar e otimizar a execução desses estudos naquele estado. Os cálculos realizados e apresentados neste trabalho foram realizados com a planilha de maio/2013.

As etapas do procedimento para análise de risco são descritas sucintamente a seguir baseadas em USEPA (1989), incluindo as equações apresentadas.

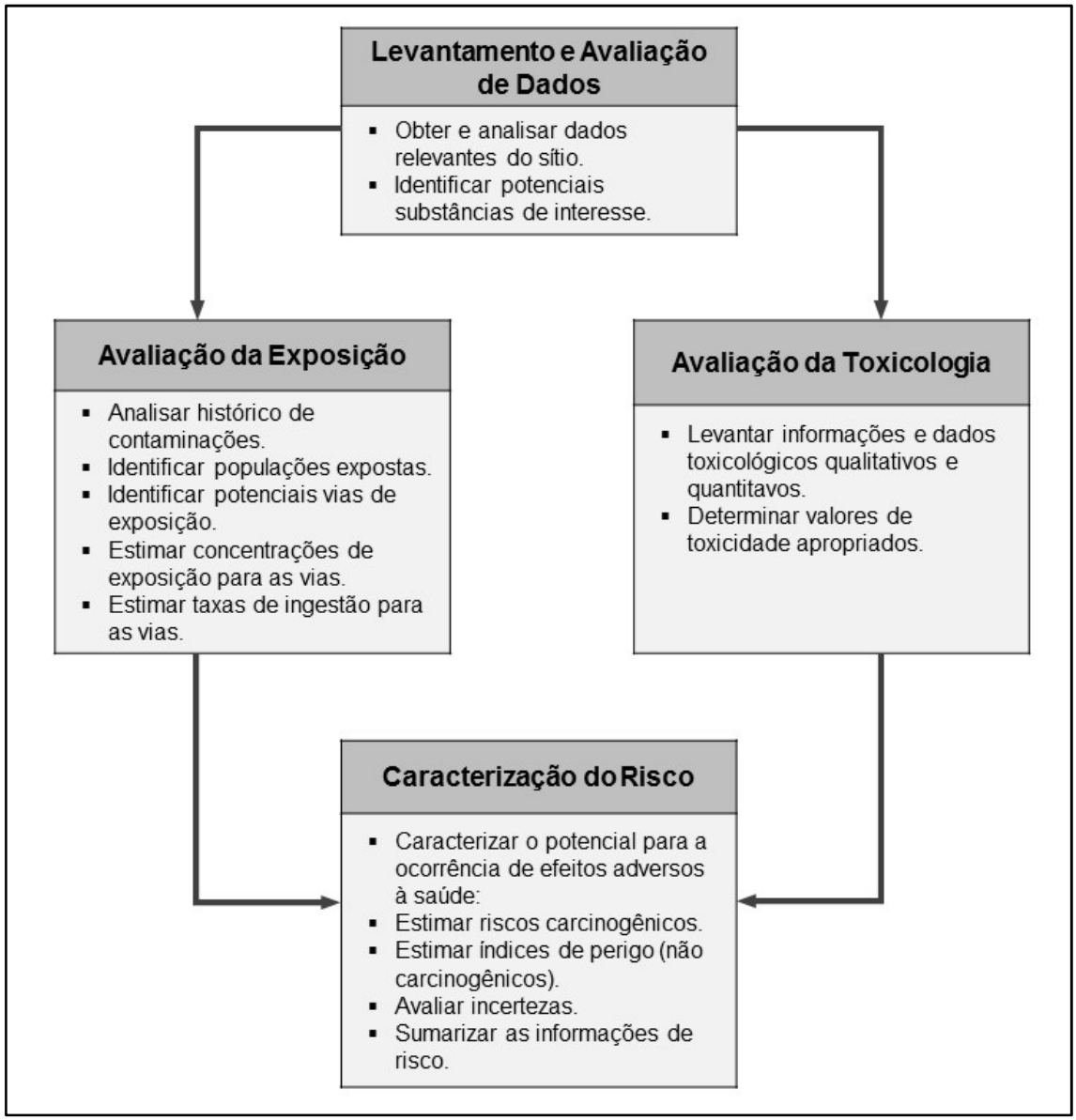
3.3.1 Identificação do Perigo (Levantamento e Avaliação de Dados)

Nesta etapa inicial, são definidas e levantadas as condições de exposição incluindo as fontes; os poluentes potenciais, bem como suas concentrações, distribuição espacial (concentrações em solo e plumas de vapores e em águas subterrâneas) e como podem se mover no meio ambiente; os pontos de exposição; e as vias de ingresso.

As concentrações utilizadas nos cálculos de risco podem ser obtidas diretamente de amostras dos compartimentos ambientais ou a partir de modelos matemáticos que podem ser analíticos ou numéricos.

Efeitos adversos à saúde humana que tenham sido observados na população de interesse podem também ser levantados nesta etapa para identificar substâncias que possam causar estes efeitos e, eventualmente, estejam presentes no local.

Figura 5 – Etapas de uma Análise de Risco à Saúde Humana.



Fonte: Adaptado de USEPA (1989)

3.3.2 Avaliação da Relação Dose-Resposta (Toxicologia)

O objetivo desta etapa é determinar a relação entre a magnitude da exposição e a probabilidade de ocorrência dos efeitos à saúde em questão.

A toxicologia de cada uma das substâncias identificadas na primeira etapa é levantada em bancos de dados de estudos técnicos toxicológicos publicados na literatura científica e internacionalmente reconhecidos. O principal deles é o Sistema de Informações Integradas de Risco (*Integrated Risk Information System* – IRIS) da USEPA. Outros bancos de dados, principalmente estadunidenses, estão disponíveis para consulta pública, a exemplo da base da agência ambiental do estado da Califórnia (CalEPA) e das Tabelas Sumárias de Avaliação de Efeitos à Saúde (*Health Effects Assessment Summary Tables* – HEAST) também da USEPA.

A toxicidade está ligada às evidências de acontecimentos de efeitos adversos à saúde humana provocados por uma exposição ao mesmo. É mensurada por meio da avaliação da relação Dose-Resposta, que é o processo de avaliação quantitativa da toxicologia da relação entre a dose de ingresso e a incidência do efeito adverso à saúde. As substâncias podem causar efeitos carcinogênicos e/ou não-carcinogênicos (USEPA, 1989). Atualmente, há duas principais classificações de carcinogenicidade das substâncias, sendo as da IARC e da USEPA.

Cada substância tem parâmetros específicos para os dois tipos de efeitos principais à saúde, denominados parâmetros toxicológicos.

O potencial de carcinogenicidade (CPF – *Carcinogenic Potency Factor*), denominado pela USEPA de Fator de Carcinogenicidade (SF – *Slope Factor*), é utilizado no cálculo do risco para efeitos carcinogênicos e é expresso como o inverso da dose ($[mg/kg.dia]^{-1}$). Corresponde à inclinação da curva Dose-Resposta (limite de confiança superior para o 95° percentil), e é estimado pela aplicação de modelos matemáticos para extrapolar as doses relativamente elevadas utilizadas nos estudos experimentais para as concentrações mais reduzidas a que podem estar expostos os seres humanos no ambiente.

Com relação aos efeitos não-carcinogênicos, estima-se uma dose limite abaixo da qual se assume que as substâncias não induzem qualquer efeito deletério à saúde humana. Este limite é conhecido como Dose de Referência (RfD – *Reference Dose*) e pode ser classificado conforme o tipo de exposição: crônico (longa duração) e subcrônico (curta duração). Para sua determinação, são utilizadas as concentrações

obtidas em estudos toxicológicos e aplicados fatores de correção em função das características dos estudos, como estudos com animais extrapolados para seres humanos, por exemplo (HALLENBECK, 1993).

Tanto as Doses de Referência (RfD) quanto os Fatores de Carcinogenicidade (SF) são obtidos para cada uma das vias de ingresso consideradas (discutidas na seção 3.3.3).

3.3.3 Avaliação da Exposição

O objetivo principal desta terceira etapa de uma Análise de Risco é quantificar a exposição de seres humanos às substâncias de interesse, que foram definidas nas duas primeiras etapas. Para tanto, são estabelecidos os receptores, as vias de ingresso e, então, calculadas as Doses de Ingresso, ou Ingresso (I) para cada um dos receptores/vias de ingresso.

Os receptores correspondem aos indivíduos da população que está potencialmente exposta às substâncias no local de estudo. Podem incluir crianças, adultos, idosos, gestantes etc., e também as características de uso e ocupação do solo no local, como rural, residencial, comercial, industrial, dentre outros. Os receptores considerados neste trabalho foram aqueles pré-definidos em planilhas da CETESB, sendo: receptor residente rural criança/adulto e receptor residente urbano criança/adulto.

Em sequência, são identificadas as vias de ingresso que podem ocorrer, ou seja, as formas em que as substâncias podem alcançar os receptores que incluem via oral/ingestão, via dermal e via aérea (por inalação). A partir dessas formas principais, são definidas as vias de ingresso. Por exemplo, a via oral/ingestão pode ser caracterizada pela ingestão de águas superficiais/subterrâneas (consumo de água como bebida), ingestão de águas superficiais durante recreação, ingestão de águas superficiais/subterrâneas durante o banho, ingestão de solo durante escavações etc.

Com a definição dos receptores e das vias de ingresso, são levantados na literatura, ou em pesquisas no próprio local de interesse, os Parâmetros de Exposição, utilizados para caracterizar os receptores quantitativamente.

Com as concentrações de exposição e caminhos de transporte definidos na primeira etapa, juntamente com os Parâmetros de Exposição dos receptores, podem

ser calculadas as Doses de Ingresso, ou simplesmente Ingresso (I) para cada uma das vias de ingresso.

A Dose de Ingresso (I) representa a quantidade de determinada substância a que o receptor poderá estar exposto por uma determinada via de ingresso em cenários de uso atual e/ou futuro do local de estudo.

Há dois tipos de Dose de Ingresso: a crônica média diária (I_C) e a integral (vida) média diária (I_V). A primeira é utilizada para a estimativa do Índice de Perigo (IP), enquanto a segunda é aplicada no cálculo do Risco Carcinogênico (RC).

Neste trabalho, foi avaliada a via de ingresso por ingestão de águas subterrâneas. Para os metais bário e cádmio, há apenas parâmetros toxicológicos para efeitos não carcinogênicos nas bases de dados toxicológicos (como a IRIS da USEPA). A definição de IP é apresentada na seção 3.3.4 a seguir neste capítulo.

A Equação 1 corresponde à fórmula geral utilizada para o cálculo das Doses de Ingresso I_C. Essa fórmula possui peculiaridade de acordo com a via de ingresso e do compartimento ambiental em que se encontra a substância e parâmetros específicos são necessários.

$$I_C = \frac{C_{ING} \times FE}{PC} \times P_{VIA} \qquad (1)$$

onde:

- I_C → Ingresso crônico médio diário ou quantidade de substância que ingressa no organismo humano por uma via de ingresso (utilizado no cálculo do Índice de Perigo) [T^{-1}].
- C_{ING} → Concentração de ingresso da substância no compartimento ambiental de interesse [ML^{-3} ou MM^{-1}].
- FE → Frequência de exposição [TT^{-1}].
- PC → Peso corporal [M].
- P_{VIA} → Parâmetros específicos de cada via de ingresso.

3.3.4 Caracterização do Risco

Na quarta e última etapa de uma Análise de Risco, são utilizados os dados do Modelo Conceitual de Exposição (fontes, caminhos e receptores) juntamente com os

aspectos toxicológicos para a quantificação do risco potencial a que está exposta uma determinada população no local em estudo.

Os valores de riscos são calculados para cada via de ingresso e cada substância, separadamente para os efeitos carcinogênicos (Risco Carcinogênico – RC) e não-carcinogênicos (Índice de Perigo – IP), individualmente por receptor.

As equações utilizadas para o cálculo do IP são apresentadas na subseção 3.3.4.1. Os valores máximos estabelecidos na legislação brasileira são descritos na subseção 3.3.4.2.

3.3.4.1 Índice de Perigo (IP)

O Índice de Perigo (IP) corresponde ao quociente entre a Dose de Ingresso do receptor e a Dose de Referência da substância avaliada conforme a Equação 2.

$$\mathrm{IP} = \frac{I_n}{RfD} \qquad (2)$$

onde:

IP → Índice de Perigo [-].

I_n → Dose de Ingresso para o Cenário de Exposição “n” [T^{-1}].

RfD → Dose de Referência [T^{-1}].

Nos casos em que um receptor esteja exposto a diferentes substâncias simultaneamente, o IP para uma determinada via de ingresso é dado pelo somatório dos IPs calculados para cada substância.

Caso diferentes vias de ingresso possam ocorrer, o IP total é dado pela soma dos riscos de cada substância em cada via de ingresso.

Os efeitos adversos à saúde causados pela exposição a mais de uma substância podem ser aditivos, sinérgicos ou até mesmo antagônicos, a depender de seus modos de ação no interior do organismo. O somatório dos riscos (efeitos aditivos) não é um procedimento toxicologicamente corroborado, porém, é o formato a favor da segurança que é adotado internacionalmente, a exemplo dos órgãos ambientais USEPA e CETESB (e que é adotado em suas Planilhas de Avaliação de Risco).

Adicionalmente, destaca-se que esses riscos são incrementais, ou seja, são adicionais àqueles riscos a que estão submetidos os indivíduos devido a hábitos de vida (fumante, alimentação, sedentarismo, emissões de veículos durante trajeto casa-trabalho-caso, por exemplo).

3.3.4.2 Valores Máximos Estabelecidos na Legislação Brasileira

As diretrizes para o gerenciamento ambiental de áreas contaminadas no Brasil foram estabelecidas na Resolução CONAMA nº 420/2009. Dentre outros aspectos, está prevista nessa resolução a realização de Análises de Risco como parte do gerenciamento de áreas contaminadas (solos e águas superficiais/subterrâneas).

Os valores máximos para riscos são definidos como “Níveis Toleráveis de Risco à Saúde Humana”.

Para as substâncias com efeitos não carcinogênicos, o valor de IP deve ser menor que 1 para que o risco seja tolerável. É importante destacar, contudo, que o IP indica o potencial de um efeito não-carcinogênico adverso à saúde, mas não se trata de um risco probabilístico. O limite de uma unidade para o índice de perigo é internacionalmente aceito como o valor a partir do qual podem ocorrer danos à saúde humana (USEPA, 1989).

Esse nível tolerável está em consonância com os valores adotados em outros locais do mundo, como EUA e países da Comunidade Europeia, por exemplo.

4. RESULTADOS DA MODELAGEM HIDROGEOQUÍMICA E DOS RISCOS À SAÚDE HUMANA E DISCUSSÕES

Os resultados da modelagem hidrogeoquímica com os dados obtidos em publicações na literatura científica são apresentados e discutidos na seção 4.1.

Os riscos à saúde humana foram calculados com os dados levantados na literatura e também com as concentrações por espécie dos metais bário e cádmio nas planilhas de Avaliação de Risco da CETESB. Os riscos estimados estão exibidos na seção 4.2 com uma análise crítica em comparação com as Concentrações Máximas Aceitáveis (CMAs) calculadas com as planilhas da CETESB.

4.1 Modelagem Hidrogeoquímica para Bário e Cádmio

Os resultados obtidos na modelagem hidrogeoquímica incluem diferentes parâmetros associados à distribuição dos íons e das espécies minerais nas águas subterrâneas. Os parâmetros mais relevantes para o contexto do trabalho incluíram: balanços iônicos (cátions e ânions) e diferenças percentuais; espécies iônicas em solução (bário e cádmio); e estados de solubilidade (precipitado/em solução) dos principais minerais do bário (barita e witherita) e do cádmio (otavita) para as condições de cada local.

Esses resultados estão apresentados nas Tabelas 7 a 9, juntamente com os principais dados de entrada do modelo, que são as concentrações e valores de parâmetros físico-químicos obtidos nas amostras de águas subterrâneas. Os dados completos estão apresentados no Anexo B (tabelas) e no Anexo C (arquivos de entrada e saída do modelo phreeqc).

Nas Tabelas 7 e 8, encontram-se os resultados das simulações relacionados ao bário, que foram detectados em amostras de quatro municípios, sendo três no estado de São Paulo (Urânia, Gália e Salto de Pirapora) e um no estado do Rio de Janeiro (Itaboraí). Em Itaboraí/RJ, as amostragens foram realizadas em duas épocas distintas e apresentadas separadamente por Gomes (2012) e Sanches (2015). Foram, dessa forma, avaliados separadamente (Tabela 8).

O cádmio foi analisado nas amostras do município de Itaboraí/RJ, e os resultados das simulações estão apresentados na Tabela 9.

4.1.1 Balanço Iônico (Cátions e Ânions)

O balanço iônico corresponde à soma dos cátions e dos ânions com suas respectivas cargas elétricas. Em uma análise química completa, a soma em miliequivalentes dos ânions deveria ser igual à soma em miliequivalentes dos cátions. Na prática, existem diferenças entre ambas as somas, devido a erros acumulados nas etapas de coleta e das determinações de cada um dos íons, e por não quantificar todas as contribuições iônicas de pequeno valor (CUSTODIO E LLAMAS, 1983).

Os valores de balanço iônico atenderam aos critérios recomendados por Friedman e Erdmann (1982) em 37 das 44 amostras de águas subterrâneas utilizadas neste trabalho (84% do total), se situando entre -14,7% (PM03) e 6,2% (PM04), ambas publicadas por Tavares (2013). Essa faixa indica boa qualidade nos procedimentos de coleta e de análises químicas seguidos em todos os trabalhos.

Em apenas 07 amostras, as diferenças foram inferiores a -18%, mas consistentes com os dados apresentados nos trabalhos originais. Foram, dessa forma, utilizados neste trabalho para as simulações hidrogeoquímicas e para os cálculos de riscos.

4.1.2 Espécies de Bário e Cádmio em Solução

Para os metais bário e cádmio, os resultados da especiação indicaram que a maior parte das concentrações detectadas correspondem às suas formas iônicas (Ba^{2+} e Cd^{2+}), que podem formar pares de íons com quaisquer dos ânions presentes na mesma amostra. Esses valores estão indicados na coluna “Ba^{2+}” nas Tabelas 7 e 8, e na coluna “Cd^{2+}” na Tabela 9.

A proporção de Ba^{2+} variou entre 82,9% na amostra PM-3C de Urânia/SP (MARCOLAN, 2009) e 100% na amostra P-05 de Itaboraí/RJ (GOMES, 2012), valendo ressaltar que nesta última amostra não foi reportada a presença de sulfato, que é o ânion principal na especiação do bário em águas. A presença do bário na forma de agregado iônico de sulfato de bário ($BaSO_4$) foi obtida na maioria das amostras, chegando a uma proporção máxima de 9,1% na amostra P-03 de Itaboraí/RJ (SANCHES, 2015), que teve uma das maiores concentrações de sulfato dentre os dados avaliados (52,1 mg/L), corroborando o controle do sulfato na especiação do bário.

O cádmio foi analisado apenas nas amostras coletadas em poços do município de Itaboraí/RJ. Ocorreu na forma de Cd^{2+} nos resultados da especiação entre 70,8% na amostra P-13 (SANCHES, 2015) e 99,9% na amostra P-05 (GOMES, 2012). A exceção foi observada na amostra P-01C (GOMES, 2012) com 50,1%, e com 45% de cádmio na espécie $CdCl^{+}$ em função da elevada concentração de cloreto detectada (626 mg/L). Proporções de $CdCl^{+}$ entre 9,0% e 21,9% foram calculadas nas amostras com as maiores concentrações de cloreto.

4.1.3 Estados de Solubilidade dos Principais Minerais de Bário e Cádmio

O estado de solubilidade dos minerais reflete o equilíbrio de um mineral entre a fase sólida e a solução. O Índice de Saturação (IS) é utilizado para avaliar se o mineral está presente na forma precipitada ou em solução na amostra, e é calculado pela fórmula apresentada na Equação 3 (PARKHURST E APPELO, 2013):

$$\mathrm{IS} = \log_{10} \frac{PAI}{K_{ps}} \qquad (3)$$

onde:

IS → Índice de Saturação [-].
PAI → Produto de Atividade Iônica [-].
K_{ps} → Produto de Solubilidade [-].

Quando IS=0, o mineral estará em equilíbrio entre as fases sólida e em solução. Para IS<0, o mineral será dissolvido na solução, enquanto que para IS>0 o mineral estará em desequilíbrio e precipitará.

O IS foi calculado em 37 das amostras para barita e 41 amostras para witherita, todas aquelas onde foi detectado sulfato e ocorreu carbonato na especiação. Em 17 amostras, foi calculado IS>0 para barita, indicando sua precipitação. Os maiores valores de IS para barita foram obtidos nas amostras com maiores proporções da espécie $BaSO_4$, como esperado, com o IS máximo igual a 0,7599 na amostra P-03 de Itaboraí/RJ (SANCHES, 2015).

Como já discutido, a especiação do bário em águas é controlada pelas concentrações de sulfato (DEUTSCH, 1997) e os resultados obtidos refletem esse

comportamento. Nessas 17 amostras, as concentrações de sulfato foram iguais ou maiores que 2,0 mg/L. Nas demais amostras com IS<0, as concentrações de sulfato foram inferiores a 2,0 mg/L.

Coeficientes de correlação linear (ou de Pearson) r_{XY} foram calculados para os seguintes conjuntos de dados (concentrações nas amostras e IS do phreeqc) para compor a avaliação, sendo o único a indicar correlação positiva o par sulfato e Índice de Saturação da barita:

- Sulfato x IS_{Barita} = 0,52 (correlação positiva moderada)
- pH x Bário = -0,23 (ausência de correlação)
- pH x IS_{Barita} = -0,26 (ausência de correlação)
- Bário x Sulfato = -0,09 (ausência de correlação)
- Bário x IS_{Barita} = 0,22 (ausência de correlação)

Todos os valores de IS para a witherita foram menores que zero (IS<0), indicando que nas condições encontradas nas amostras, este mineral está em solução.

O principal mineral do cádmio encontrado na natureza é a greenockita (CdS), em geral, associado com esfalerita (ZnS). Os resultados não incluíram a determinação de sulfeto, que não é esperado nas condições encontradas nos poços dos estudos referenciados. Assim, não foi possível verificar se poderia ocorrer nas condições das amostras dos poços.

Para o cádmio, foram calculados valores de IS para o mineral otavita ($CdCO_3$), de ocorrência mais provável nas condições estudadas. Todos os valores de IS foram abaixo de zero (IS<0), indicando que o mineral se encontra em solução.

Os maiores valores de IS (mais próximos de zero), foram calculados para as 04 amostras com valores de pH acima de 8, sendo P-13 com pH de 8,40 (SANCHES, 2015) e P-01A (pH igual a 8,0), P-03A (pH igual a 8,8) e P-03B (pH igual a 8,6), de Gomes (2012).

Os coeficientes de correlação linear (ou de Pearson) r_{XY} calculados para os pares de dados de pH e Cd medidos nas amostras e IS da otavita obtido no phreeqc foram os seguintes:

- pH x Cádmio = -0,41 (correlação negativa)
- pH x $IS_{Otavita}$ = 0,98 (correlação positiva forte)
- Cádmio x $IS_{Otavita}$ = -0,35 (correlação negativa)

A relação do Diagrama de equilíbrio potencial-pH para o sistema Cd-C-S-O-H (ver Figura 4) prevê a formação do $CdCO_3$ (fórmula da otavita) em soluções com pH acima de 8, como foi encontrado nos dados e corroborado com o maior valor de correlação.

Tabela 7 – Resultados da modelagem hidrogeoquímica em poços dos municípios do estado de São Paulo (Urânia, Gália e Salto de Pirapora): balanço iônico, espécies iônicas em solução e estados de solubilidade da barita.

Poço	Concentrações na Fração Dissolvida (mg/L)				Balanço Iônico (%)	IS [b] Barita
	Bário [a] (espécies)	Ba^{2+}	$BaSO_4$	SO_4^{2-}		
Marcolan (2009) - Poços em Urânia/SP						
PM-1	0,419	0,409	<0,001	0,27	-18,0%	-1,6
PM-2	0,017	0,016	<0,001	1,70	2,4%	-2,1
PM-3A	0,217	0,214	<0,001	0,28	-11,6%	-1,8
PM-3B	0,116	0,113	<0,001	0,11	5,1%	-2,5
PM-3C	0,055	0,046	0,002	14,00	4,7%	-0,8
Tavares (2013) - Poços em Gália/SP e em Salto de Pirapora/SP						
G PM-03	0,280	0,271	0,003	4,43	-3,3%	-0,6
G PM-02	1,540	1,466	0,005	1,29	2,3%	-0,3
G PM-01	0,340	0,314	0,007	7,78	-9,5%	-0,1
PM01	0,070	0,070	<0,001	0,08	-64,7%	-2,6
PM07	0,220	0,219	<0,001	0,31	5,8%	-1,6
PM03	0,740	0,728	0,007	3,26	-14,7%	-0,1
PM04	1,480	1,421	0,001	0,24	6,2%	-1,2
PM19	1,900	1,805	0,025	15,58	-6,0%	0,4
PM24/45	0,610	0,604	0,001	0,49	-2,7%	-1,1
PM25	0,900	0,888	0,006	1,99	-0,6%	-0,2
PM27	8,110	7,794	0,001	0,06	-41,1%	-0,9

Legenda:

a) Soma das concentrações das espécies detectadas na fração dissolvida.

b) IS = Índice de Saturação. Valores positivos (IS>0) indicam a precipitação do mineral. Valores negativos (IS<0) indicam que o mineral está em solução.

Tabela 8 – Resultados da modelagem hidrogeoquímica em poços do município de Itaboraí/RJ: balanço iônico, espécies iônicas em solução e estados de solubilidade da barita.

Poço	Concentrações na Fração Dissolvida (mg/L)				Balanço Iônico (%)	IS [(b)] Barita
	Bário [(a)] (espécies)	Ba^{2+}	$BaSO_4$	SO_4^{2-}		
Gomes (2012) - Poços em Itaboraí/RJ						
P-01A (08/09)	1,050	1,014	0,002	0,80	-1,2%	-0,6
P-01B (08/09)	0,370	0,342	0,021	20,00	-6,9%	0,3
P-01C (08/09)	1,760	1,686	<0,001	-	-5,7%	-
P-02A (08/09)	0,580	0,561	0,006	4,00	-8,2%	-0,2
P-02B (08/09)	0,080	0,080	<0,001	0,00	-7,2%	-
P-02C (08/09)	0,170	0,168	<0,001	0,00	1,5%	-
P-03A (08/09)	0,430	0,393	<0,001	-	-84,4%	-
P-03B (08/09)	0,190	0,178	0,003	5,20	-1,2%	-0,6
P-04A (08/09)	0,260	0,242	0,014	22,50	-24,0%	0,2
P-04B (08/09)	0,220	0,209	0,007	15,00	0,8%	-0,1
P-05 (08/09)	0,070	0,070	<0,001	-	-5,2%	-
Sanches (2015) - Poços em Itaboraí/RJ						
P-01 (06/13)	<0,002	-	-	73,10	-27,0%	-
P-02 (06/13)	1,170	1,092	0,040	18,20	-2,5%	0,6
P-03 (06/13)	0,620	0,547	0,057	52,10	-0,7%	0,8
P-04 (06/13)	1,370	1,245	0,052	55,60	0,4%	0,7
P-05 (10/13)	2,810	2,748	0,040	4,30	-8,5%	0,6
P-06 (10/13)	1,800	1,771	0,013	2,70	-28,2%	0,1
P-07 (10/13)	1,510	1,454	0,010	2,90	-1,2%	0,0
P-08 (10/13)	0,800	0,761	0,033	13,00	-11,9%	0,5
P-09 (10/13)	1,200	1,145	0,043	12,10	-9,3%	0,7
P-10 (10/13)	1,790	1,756	0,011	2,00	-7,6%	0,0
P-11 (10/13)	0,750	0,719	0,006	3,60	-6,2%	-0,2
P-12 (10/13)	2,520	2,448	0,033	4,80	-2,3%	0,5
P-13 (10/13)	1,980	1,766	0,012	3,60	-4,6%	0,1
P-14 (10/13)	0,980	0,918	0,033	17,20	-2,8%	0,5
P-15 (10/13)	<0,002	-	-	6,90	-4,9%	-
P-16 (10/13)	1,610	1,561	0,019	4,90	-14,3%	0,3
P-17 (10/13)	2,310	2,252	0,021	3,50	-7,6%	0,3

Legenda:

a) Soma das concentrações das espécies detectadas na fração dissolvida.

b) IS = Índice de Saturação. Valores positivos (IS>0) indicam a precipitação do mineral. Valores negativos (IS<0) indicam que o mineral está em solução.

Tabela 9 – Resultados da modelagem hidrogeoquímica em poços do município de Itaboraí/RJ: balanço iônico, espécies iônicas em solução e estados de solubilidade da otavita.

Poço	Concentrações na Fração Dissolvida (µg/L)				Balanço Iônico (%)	IS [(b)] Otavita
	Cádmio [(a)] (espécies)	Cd^{2+}	$CdCO_3$	pH		
Gomes (2012) - Poços em Itaboraí/RJ						
P-01A (08/09)	0,730	0,655	0,006	8,0	-1,2%	-1,0
P-01B (08/09)	0,660	0,600	<0,001	6,0	-6,9%	-3,2
P-01C (08/09)	0,690	0,346	<0,001	7,0	-5,7%	-2,6
P-02A (08/09)	0,680	0,623	0,001	7,2	-8,2%	-2,0
P-02B (08/09)	0,790	0,767	<0,001	6,0	-7,2%	-3,8
P-02C (08/09)	0,990	0,949	<0,001	6,7	1,5%	-2,6
P-03A (08/09)	0,940	0,723	0,062	8,8	-84,4%	-0,1
P-03B (08/09)	0,880	0,739	0,028	8,6	-1,2%	-0,4
P-04A (08/09)	0,690	0,527	0,001	7,7	-24,0%	-2,1
P-04B (08/09)	0,680	0,505	<0,001	6,8	0,8%	-2,9
P-05 (08/09)	0,670	0,669	<0,001	-	-5,2%	-
Sanches (2015) - Poços em Itaboraí/RJ						
P-01 (06/13)	-	-	-	5,5	-27,0%	-
P-02 (06/13)	-	-	-	6,5	-2,5%	-
P-03 (06/13)	-	-	-	7,2	-0,7%	-
P-04 (06/13)	-	-	-	5,9	0,4%	-
P-05 (10/13)	0,920	0,872	<0,001	5,2	-8,5%	-4,3
P-06 (10/13)	1,300	1,129	<0,001	4,2	-28,2%	-5,4
P-07 (10/13)	0,830	0,730	<0,001	6,5	-1,2%	-2,5
P-08 (10/13)	0,880	0,824	<0,001	4,4	-11,9%	-5,2
P-09 (10/13)	1,020	0,948	<0,001	6,1	-9,3%	-3,2
P-10 (10/13)	0,610	0,578	<0,001	6,4	-7,6%	-3,0
P-11 (10/13)	0,910	0,793	0,001	6,9	-6,2%	-2,0
P-12 (10/13)	0,650	0,595	<0,001	5,8	-2,3%	-3,6
P-13 (10/13)	0,830	0,588	0,036	8,4	-4,6%	-0,3
P-14 (10/13)	0,770	0,629	0,002	7,5	-2,8%	-1,6
P-15 (10/13)	0,710	0,604	0,001	7,2	-4,9%	-1,8
P-16 (10/13)	0,980	0,871	<0,001	4,6	-14,3%	-4,5
P-17 (10/13)	1,030	0,944	<0,001	5,0	-7,6%	-4,1

Legenda:

a) Soma das concentrações das espécies detectadas na fração dissolvida.

b) IS = Índice de Saturação. Valores positivos (IS>0) indicam a precipitação do mineral. Valores negativos (IS<0) indicam que o mineral está em solução.

4.2 Riscos à Saúde Humana para Via de Ingestão de Água

Os riscos à saúde humana para a via de ingestão de águas subterrâneas calculados neste trabalho com as Planilhas de Avaliação de Risco da CETESB são apresentados em tabelas no Anexo D. Resumo com os maiores valores de IPs calculados para cada um dos quatro conjuntos de dados utilizados são apresentados na Tabela 10 para os poços de municípios no estado de São Paulo (MARCOLAN, 2009; TAVARES, 2013) e na Tabela 11 para os poços de município no estado do Rio de Janeiro (GOMES, 2012; SANCHES, 2015).

Os parâmetros toxicológicos para os metais bário e cádmio publicados na literatura possibilitaram a obtenção de Doses de Referência (*RfD – Reference Dose*) para efeitos não carcinogênicos voltados ao cálculo de Índices de Perigo (IP). Os valores apresentados nestas tabelas correspondem aos IPs calculados. Não há estudos que indiquem a ocorrência de efeitos carcinogênicos para ambos os metais para a via de ingestão de água (USEPA, 2007; USEPA, 2012).

Na Resolução CONAMA n° 420/2009, é estabelecido para substâncias não carcinogênicas que o ingresso diário de contaminantes deve ser igual ou inferior ao ingresso diário tolerável a que uma pessoa possa estar exposta por toda a sua vida. Isso equivale a valores de IP igual ou inferior a 1. Essa referência segue as recomendações adotadas nos EUA e na Europa e reconhecidas internacionalmente.

Dentre os receptores padrões considerados pela CETESB em suas planilhas, foram avaliados os residentes em área rural e em área urbana para crianças e adultos. A exposição foi simulada para o receptor diretamente sobre a fonte, que representa as condições dos poços amostrados.

Os resultados de IP para o bário são apresentados nas Tabelas D.1 a D.6 (Anexo D) para os municípios de Urânia/SP, Gália/SP, Salto de Pirapora/SP e Itaboraí/RJ. Estas tabelas incluem os valores de IP para as concentrações detectadas nas amostras dos poços e também concentrações de bário subtraídas dos valores encontrados para a espécie $BaSO_4$ nas simulações hidrogeoquímicas nos casos em que o IS foi positivo (IS>0), visto que o sulfato de bário não é tóxico para os seres humanos.

Valores de IP acima de 1 foram calculados para a amostra do poço PM27 do município de Salto de Pirapora/SP para todos os quatro receptores avaliados. A concentração de bário neste poço foi igual a 8,11, superior ao Valor Orientador (VO)

estabelecido na Resolução CONAMA 420/2009. Concentrações de bário acima desse VO foram também detectadas em outros poços, mas todas resultaram em IP abaixo de 1 (dentro da faixa aceitável).

O valor de IS para barita na amostra do poço PM27 foi de -0,91, indicando que se encontra em solução e, portanto, não foi possível subtrair sua concentração para redução dos riscos neste caso. Nas demais amostras, a subtração das concentrações de $BaSO_4$ quando o IS foi positivo (IS>0) levou a reduções nos riscos de até 10%, como no caso da amostra P-03 (06/13) de Itaboraí/RJ publicada por Sanches (2015). Isso é favorável e torna a Avaliação de Risco mais representativa da realidade local. Esse entendimento segue a mesma linha de Menzie *et al.* (2008).

Nas Tabelas D.7 e D.8 (Anexo D), são encontrados os valores de IP para o cádmio para o município de Itaboraí/RJ, com os dados publicados por Gomes (2012) e por Sanches (2015). Os valores de IS para os minerais do cádmio foram negativos (IS<0) e, dessa forma, não foi houve redução dos riscos em função de precipitação do metal.

Os valores de IP calculados para cádmio foram todos abaixo de 1, dentro da faixa tolerável de riscos à saúde humana.

A soma dos IPs para bário e cádmio para as amostras dos poços de Itaboraí/RJ são apresentados nas Tabelas D.9 e D.12 (Anexo D), relativos ao bário detectado nas amostras e aos valores subtraídos do $BaSO_4$ quando IS>0.

Os riscos para a exposição aos dois metais (múltiplas substâncias), que é a situação existente nos locais estudados, levou a valores de IP acima de 1 para os receptores: residente rural criança e residente urbano criança. Para a soma de bário e cádmio detectados na amostra do poço P-05 (10/13) de Itaboraí/RJ publicada por Sanches (2015), os valores de IP foram iguais a 1,02, pouco acima da unidade. Já quando o bário foi subtraído da espécie $BaSO_4$ nos casos em que o IS foi maior que zero (IS>0), a soma dos IPs de bário e cádmio foi igual a 1,0 para os dois receptores, indicando que ao se considerar a especiação dos metais os riscos calculados podem atender a legislação, além de serem mais representativos das condições de exposição reais.

A título ilustrativo, são apresentadas na Tabela 12 as Concentrações Máximas Aceitáveis (CMAs) calculadas com as Planilhas de Avaliação de Risco da CETESB para os metais bário e cádmio em exposições dos mesmos receptores considerados neste trabalho (residentes rural/urbano, criança e adulto).

As concentrações utilizadas como entrada neste trabalho foram inferiores às CMAs, indicando que as condições encontradas possibilitam o uso das águas subterrâneas para o consumo humano (via de ingestão).

Tabela 10 – Valores máximos de IP calculados para os dados dos poços dos municípios do estado de São Paulo (Urânia, Gália e Salto de Pirapora) utilizados no trabalho para o metal bário para os receptores residente rural/urbano (criança/adulto).

Poço	Dados de campo (mg/L)		Concentrações de entrada na Avaliação de Risco	Valores de IP (Acima de 1 indicados em vermelho)			
	Ba^{2+}	Cd^{2+}		Residente Rural Criança	Residente Rural Adulto	Residente Urbano Criança	Residente Urbano Adulto
Marcolan (2009) - Poços de Urânia/SP							
PM-3A	0,217	-	Bário	0,07	0,03	0,07	0,03
			Bário - $BaSO_4$	-	-	-	-
			Cádmio	-	-	-	-
			Bário + Cádmio	-	-	-	-
			(Bário - $BaSO_4$) + Cádmio	-	-	-	-
Tavares (2013) - Poços de Gália/SP e Salto de Pirapora/SP							
PM27	8,110	-	Bário	2,59	1,23	2,59	1,11
			Bário - $BaSO_4$	-	-	-	-
			Cádmio	-	-	-	-
			Bário + Cádmio	-	-	-	-
			(Bário - $BaSO_4$) + Cádmio	-	-	-	-

Tabela 11 – Valores máximos de IP calculados para os dados dos poços do município do estado do Rio de Janeiro (Itaboraí) utilizados no trabalho para os metais bário e cádmio para os receptores residente rural/urbano (criança/adulto).

Poço	Dados de campo (mg/L)		Concentrações de entrada na Avaliação de Risco	Valores de IP (Acima de 1 indicados em vermelho)			
	Ba^{2+}	Cd^{2+}		Residente Rural Criança	Residente Rural Adulto	Residente Urbano Criança	Residente Urbano Adulto
Gomes (2012) - Poços de Itaboraí/RJ							
P-01C (08/09)	1,760	0,000690	Bário	0,56	0,27	0,56	0,24
			Bário - $BaSO_4$	0,56	0,27	0,56	0,24
			Cádmio	0,09	0,04	0,09	0,04
			Bário + Cádmio	0,65	0,31	0,65	0,28
			(Bário - $BaSO_4$) + Cádmio	0,65	0,31	0,65	0,28
Sanches (2015) - Poços de Itaboraí/RJ							
P-05 (10/13)	2,810	0,000920	Bário	0,90	0,43	0,90	0,38
			Bário - $BaSO_4$	0,89	0,42	0,89	0,38
			Cádmio	0,12	0,06	0,12	0,05
			Bário + Cádmio	1,02	0,48	1,02	0,44
			(Bário - $BaSO_4$) + Cádmio	1,00	0,48	1,00	0,43

Tabela 12 – Concentrações Máximas Aceitáveis (CMAs) calculadas com as Planilhas de Avaliação de Risco da CETESB para os metais bário e cádmio para os receptores residente rural/urbano (criança/adulto).

Receptor	CMAs para Via de Ingestão de Água (mg/L)	
	Bário	Cádmio
	7440-30-3	7440-43-9
Residente Rural Criança	3,13	0,01
Residente Rural Adulto	6,57	0,02
Residente Urbano Criança	3,13	0,01
Residente Urbano Adulto	7,30	0,02

5. CONCLUSÕES

Uma modelagem hidrogeoquímica com o modelo phreeqc foi realizada para avaliar a especiação dos metais bário e cádmio em amostras de águas subterrâneas e os estados de solubilidade de seus principais minerais (barita e witherita para bário; otavita para cádmio). As concentrações obtidas nas amostras e na especiação foram utilizadas para avaliação de riscos à saúde humana com as Planilhas da CETESB. Foram utilizados resultados analíticos de amostras coletadas em poços de municípios nos estados de São Paulo (Urânia, Gália e Salto de Pirapora) e do Rio de Janeiro (Itaboraí).

As espécies iônicas que formam os principais minerais de bário ($BaSO_4$ e $BaCO_3$) e de cádmio ($CdCO_3$) foram encontradas na modelagem. Valores de Índice de Saturação (IS) indicando a precipitação do mineral (IS>0) foram obtidos apenas para a barita. Os minerais do cádmio se mantiveram em solução, de acordo com o modelo (IS<0).

Segundo a literatura técnica, a especiação em águas subterrâneas do bário é controlada pelas concentrações de sulfato, enquanto que a especiação do cádmio é controlada pelo pH. Os resultados obtidos com o phreeqc para os resultados analíticos das amostras dos poços refletiram esses condicionantes.

Os valores de índice de Perigo (IP) para efeitos não carcinogênicos individuais foram acima de 1 apenas para o bário no poço PM27 de Salto de Pirapora/SP, para os receptores residentes rural/urbano (criança/adulto). Nos demais poços, ainda que tenham sido inferiores a 1 e dentro da faixa aceitável, os riscos foram reduzidos quando subtraídas as concentrações de bário na forma de $BaSO_4$ (barita precipitada).

Os riscos totais para bário e cádmio em conjunto foram iguais a 1,02 para os receptores residentes rural/urbano criança. Esse valor reduziu para 1, atendendo a legislação, quando foi considerada a precipitação de bário na forma de barita. Ou seja, a exposição a múltiplas substâncias pode acarretar em riscos fora da faixa aceitável, mas isso pode ser atenuado ao se levar em conta as formas/espécies em que os metais se encontram nas águas subterrâneas e as toxicidades associadas a essas espécies.

A especiação dos metais se mostrou importante, principalmente para o bário, mesmo nas amostras estudadas que foram coletadas em áreas sem contaminação.

Em áreas contaminadas, essa avaliação se torna mais relevante e importante como parte das atividades de gerenciamento.

A necessidade de ações de intervenção em função do uso do solo (atual e possíveis usos futuros) para uma determinada área deve ser baseada nos resultados de uma avaliação de riscos à saúde humana. Nos casos de contaminações por metais, esta avaliação deve, essencialmente, considerar as espécies em que os metais estão presentes e também os estados de solubilidade de seus minerais (precipitados/em solução), de forma a tornar mais fidedigna à realidade a avaliação de risco. Isto, no entanto, não foi observado na Resolução CONAMA nº 420/2009, sendo importante que estes aspectos técnicos sejam sempre levados em consideração pelos órgãos ambientais (e outros órgãos públicos envolvidos) nas etapas de GAC. Ademais, uma atualização dos regulamentos técnicos e legais é necessária para embasar decisões que sejam tomadas pelos profissionais dos órgãos públicos com base em conceitos científicos, resguardando-os assim como os proprietários/responsáveis legais pelas áreas contaminadas.

As seguintes linhas de pesquisa adicionais são recomendadas como continuidade dos estudos da influência da especiação dos metais de bário e cádmio em riscos à saúde humana, além de servirem de base para outros metais:

- Hidrogeoquímica de áreas contaminadas com cádmio para análise de íons necessários em condições impactadas e em que haja riscos à saúde humana para o consumo de água.
- Influência de filtração com membranas menores (0,22 µm ou 0,10 µm, por exemplo) para retenção do sulfato de bário na forma coloidal em águas subterrâneas.
- Especiação dos metais bário e do cádmio em soluções com pH estomacal (<1,5), representativa das condições após a entrada nos organismos humanos.
- Tratamento por meio da adição de sulfato em concentrações dentro do padrão de potabilidade (<250 mg/L) como alternativa para águas subterrâneas com presença natural de bário acima do padrão CONAMA 420/2009, como é o caso de alguns aquíferos no interior do estado de São Paulo.

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Anexo A

Dados de campo utilizados como entrada no trabalho

Tabela A.1 – Parâmetros físico-químicos e resultados analíticos de metais em amostras de águas subterrâneas coletadas em poços de municípios no estado de São Paulo (Urânia, Gália e Salto de Pirapora).

Poço	Data	BI	Temperatura	pe	pH	Eh	CE	OD	TDS	Na+	K+	Ca2+	Mg2+	Fe Total	Mn2+
		%	(ºC)	-	-	mV	µS/cm	mgO2/L	mg/L	mg/L	mg/L	mg/L	mg/L	mg/L	mg/L
Marcolan (2009)															
PM-1	Sep-07	2,99	26,20	7,037	7,47	418,0	413,0	0,80	-	8,40	6,40	44,00	21,00	<0,001	<0,001
PM-2	Sep-07	2,17	26,90	6,483	9,17	386,0	196,0	3,30	-	45,00	3,60	1,90	0,20	0,00	<0,001
PM-3A	Sep-07	4,61	30,50	8,149	6,33	491,0	162,5	4,20	-	9,20	4,30	15,00	5,70	<0,001	0,02
PM-3B	Sep-07	5,11	30,40	7,653	7,77	461,0	236,0	2,40	-	8,40	4,30	23,00	13,00	<0,001	0,01
PM-3C	Sep-07	-0,29	28,10	4,349	11,13	260,0	599,0	1,00	-	23,00	10,70	39,00	<0,1	<0,001	<0,001
Tavares (2013)															
G PM-03	Jul-10	6,69	23,80	4,883	7,04	287,7	443,0	-	-	2,70	2,30	63,09	16,16	<0,05	0,03
G PM-02	Jul-10	3,45	27,00	4,473	8,86	266,4	276,0	-	-	4,70	5,70	21,08	18,48	<0,05	0,03
G PM-01	Jul-10	-0,54	24,10	6,553	9,37	386,5	264,0	-	-	21,60	16,80	7,42	7,29	<0,05	0,03
PM01	Oct-10	-66,38	22,50	5,386	5,58	316,0	277,0	4,72	-	0,50	0,20	0,56	0,05	0,09	0,01
PM07	Oct-10	2,45	23,40	1,592	5,32	93,7	148,4	0,63	-	17,00	2,10	1,20	1,06	2,01	0,05
PM03	Oct-10	-10,64	22,70	1,724	5,21	101,2	351,0	0,58	-	26,00	5,60	4,94	6,40	0,11	0,56
PM04	Oct-10	5,67	21,20	-1,471	7,07	-85,9	755,0	0,87	-	10,10	3,30	67,37	56,38	1,84	0,19
PM19	Oct-10	-1,59	25,00	3,135	5,65	185,5	2.530,0	1,16	-	128,00	5,90	81,11	160,83	0,05	1,14
PM24/45	Oct-10	0,04	21,50	3,315	5,36	193,8	408,0	1,29	-	3,50	3,10	12,10	28,19	0,08	0,13
PM25	Oct-10	-16,22	23,70	1,241	5,52	73,1	164,4	0,88	-	15,00	1,10	1,05	0,97	10,15	3,44
PM27	Oct-10	-47,34	23,30	-1,312	6,52	-77,2	892,0	0,75	-	23,00	15,00	7,23	5,20	15,23	9,24

Fonte: Marcolan (2009) e Tavares (2013).

Tabela A.2 – Parâmetros físico-químicos e resultados analíticos de metais em amostras de águas subterrâneas coletadas em poços de município no estado do Rio de Janeiro (Itaboraí).

Poço	Data	BI	Temperatura	pe	pH	Eh	CE	OD	TDS	Na+	K+	Ca2+	Mg2+	Fe Total	Mn2+
		%	(ºC)	-	-	mV	µS/cm	mgO2/L	mg/L	mg/L	mg/L	mg/L	mg/L	mg/L	mg/L
Gomes (2012)															
P-01A (08/09)	Aug-09	-	24,94	-1,995	8,00	-118,0	366,0	-	182	76,40	2,40	6,40	0,87	0,11	0,09
P-01B (08/09)	Aug-09	-	24,81	-2,317	6,00	-137,0	183,0	-	91	48,40	4,20	5,60	1,22	0,73	0,14
P-01C (08/09)	Aug-09	-	24,74	-2,047	7,00	-121,0	2.550,0	-	1.268	144,00	18,80	181,00	19,03	23,56	4,54
P-02A (08/09)	Aug-09	-	25,78	1,113	7,20	66,0	376,0	-	187	9,10	5,90	38,10	3,72	0,02	0,02
P-02B (08/09)	Aug-09	-	25,95	1,803	6,00	107,0	90,0	-	45	4,20	2,20	5,20	1,35	0,02	0,06
P-02C (08/09)	Aug-09	-	26,24	1,481	6,70	88,0	197,0	-	98	18,40	5,20	7,30	2,08	0,01	0,29
P-03A (08/09)	Aug-09	-	25,24	-2,010	8,80	-119,0	375,0	-	186	3,20	1,60	4,90	0,79	0,09	0,30
P-03B (08/09)	Aug-09	-	25,40	-0,422	8,60	-25,0	373,0	-	185	90,20	1,10	4,10	0,88	0,02	0,59
P-04A (08/09)	Aug-09	-	25,56	-2,682	7,70	-159,0	1.104,0	-	549	33,60	8,00	16,10	6,65	1,52	1,35
P-04B (08/09)	Aug-09	-	25,60	-1,839	6,80	-109,0	900,0	-	448	97,00	6,00	19,00	8,00	0,02	0,48
P-05 (08/09)	Aug-09	-	-	-	-	-	-	-	-	-	-	-	-	0,35	0,36

Fonte: Gomes (2012).

Tabela A.3 – Parâmetros físico-químicos e resultados analíticos de metais em amostras de águas subterrâneas coletadas em poços de município no estado do Rio de Janeiro (Itaboraí).

Poço	Data	BI	Temperatura	pe	pH	Eh	CE	OD	TDS	Na+	K+	Ca2+	Mg2+	Fe Total	Mn2+
		%	(ºC)	-	-	mV	µS/cm	mgO2/L	mg/L	mg/L	mg/L	mg/L	mg/L	mg/L	mg/L
Sanches (2015)															
P-01 (06/13)	Jun-13	-	23,06	0,371	5,50	40,0	363,0	-	182	52,30	7,00	18,50	4,26	-	-
P-02 (06/13)	Jun-13	-	24,78	0,447	6,50	6,0	418,0	-	211	65,10	5,30	71,00	5,41	-	-
P-03 (06/13)	Jun-13	-	25,08	0,406	7,20	38,0	728,0	-	365	141,00	4,30	49,00	5,14	-	-
P-04 (06/13)	Jun-13	-	25,89	0,454	5,90	14,0	3.138,0	-	1.572	193,50	16,20	337,90	85,95	-	-
P-05 (10/13)	Oct-13	-	24,52	0,276	5,20	175,0	47,0	-	24	13,40	2,50	9,10	2,34	0,85189	0,01740
P-06 (10/13)	Oct-13	-	24,48	0,145	4,20	576,0	313,0	-	154	20,50	8,20	13,30	7,55	0,02407	0,08004
P-07 (10/13)	Oct-13	-	25,80	0,269	6,50	211,0	289,0	-	145	62,30	3,20	29,80	6,74	0,03211	0,00646
P-08 (10/13)	Oct-13	-	26,22	0,227	4,40	310,0	48,0	-	24	13,30	2,50	8,60	2,81	0,03947	0,05055
P-09 (10/13)	Oct-13	-	24,26	0,280	6,10	163,0	62,0	-	31	15,30	2,80	14,50	3,73	0,17229	0,09200
P-10 (10/13)	Oct-13	-	25,37	0,313	6,40	135,0	80,0	-	40	18,00	2,00	14,00	4,00	0,00789	0,00413
P-11 (10/13)	Oct-13	-	24,83	0,437	6,90	13,0	318,0	-	159	58,00	4,60	36,30	7,42	0,07531	0,13665
P-12 (10/13)	Oct-13	-	27,33	0,447	5,80	35,0	155,0	-	78	21,30	4,00	17,60	9,18	0,46189	0,03012
P-13 (10/13)	Oct-13	-	26,74	0,404	8,40	60,0	1.367,0	-	684	239,20	3,30	20,00	13,54	0,03058	0,00559
P-14 (10/13)	Oct-13	-	24,93	0,441	7,50	12,0	586,0	-	293	50,80	5,40	54,10	14,24	0,04925	0,06439
P-15 (10/13)	Oct-13	-	25,54	0,343	7,20	102,0	446,0	-	223	29,60	3,10	42,80	27,40	0,17304	0,11577
P-16 (10/13)	Oct-13	-	24,63	0,223	4,60	283,0	125,0	-	63	24,10	7,50	14,10	16,74	0,02525	0,06763
P-17 (10/13)	Oct-13	-	25,06	0,253	5,00	227,0	67,0	-	34	16,50	4,50	20,30	12,12	0,03198	0,01180

Fonte: Sanches (2015).

Tabela A.4 – Resultados analíticos de ânions inorgânicos em amostras de águas subterrâneas coletadas em poços de municípios no estado de São Paulo (Urânia, Gália e Salto de Pirapora).

Poço	Data	Alcalinidade total	HCO3-	CO3=	SO42-	Cl-	F-	NH4+	NO2-	NO3-	PO43-	Si
		mg CaCO3/L	mg/L	mg/L	mg/L	mg/L	mg/L	mg/L	mg/L	mg/L	mg/L	mg/L
Marcolan (2009)												
PM-1	Sep-07	165,05	201,36	0,35	0,27	8,20	0,28	<0,02	<0,02	40,00	<0,05	65,60
PM-2	Sep-07	97,91	117,97	0,73	1,70	1,20	0,32	<0,02	<0,02	0,23	0,240	17,50
PM-3A	Sep-07	65,19	79,53	0,01	0,28	3,00	0,14	<0,02	<0,02	11,00	0,100	26,30
PM-3B	Sep-07	121,69	148,46	-	0,11	0,25	0,17	<0,02	<0,02	0,06	0,012	62,60
PM-3C	Sep-07	139,88	18,16	74,84	14,00	3,30	0,44	<0,02	0,230	0,25	0,050	10,10
Tavares (2013)												
G PM-03	Jul-10	180,17	219,56	0,12	4,43	4,58	0,07	-	0,020	16,13	0,050	14,37
G PM-02	Jul-10	131,66	159,38	0,61	1,29	2,85	0,08	-	0,009	1,25	0,040	11,58
G PM-01	Jul-10	86,52	93,94	5,71	7,78	13,45	0,12	-	0,020	7,97	0,060	5,27
PM01	Oct-10	15,02	18,32	-	0,08	0,23	0,03	-	-	0,23	0,030	0,35
PM07	Oct-10	10,01	12,21	-	0,31	24,62	0,06	-	0,070	0,05	0,020	6,08
PM03	Oct-10	7,51	9,16	-	3,26	81,53	0,08	-	0,160	4,03	0,040	6,98
PM04	Oct-10	375,34	457,39	0,26	0,24	4,51	0,13	-	0,010	0,16	0,020	13,74
PM19	Oct-10	40,03	48,84	-	15,58	783,49	0,13	-	0,090	37,85	0,150	8,60
PM24/45	Oct-10	25,02	30,53	-	0,49	92,35	0,14	-	0,160	3,14	0,060	8,07
PM25	Oct-10	35,03	42,74	-	1,99	20,36	0,08	-	0,050	0,15	0,010	3,40
PM27	Oct-10	285,26	347,90	0,06	0,06	57,79	0,53	-	0,030	0,15	0,030	2,19

Fonte: Marcolan (2009) e Tavares (2013).

Tabela A.5 – Resultados analíticos de ânions inorgânicos em amostras de águas subterrâneas coletadas em poços de município no estado do Rio de Janeiro (Itaboraí).

Poço	Data	Alcalinidade total	HCO3-	CO3=	SO42-	Cl-	F-	NH4+	NO2-	NO3-	PO43-	Si
		mg CaCO3/L	mg/L	mg/L	mg/L	mg/L	mg/L	mg/L	mg/L	mg/L	mg/L	mg/L
Gomes (2012)												
P-01A (08/09)	Aug-09	187,70	229,00	-	0,80	3,70	0,28	0,006	0,004	0,051	0,068	30,40
P-01B (08/09)	Aug-09	128,69	157,00	-	20,00	-	0,21	0,010	0,005	0,083	0,443	71,80
P-01C (08/09)	Aug-09	144,26	176,00	-	-	626,00	-	0,076	0,015	0,058	0,065	70,00
P-02A (08/09)	Aug-09	149,18	182,00	-	4,00	5,70	0,40	0,003	0,005	0,054	0,055	28,10
P-02B (08/09)	Aug-09	24,59	30,00	-	0,00	6,80	0,09	0,007	0,005	0,329	0,016	9,40
P-02C (08/09)	Aug-09	65,57	80,00	-	0,00	3,80	0,37	0,004	0,004	0,044	0,059	5,20
P-03A (08/09)	Aug-09	268,85	328,00	-	-	-	-	0,011	0,004	0,021	0,127	19,50
P-03B (08/09)	Aug-09	196,72	240,00	-	5,20	7,80	1,82	0,007	0,006	0,061	0,095	18,90
P-04A (08/09)	Aug-09	40,98	50,00	-	22,50	122,00	6,14	0,049	0,007	0,018	0,004	37,50
P-04B (08/09)	Aug-09	55,74	68,00	-	15,00	158,00	0,37	0,009	0,004	0,023	0,030	22,50
P-05 (08/09)	Aug-09	-	-	-	-	-	0,65	0,161	0,014	0,014	0,048	14,50

Fonte: Gomes (2012).

Tabela A.6 – Resultados analíticos de ânions inorgânicos em amostras de águas subterrâneas coletadas em poços de município no estado do Rio de Janeiro (Itaboraí).

Poço	Data	Alcalinidade total	HCO3-	CO3=	SO42-	Cl-	F-	NH4+	NO2-	NO3-	PO43-	Si
		mg CaCO3/L	mg/L	mg/L	mg/L	mg/L	mg/L	mg/L	mg/L	mg/L	mg/L	mg/L
Sanches (2015)												
P-01 (06/13)	Jun-13	24,59	30,00	-	73,10	66,80	0,01	-	<0,002	35,01	0,010	-
P-02 (06/13)	Jun-13	238,52	291,00	-	18,20	73,80	0,06	-	<0,002	1,17	0,060	-
P-03 (06/13)	Jun-13	150,00	183,00	-	52,10	174,00	0,07	-	0,060	3,26	0,070	-
P-04 (06/13)	Jun-13	220,49	269,00	-	55,60	950,00	0,02	-	<0,002	1,46	0,020	-
P-05 (10/13)	Oct-13	47,54	58,00	-	4,30	9,60	1,07	-	<0,002	3,56	0,008	-
P-06 (10/13)	Oct-13	27,87	34,00	-	2,70	63,00	1,19	-	<0,002	28,54	0,061	-
P-07 (10/13)	Oct-13	215,57	263,00	-	2,90	17,90	1,24	-	<0,002	0,46	0,143	-
P-08 (10/13)	Oct-13	38,52	47,00	-	13,00	9,20	1,08	-	0,020	4,62	0,003	-
P-09 (10/13)	Oct-13	65,57	80,00	-	12,10	9,00	1,10	-	<0,002	4,12	0,056	-
P-10 (10/13)	Oct-13	81,97	100,00	-	2,00	4,00	1,02	-	<0,002	4,96	0,003	-
P-11 (10/13)	Oct-13	245,90	300,00	-	3,60	16,00	1,22	-	<0,002	3,21	0,114	-
P-12 (10/13)	Oct-13	93,44	114,00	-	4,80	18,00	1,06	-	<0,002	4,37	0,029	-
P-13 (10/13)	Oct-13	609,02	743,00	-	3,60	37,00	6,03	-	<0,002	2,84	0,012	-
P-14 (10/13)	Oct-13	202,46	247,00	-	17,20	60,40	1,05	-	<0,002	5,87	0,102	-
P-15 (10/13)	Oct-13	236,07	288,00	-	6,90	33,20	2,00	-	0,320	5,84	0,087	-
P-16 (10/13)	Oct-13	118,85	145,00	-	4,90	29,70	1,16	-	0,020	15,22	0,003	-
P-17 (10/13)	Oct-13	103,28	126,00	-	3,50	16,60	1,09	-	0,010	9,57	0,009	-

Fonte: Sanches (2015).

Tabela A.7 – Resultados analíticos de metais traço em amostras de águas subterrâneas coletadas em poços de municípios no estado de São Paulo (Urânia, Gália e Salto de Pirapora).

Poço	Data	Ba2+	Cd2+	Al3+	Br	B	Pb	Cu	Ni	Sr	Zn
		mg/L	mg/L	mg/L	mg/L	mg/L	mg/L	mg/L	mg/L	mg/L	mg/L
Marcolan (2009)											
PM-1	Sep-07	0,419	-	<0,01	<0,02	-	-	<0,001	<0,001	0,55	0,01000
PM-2	Sep-07	0,017	-	0,05000	<0,02	-	-	<0,001	<0,001	0,09	0,01000
PM-3A	Sep-07	0,217	-	<0,01	<0,02	-	-	<0,001	0,00200	0,12	0,04000
PM-3B	Sep-07	0,116	-	0,01000	<0,02	-	-	<0,001	<0,001	0,83	0,01000
PM-3C	Sep-07	0,055	-	2,01000	<0,02	-	-	<0,001	0,00100	0,90	<0,01
Tavares (2013)											
G PM-03	Jul-10	0,280	-	<0,030	-	-	-	-	-	0,53	-
G PM-02	Jul-10	1,540	-	<0,030	-	-	-	-	-	0,58	-
G PM-01	Jul-10	0,340	-	<0,030	-	-	-	-	-	1,46	-
PM01	Oct-10	0,070	-	0,020	-	-	-	-	0,00730	0,15	-
PM07	Oct-10	0,220	-	0,025	-	-	-	-	0,00550	0,22	-
PM03	Oct-10	0,740	-	0,067	-	-	0,00210	-	0,01300	0,50	-
PM04	Oct-10	1,480	-	0,013	-	-	-	-	0,00051	0,53	-
PM19	Oct-10	1,900	-	0,014	-	-	0,00100	-	0,55000	1,21	-
PM24/45	Oct-10	0,610	-	0,028	-	-	0,02200	-	0,63000	0,31	-
PM25	Oct-10	0,900	-	0,019	-	-	0,01800	-	0,00350	0,10	-
PM27	Oct-10	8,110	-	0,035	-	-	0,00058	-	0,01100	0,20	-

Fonte: Marcolan (2009) e Tavares (2013).

Tabela A.8 – Resultados analíticos de metais traço em amostras de águas subterrâneas coletadas em poços de município no estado do Rio de Janeiro (Itaboraí).

Poço	Data	Ba2+	Cd2+	Al3+	Br	B	Pb	Cu	Ni	Sr	Zn
		mg/L	mg/L	mg/L	mg/L	mg/L	mg/L	mg/L	mg/L	mg/L	mg/L
Gomes (2012)											
P-01A (08/09)	Aug-09	1,050	0,00073	0,00849	-	0,05670	0,00363	0,00551	0,00673	-	0,13820
P-01B (08/09)	Aug-09	0,370	0,00066	0,00672	-	0,02300	0,00147	0,00093	nd	-	0,10300
P-01C (08/09)	Aug-09	1,760	0,00069	0,00151	-	0,02420	0,00243	0,00165	0,00337	-	0,09620
P-02A (08/09)	Aug-09	0,580	0,00068	0,00508	-	0,02220	0,00187	0,00726	0,00095	-	0,09850
P-02B (08/09)	Aug-09	0,080	0,00079	0,01108	-	0,00780	0,00620	0,01091	0,00370	-	0,03670
P-02C (08/09)	Aug-09	0,170	0,00099	0,00818	-	0,01050	0,00576	0,06238	0,00946	-	0,07650
P-03A (08/09)	Aug-09	0,430	0,00094	0,01562	-	0,02660	0,00166	0,00088	nd	-	0,01990
P-03B (08/09)	Aug-09	0,190	0,00088	0,04564	-	0,01410	0,00167	0,00211	nd	-	0,01200
P-04A (08/09)	Aug-09	0,260	0,00069	0,00115	-	0,01220	0,00317	0,00336	0,00112	-	0,00980
P-04B (08/09)	Aug-09	0,220	0,00068	0,00210	-	0,03170	0,00337	0,00317	nd	-	0,00580
P-05 (08/09)	Aug-09	0,070	0,00067	0,00803	-	0,73410	0,00233	0,00474	0,00180	-	0,01190

Fonte: Gomes (2012).

Tabela A.9 – Resultados analíticos de metais traço em amostras de águas subterrâneas coletadas em poços de município no estado do Rio de Janeiro (Itaboraí).

Poço	Data	Ba2+	Cd2+	Al3+	Br	B	Pb	Cu	Ni	Sr	Zn
		mg/L	mg/L	mg/L	mg/L	mg/L	mg/L	mg/L	mg/L	mg/L	mg/L
Sanches (2015)											
P-01 (06/13)	Jun-13	<0,002	-	-	0,500	-	-	-	-	-	-
P-02 (06/13)	Jun-13	1,170	-	-	0,600	-	-	-	-	-	-
P-03 (06/13)	Jun-13	0,620	-	-	0,710	-	-	-	-	-	-
P-04 (06/13)	Jun-13	1,370	-	-	3,380	-	-	-	-	-	-
P-05 (10/13)	Oct-13	2,810	0,000920	0,017550	<0,002	0,117500	0,000840	0,009180	0,003600	-	0,121990
P-06 (10/13)	Oct-13	1,800	0,001300	0,857480	0,340	0,169000	0,002960	0,005360	0,004190	-	0,261140
P-07 (10/13)	Oct-13	1,510	0,000830	0,029020	0,440	0,140400	0,000530	0,002660	0,000660	-	0,154260
P-08 (10/13)	Oct-13	0,800	0,000880	0,052510	0,170	0,126500	0,000160	0,002030	0,000280	-	0,110260
P-09 (10/13)	Oct-13	1,200	0,001020	0,127960	0,450	0,132000	0,001050	0,004470	0,001260	-	0,099310
P-10 (10/13)	Oct-13	1,790	0,000610	0,022130	0,400	0,124000	0,000650	0,002050	<0,000003	-	0,125930
P-11 (10/13)	Oct-13	0,750	0,000910	0,006210	0,440	0,079150	0,001360	0,001940	0,000690	-	0,006760
P-12 (10/13)	Oct-13	2,520	0,000650	0,008590	0,460	0,114400	0,004510	0,003870	0,000940	-	0,106560
P-13 (10/13)	Oct-13	1,980	0,000830	0,061920	0,490	0,605100	0,001080	0,002480	0,001610	-	0,131580
P-14 (10/13)	Oct-13	0,980	0,000770	0,048810	0,540	0,134300	0,000520	0,001380	<0,000003	-	0,108080
P-15 (10/13)	Oct-13	<0,002	0,000710	0,026650	0,500	0,130900	0,000640	0,001690	0,000670	-	0,121360
P-16 (10/13)	Oct-13	1,610	0,000980	0,041990	0,480	0,136200	0,000460	0,006080	0,001900	-	0,155290
P-17 (10/13)	Oct-13	2,310	0,001030	0,025670	0,450	0,136300	0,000710	0,002630	0,001420	-	0,118400

Fonte: Sanches (2015).

Anexo B

Resultados das simulações com o modelo phreeqc: equilíbrio hidrogeoquímico, especiação e estados de solubilidade de minerais

Tabela B.1 – Resultados do modelo phreeqc (equilíbrio hidrogeoquímico, especiação e estados de solubilidade de minerais para o metal bário) para os dados de poços de municípios no estado de São Paulo (Urânia, Gália e Salto de Pirapora).

Parâmetro		Unidade	Poços de Urânia/SP (Marcolan, 2009)					Poços de Gália/SP e Salto de Pirapora/SP (Tavares, 2013)										
			PM-1	PM-2	PM-3A	PM-3B	PM-3C	G PM-03	G PM-02	G PM-01	PM01	PM07	PM03	PM04	PM19	PM24/45	PM25	PM27
Dados de Campo (íons na "fração dissolvida")																		
pH		-	7,47	9,17	6,33	7,77	11,13	7,04	8,86	9,37	5,58	5,32	5,21	7,07	5,65	5,36	5,52	6,52
pe [(a)]		-	7,037	6,483	8,149	7,653	4,349	4,883	4,473	6,553	5,386	1,592	1,724	-1,471	3,135	3,315	1,241	-1,312
Bário (Ba^{2+})		mg/L	0,419	0,017	0,217	0,116	0,055	0,280	1,540	0,340	0,070	0,220	0,740	1,480	1,900	0,610	0,900	8,110
Sulfato (SO_4^{2-})		mg/L	0,3	1,7	0,3	0,1	14,0	4,4	1,3	7,8	0,1	0,3	3,3	0,2	15,6	0,5	2,0	0,1
Resultados do modelo phreeqc																		
Balanço Cátion-Ânion		%	-18%	2%	-12%	5%	5%	-3%	2%	-9%	-65%	6%	-15%	6%	-6%	-3%	-1%	-41%
Espécies iônicas de bário em solução [(d)] (valores em mg/L de bário)	Ba^{2+}	mg/L	0,409	0,016	0,214	0,113	0,046	0,271	1,466	0,314	0,070	0,219	0,728	1,421	1,805	0,604	0,888	7,794
	$BaSO_4$	mg/L	<0,001	<0,001	<0,001	<0,001	0,007	<0,001	0,044	0,016	<0,001	<0,001	<0,001	0,001	<0,001	<0,001	<0,001	0,002
	$BaCO_3$	mg/L	<0,001	<0,001	<0,001	<0,001	0,002	0,003	0,005	0,007	<0,001	<0,001	0,007	<0,001	0,025	<0,001	0,006	0,001
	$BaHCO_3^+$	mg/L	0,009	<0,001	0,003	0,002	<0,001	0,006	0,025	0,003	<0,001	<0,001	<0,001	0,057	0,007	0,002	0,005	0,284
	$BaOH^+$	mg/L	<0,001	<0,001	<0,001	<0,001	<0,001	<0,001	<0,001	<0,001	<0,001	<0,001	<0,001	<0,001	<0,001	<0,001	<0,001	<0,001
	$BaCl^+$	mg/L	<0,001	<0,001	<0,001	<0,001	<0,001	<0,001	<0,001	<0,001	<0,001	<0,001	0,004	<0,001	0,062	0,003	0,001	0,028
	$BaNO_3^+$	mg/L	<0,001	<0,001	<0,001	<0,001	<0,001	<0,001	<0,001	<0,001	<0,001	<0,001	<0,001	<0,001	<0,001	<0,001	<0,001	<0,001
Índice de Saturação (IS) [(b)]	Barita [(c)]	-	-1,63	-2,05	-1,78	-2,52	-0,76	-0,57	-0,32	-0,12	-2,57	-1,57	-0,11	-1,20	0,41	-1,09	-0,19	-0,91
	Witherita [(c)]	-	-2,50	-2,44	-4,21	-2,81	-1,45	-3,08	-0,67	-1,08	-6,05	-6,03	-5,78	-2,08	-4,48	-5,25	-4,70	-1,94

Observações:

a) Potencial de elétrons calculado a partir do potencial redox medido (ORP) e da temperatura medidos em campo.

b) Índice de saturação corresponde ao log (IAP/K_{sp}). Para valores de IS>0, o mineral precipita e para valores de IS<0 o mineral fica em solução.

c) Barita é um mineral formado por sulfato de bário ($BaSO_4$). Witherita é um mineral formado por carbonato de bário ($BaCO_3$).

d) A soma das concentrações das espécies é igual a soma das concentrações dos dados de campo.

Tabela B.2 – Resultados do modelo phreeqc (equilíbrio hidrogeoquímico, especiação e estados de solubilidade de minerais para o metal bário) para os dados de poços de município no estado do Rio de Janeiro (Itaboraí).

Parâmetro		Unidade	Poços de Itaboraí/RJ (Gomes, 2012)										
			P-01A (08/09)	P-01B (08/09)	P-01C (08/09)	P-02A (08/09)	P-02B (08/09)	P-02C (08/09)	P-03A (08/09)	P-03B (08/09)	P-04A (08/09)	P-04B (08/09)	P-05 (08/09)
Dados de Campo (íons na "fração dissolvida")													
pH		-	8,00	6,00	7,00	7,20	6,00	6,70	8,80	8,60	7,70	6,80	-
pe [(a)]		-	-1,995	-2,317	-2,047	1,113	1,803	1,481	-2,010	-0,422	-2,682	-1,839	4,000
Bário (Ba^{2+})		mg/L	1,050	0,370	1,760	0,580	0,080	0,170	0,430	0,190	0,260	0,220	0,070
Sulfato (SO_4^{2-})		mg/L	0,8	20,0	-	4,0	0,0	0,0	-	5,2	22,5	15,0	-
Resultados do modelo phreeqc													
Balanço Cátion-Ânion		%	-1%	-7%	-6%	-8%	-7%	2%	-84%	-1%	-24%	1%	-5%
Espécies iônicas de bário em solução [(d)] (valores em mg/L de bário)	Ba^{2+}	mg/L	1,014	0,342	1,686	0,561	0,080	0,168	0,393	0,178	0,242	0,209	0,070
	$BaSO_4$	mg/L	0,006	<0,001	<0,001	<0,001	<0,001	<0,001	0,022	0,004	<0,001	<0,001	<0,001
	$BaCO_3$	mg/L	0,002	0,021	<0,001	0,006	<0,001	<0,001	<0,001	0,003	0,014	0,007	<0,001
	$BaHCO_3^+$	mg/L	0,027	0,007	0,024	0,012	<0,001	0,002	0,015	0,005	0,001	0,002	<0,001
	$BaOH^+$	mg/L	<0,001	<0,001	<0,001	<0,001	<0,001	<0,001	<0,001	<0,001	<0,001	<0,001	<0,001
	$BaCl^+$	mg/L	<0,001	<0,001	0,050	<0,001	<0,001	<0,001	<0,001	<0,001	0,002	0,002	<0,001
	$BaNO_3^+$	mg/L	<0,001	<0,001	<0,001	<0,001	<0,001	<0,001	<0,001	<0,001	<0,001	<0,001	<0,001
Índice de Saturação (IS) [(b)]	Barita [(c)]	-	-0,62	0,33	-	-0,22	-	-	-	-0,58	0,16	-0,13	-
	Witherita [(c)]	-	-1,48	-4,10	-2,57	-2,63	-5,38	-3,96	-0,95	-1,64	-3,08	-3,93	-

Observações:

a) Potencial de elétrons calculado a partir do potencial redox medido (ORP) e da temperatura medidos em campo.

b) Índice de saturação corresponde ao log (IAP/K_{sp}). Para valores de IS>0, o mineral precipita e para valores de IS<0 o mineral fica em solução.

c) Barita é um mineral formado por sulfato de bário ($BaSO_4$). Witherita é um mineral formado por carbonato de bário ($BaCO_3$).

d) A soma das concentrações das espécies é igual a soma das concentrações dos dados de campo.

Tabela B.3 – Resultados do modelo phreeqc (equilíbrio hidrogeoquímico, especiação e estados de solubilidade de minerais para o metal bário) para os dados de poços de município no estado do Rio de Janeiro (Itaboraí).

Parâmetro		Unidade	Poços de Itaboraí/RJ (Sanches, 2015)																
			P-01 (06/13)	P-02 (06/13)	P-03 (06/13)	P-04 (06/13)	P-05 (06/13)	P-06 (10/13)	P-07 (10/13)	P-08 (10/13)	P-09 (10/13)	P-10 (10/13)	P-11 (10/13)	P-12 (10/13)	P-13 (10/13)	P-14 (10/13)	P-15 (10/13)	P-16 (10/13)	P-17 (10/13)
Dados de Campo (íons na "fração dissolvida")																			
pH		-	5,50	6,50	7,20	5,90	5,20	4,20	6,50	4,40	6,10	6,40	6,90	5,80	8,40	7,50	7,20	4,60	5,00
pe [(a)]		-	0,371	0,447	0,406	0,454	0,276	0,145	0,269	0,227	0,28	0,313	0,437	0,447	0,404	0,441	0,343	0,223	0,253
Bário (Ba^{2+})		mg/L	<0,002	1,170	0,620	1,370	2,810	1,800	1,510	0,800	1,200	1,790	0,750	2,520	1,980	0,980	<0,002	1,610	2,310
Sulfato (SO_4^{2-})		mg/L	73,1	18,2	52,1	55,6	4,3	2,7	2,9	13,0	12,1	2,0	3,6	4,8	3,6	17,2	6,9	4,9	3,5
Resultados do modelo phreeqc																			
Balanço Cátion-Ânion		%	-27%	-3%	-1%	0%	-9%	-28%	-1%	-12%	-9%	-8%	-6%	-2%	-5%	-3%	-5%	-14%	-8%
Espécies iônicas de bário em solução [(d)] (valores em mg/L de bário)	Ba^{2+}	mg/L	-	1,092	0,547	1,245	2,748	1,771	1,454	0,761	1,145	1,756	0,719	2,448	1,766	0,918	-	1,561	2,252
	$BaSO_4$	mg/L	-	<0,001	<0,001	<0,001	<0,001	<0,001	<0,001	<0,001	<0,001	<0,001	<0,001	<0,001	0,072	0,002	-	<0,001	<0,001
	$BaCO_3$	mg/L	-	0,040	0,057	0,052	0,040	0,013	0,010	0,033	0,043	0,011	0,006	0,033	0,012	0,033	-	0,019	0,021
	$BaHCO_3^+$	mg/L	-	0,033	0,010	0,024	0,020	0,008	0,044	0,005	0,011	0,022	0,024	0,036	0,127	0,024	-	0,026	0,034
	$BaOH^+$	mg/L	-	<0,001	<0,001	<0,001	<0,001	<0,001	<0,001	<0,001	<0,001	<0,001	<0,001	<0,001	<0,001	<0,001	-	<0,001	<0,001
	$BaCl^+$	mg/L	-	0,005	0,005	0,048	0,002	0,007	0,002	<0,001	<0,001	<0,001	<0,001	0,003	0,004	0,003	-	0,003	0,003
	$BaNO_3^+$	mg/L	-	<0,001	<0,001	<0,001	<0,001	<0,001	<0,001	<0,001	<0,001	<0,001	<0,001	<0,001	<0,001	<0,001	-	<0,001	<0,001
Índice de Saturação (IS) [(b)]	Barita [(c)]	-	-	0,62	0,76	0,72	0,61	0,13	0,01	0,51	0,65	0,04	-0,21	0,50	0,06	0,53	-	0,30	0,33
	Witherita [(c)]	-	-	-2,91	-2,73	-3,69	-4,39	-5,82	-2,78	-5,81	-3,76	-3,17	-2,65	-3,57	-0,45	-2,05	-	-4,90	-4,39

Observações:

a) Potencial de elétrons calculado a partir do potencial redox medido (ORP) e da temperatura medidos em campo.

b) Índice de saturação corresponde ao log (IAP/K_{sp}). Para valores de IS>0, o mineral precipita e para valores de IS<0 o mineral fica em solução.

c) Barita é um mineral formado por sulfato de bário ($BaSO_4$). Witherita é um mineral formado por carbonato de bário ($BaCO_3$).

d) A soma das concentrações das espécies é igual a soma das concentrações dos dados de campo.

Tabela B.4 – Resultados do modelo phreeqc (equilíbrio hidrogeoquímico, especiação e estados de solubilidade de minerais para o metal cádmio) para os dados de poços de município no estado do Rio de Janeiro (Itaboraí).

Parâmetro		Unidade	Poços de Itaboraí/RJ (Gomes, 2012)										
			P-01A (08/09)	P-01B (08/09)	P-01C (08/09)	P-02A (08/09)	P-02B (08/09)	P-02C (08/09)	P-03A (08/09)	P-03B (08/09)	P-04A (08/09)	P-04B (08/09)	P-05 (08/09)
Dados de Campo (íons na "fração dissolvida")													
pH		-	8,00	6,00	7,00	7,20	6,00	6,70	8,80	8,60	7,70	6,80	-
pe [a]		-	-1,995	-2,317	-2,047	1,113	1,803	1,481	-2,010	-0,422	-2,682	-1,839	4,000
Cádmio (Cd^{2+})		mg/L	0,000730	0,000660	0,000690	0,000680	0,000790	0,000990	0,000940	0,000880	0,000690	0,000680	0,000670
Resultados do modelo phreeqc													
Balanço Cátion-Ânion		%	-1%	-7%	-6%	-8%	-7%	2%	-84%	-1%	-24%	1%	-5%
Espécies iônicas de cádmio em solução [d] (valores em mg/L de cádmio)	Cd^{2+}	mg/L	0,000655	0,000600	0,000346	0,000623	0,000767	0,000949	0,000723	0,000739	0,000527	0,000505	0,000669
	$CdHCO_3^+$	mg/L	0,000058	0,000038	0,000016	0,000044	0,000010	0,000032	0,000088	0,000064	0,000010	0,000012	<0,000001
	$CdCO_3$	mg/L	0,000006	<0,000001	<0,000001	<0,000001	<0,000001	<0,000001	0,000062	0,000028	<0,000001	<0,000001	<0,000001
	$CdCl^+$	mg/L	0,000005	<0,000001	0,000310	0,000007	0,000012	0,000008	<0,000001	0,000011	0,000127	0,000149	<0,000001
	$CdSO_4$	mg/L	<0,000001	0,000021	<0,000001	0,000004	<0,000001	<0,000001	<0,000001	0,000006	0,000018	0,000010	<0,000001
Índice de Saturação (IS) [b]	Otavita [c]	-	-1,05	-3,23	-2,64	-1,96	-3,77	-2,58	-0,06	-0,40	-2,12	-2,92	-

Observações:

a) Potencial de elétrons calculado a partir do potencial redox medido (ORP) e da temperatura medidos em campo.

b) Índice de saturação corresponde ao log (IAP/K_{sp}). Para valores de IS>0, o mineral precipita e para valores de IS<0 o mineral fica em solução.

c) Otavita é um mineral formado por carbonato de cádmio ($CdCO_3$).

d) A soma das concentrações das espécies é igual a soma das concentrações dos dados de campo.

Tabela B.5 – Resultados do modelo phreeqc (equilíbrio hidrogeoquímico, especiação e estados de solubilidade de minerais para o metal cádmio) para os dados de poços de município no estado do Rio de Janeiro (Itaboraí).

Parâmetro		Unidade	Poços de Itaboraí/RJ (Sanches, 2015)																
			P-01 (06/13)	P-02 (06/13)	P-03 (06/13)	P-04 (06/13)	P-05 (06/13)	P-06 (10/13)	P-07 (10/13)	P-08 (10/13)	P-09 (10/13)	P-10 (10/13)	P-11 (10/13)	P-12 (10/13)	P-13 (10/13)	P-14 (10/13)	P-15 (10/13)	P-16 (10/13)	P-17 (10/13)
Dados de Campo (íons na "fração dissolvida")																			
pH		-	5,50	6,50	7,20	5,90	5,20	4,20	6,50	4,40	6,10	6,40	6,90	5,80	8,40	7,50	7,20	4,60	5,00
pe [a]		-	0,371	0,447	0,406	0,454	0,276	0,145	0,269	0,227	0,28	0,313	0,437	0,447	0,404	0,441	0,343	0,223	0,253
Cádmio (Cd^{2+})		mg/L	-	-	-	-	0,000920	0,001300	0,000830	0,000880	0,001020	0,000610	0,000910	0,000650	0,000830	0,000770	0,000710	0,000980	0,001030
Resultados do modelo phreeqc																			
Balanço Cátion-Ânion		%	-27%	-3%	-1%	0%	-9%	-28%	-1%	-12%	-9%	-8%	-6%	-2%	-5%	-3%	-5%	-14%	-8%
Espécies iônicas de cádmio em solução [d] (valores em mg/L de cádmio)	Cd^{2+}	mg/L	-	-	-	-	0,000872	0,001129	0,000730	0,000824	0,000948	0,000578	0,000793	0,000595	0,000588	0,000629	0,000604	0,000871	0,000944
	$CdHCO_3^+$	mg/L	-	-	-	-	0,000022	0,000017	0,000071	0,000017	0,000031	0,000024	0,000087	0,000027	0,000132	0,000054	0,000061	0,000049	0,000047
	$CdCO_3$	mg/L	-	-	-	-	<0,000001	<0,000001	<0,000001	<0,000001	<0,000001	<0,000001	<0,000001	<0,000001	0,000036	0,000002	0,000001	<0,000001	<0,000001
	$CdCl^+$	mg/L	-	-	-	-	0,000018	0,000144	0,000025	0,000017	0,000018	0,000005	0,000024	0,000022	0,000035	0,000069	0,000037	0,000051	0,000032
	$CdSO_4$	mg/L	-	-	-	-	0,000007	0,000005	0,000003	0,000021	0,000021	0,000002	0,000004	0,000005	0,000002	0,000013	0,000005	0,000006	0,000005
Índice de Saturação (IS) [b]	Otavita [c]	-	-	-	-	-	-4,27	-5,39	-2,46	-5,15	-3,22	-3,02	-1,98	-3,56	-0,30	-1,59	-1,83	-4,53	-4,14

Observações:

a) Potencial de elétrons calculado a partir do potencial redox medido (ORP) e da temperatura medidos em campo.

b) Índice de saturação corresponde ao log (IAP/K_{sp}). Para valores de IS>0, o mineral precipita e para valores de IS<0 o mineral fica em solução.

c) Otavita é um mineral formado por carbonato de cádmio ($CdCO_3$).

d) A soma das concentrações das espécies é igual a soma das concentrações dos dados de campo.

Anexo C

Arquivos de entrada e de saída do modelo phreeqc

```
SOLUTION 1 # (Tavares, 2013) Gália/SP - G PM-03 jul/10 (Tabela 7.1.2.1 - página 154)
# Below detection limits values included as zero.
    temp      23.8
    pe        4.883 # Calculated with eh-to-pe.xls file
    pH        7.04
#   ORP       287.7 mV
#   EC        443 µS/cm # Electrical conductivity
    redox     pe
    units     mg/l
    density   1
#    O(0)      -
    Ba        0.28
#    Cd        -
    Na        2.7
    K         2.3
    Ca        63.09
    Mg        16.16
    Fe        0 # Dissolved Iron
#    Fe(2)     -
#    Fe(3)     -
    Mn        0.03
    Alkalinity 180.17 as Ca.5(CO3).5 # Total Alkalinity calculated as mgCaCO3/L
#    C         0.12
    S(6)      4.43
#    S(-2)     - # Sulfide (sulfite SO3(-2) is not included in phreeqc database and
implies in differences in Ionic Balance for some wells)
#    S(4)      - # Sulfite included by Paulo Alencar in wateq4f.dat database considering
discussions at http://phreeqcusers.org/index.php?topic=963.0
    Cl        4.58
    F         0.07
#    N(-3)     - # NH3 reported as N
    N(+3)     0.02 # Nitrite reported as N
    N(+5)     16.13 # Nitrate reported as N
#    N(0)      - # Total nitrogen
    P         0.05 # Phosphate reported as P
    Si        14.37
    Al        0
#    As        -
#    Ag        -
#    Br        -
#    B         -
#    Co        -
#    Pb        -
#    Cr        -
#    Cr(+6)    -
#    Cu        -
#    Mo        -
#    Ni        -
#    Se(6)     - # Dissolved Selenium considered as selenate
    Sr        0.53
#    V         -
#    Zn        -
    -water    1 # kg

SOLUTION 2 # (Tavares, 2013) Gália/SP - G PM-02 jul/10 (Tabela 7.1.2.1 - página 154)
# Below detection limits values included as zero.
    temp      27
    pe        4.473 # Calculated with eh-to-pe.xls file
    pH        8.86
#   ORP       266.4 mV
#   EC        276 µS/cm # Electrical conductivity
    redox     pe
    units     mg/l
    density   1
#    O(0)      -
    Ba        1.54
#    Cd        -
    Na        4.7
```

```
    K         5.7
    Ca        21.08
    Mg        18.48
    Fe        0 # Dissolved Iron
#    Fe(2)     -
#    Fe(3)     -
    Mn        0.03
    Alkalinity 131.66 as Ca.5(CO3).5 # Total Alkalinity calculated as mgCaCO3/L
#    C         0.61
    S(6)      1.29
#    S(-2)     - # Sulfide (sulfite SO3(-2) is not included in phreeqc database and
implies in differences in Ionic Balance for some wells)
#    S(4)      - # Sulfite included by Paulo Alencar in wateq4f.dat database considering
discussions at http://phreeqcusers.org/index.php?topic=963.0
    Cl        2.85
    F         0.08
#    N(-3)     - # NH3 reported as N
    N(+3)     0.009 # Nitrite reported as N
    N(+5)     1.25 # Nitrate reported as N
#    N(0)      - # Total nitrogen
    P         0.04 # Phosphate reported as P
    Si        11.58
    Al        0
#    As        -
#    Ag        -
#    Br        -
#    B         -
#    Co        -
#    Pb        -
#    Cr        -
#    Cr(+6)    -
#    Cu        -
#    Mo        -
#    Ni        -
#    Se(6)     - # Dissolved Selenium considered as selenate
    Sr        0.58
#    V         -
#    Zn        -
    -water    1 # kg

SOLUTION 3 # (Tavares, 2013) Gália/SP - G PM-01 jul/10 (Tabela 7.1.2.1 - página 154)
# Below detection limits values included as zero.
    temp      24.1
    pe        6.553 # Calculated with eh-to-pe.xls file
    pH        9.37
#   ORP       386.5 mV
#   EC        264 µS/cm # Electrical conductivity
    redox     pe
    units     mg/l
    density   1
#    O(0)      -
    Ba        0.34
#    Cd        -
    Na        21.6
    K         16.8
    Ca        7.42
    Mg        7.29
    Fe        0 # Dissolved Iron
#    Fe(2)     -
#    Fe(3)     -
    Mn        0.03
    Alkalinity 86.52 as Ca.5(CO3).5 # Total Alkalinity calculated as mgCaCO3/L
#    C         5.71
    S(6)      7.78
#    S(-2)     - # Sulfide (sulfite SO3(-2) is not included in phreeqc database and
implies in differences in Ionic Balance for some wells)
#    S(4)      - # Sulfite included by Paulo Alencar in wateq4f.dat database considering
discussions at http://phreeqcusers.org/index.php?topic=963.0
```

```
    Cl        13.45
    F         0.12
#    N(-3)     - # NH3 reported as N
    N(+3)     0.02 # Nitrite reported as N
    N(+5)     7.97 # Nitrate reported as N
#    N(0)      - # Total nitrogen
    P         0.06 # Phosphate reported as P
    Si        5.27
    Al        0
#    As        -
#    Ag        -
#    Br        -
#    B         -
#    Co        -
#    Pb        -
#    Cr        -
#    Cr(+6)    -
#    Cu        -
#    Mo        -
#    Ni        -
#    Se(6)     - # Dissolved Selenium considered as selenate
    Sr        1.46
#    V         -
#    Zn        -
    -water    1 # kg

SOLUTION 4 # (Tavares, 2013) Salto de Pirapora/SP - PM01 out/10 (Tabela 7.1.3.1 - página
164)
# Below detection limits values included as zero.
    temp      22.5
    pe        5.386 # Calculated with eh-to-pe.xls file
    pH        5.58
#   ORP       316 mV
#   EC        277 µS/cm # Electrical conductivity
    redox     pe
    units     mg/l
    density   1
    O(0)      4.72
    Ba        0.07
#    Cd        -
    Na        0.5
    K         0.2
    Ca        0.56
    Mg        0.05
    Fe        0.09 # Dissolved Iron
#    Fe(2)     -
#    Fe(3)     -
    Mn        0.01
    Alkalinity 15.02 as Ca.5(CO3).5 # Total Alkalinity calculated as mgCaCO3/L
#    C         -
    S(6)      0.08
#    S(-2)     - # Sulfide (sulfite SO3(-2) is not included in phreeqc database and
implies in differences in Ionic Balance for some wells)
#    S(4)      - # Sulfite included by Paulo Alencar in wateq4f.dat database considering
discussions at http://phreeqcusers.org/index.php?topic=963.0
    Cl        0.23
    F         0.04
#    N(-3)     - # NH3 reported as N
#    N(+3)     - # Nitrite reported as N
    N(+5)     0.23 # Nitrate reported as N
#    N(0)      - # Total nitrogen
    P         0.03 # Phosphate reported as P
    Si        0.35
    Al        0.02
#    As        -
#    Ag        -
#    Br        -
#    B         -
```

```
#    Co        -
#    Pb        -
#    Cr        -
#    Cr(+6)    -
#    Cu        -
#    Mo        -
#    Ni        0.0073
#    Se(6)     - # Dissolved Selenium considered as selenate
    Sr        0.15
#    V         -
#    Zn        -
    -water    1 # kg

SOLUTION 5 # (Tavares, 2013) Salto de Pirapora/SP - PM07 out/10 (Tabela 7.1.3.1 - página
164)
# Below detection limits values included as zero.
    temp      23.4
    pe        1.592 # Calculated with eh-to-pe.xls file
    pH        5.32
#   ORP       93.7 mV
#   EC        148.4 µS/cm # Electrical conductivity
    redox     pe
    units     mg/l
    density   1
    O(0)      0.63
    Ba        0.22
#    Cd        -
    Na        17
    K         2.1
    Ca        1.2
    Mg        1.06
    Fe        2.01 # Dissolved Iron
#    Fe(2)     -
#    Fe(3)     -
    Mn        0.05
    Alkalinity 10.01 as Ca.5(CO3).5 # Total Alkalinity calculated as mgCaCO3/L
#    C         -
    S(6)      0.31
#    S(-2)     - # Sulfide (sulfite SO3(-2) is not included in phreeqc database and
implies in differences in Ionic Balance for some wells)
#    S(4)      - # Sulfite included by Paulo Alencar in wateq4f.dat database considering
discussions at http://phreeqcusers.org/index.php?topic=963.0
    Cl        24.62
    F         0.06
#    N(-3)     - # NH3 reported as N
    N(+3)     0.07 # Nitrite reported as N
    N(+5)     0.05 # Nitrate reported as N
#    N(0)      - # Total nitrogen
    P         0.02 # Phosphate reported as P
    Si        6.08
    Al        0.025
#    As        -
#    Ag        -
#    Br        -
#    B         -
#    Co        -
#    Pb        -
#    Cr        -
#    Cr(+6)    -
#    Cu        -
#    Mo        -
#    Ni        0.0055
#    Se(6)     - # Dissolved Selenium considered as selenate
    Sr        0.22
#    V         -
#    Zn        -
    -water    1 # kg
```

```
SOLUTION 6 # (Tavares, 2013) Salto de Pirapora/SP - PM03 out/10 (Tabela 7.1.3.1 - página
164)
# Below detection limits values included as zero.
    temp      22.7
    pe        1.724 # Calculated with eh-to-pe.xls file
    pH        5.21
#   ORP       101.2 mV
#   EC        351 µS/cm # Electrical conductivity
    redox     pe
    units     mg/l
    density   1
    O(0)      0.58
    Ba        0.74
#    Cd        -
    Na        26
    K         5.6
    Ca        4.94
    Mg        6.4
    Fe        0.11 # Dissolved Iron
#    Fe(2)     -
#    Fe(3)     -
    Mn        0.56
    Alkalinity 7.51 as Ca.5(CO3).5 # Total Alkalinity calculated as mgCaCO3/L
#    C         -
    S(6)      3.26
#    S(-2)     - # Sulfide (sulfite SO3(-2) is not included in phreeqc database and
implies in differences in Ionic Balance for some wells)
#    S(4)      - # Sulfite included by Paulo Alencar in wateq4f.dat database considering
discussions at http://phreeqcusers.org/index.php?topic=963.0
    Cl        81.53
    F         0.08
#    N(-3)     - # NH3 reported as N
    N(+3)     0.16 # Nitrite reported as N
    N(+5)     4.03 # Nitrate reported as N
#    N(0)      - # Total nitrogen
    P         0.04 # Phosphate reported as P
    Si        6.98
    Al        0.067
#    As        -
#    Ag        -
#    Br        -
#    B         -
#    Co        0.0125
#    Pb        0.0021
#    Cr        -
#    Cr(+6)    -
#    Cu        -
#    Mo        -
#    Ni        0.013
#    Se(6)     - # Dissolved Selenium considered as selenate
    Sr        0.5
#    V         -
#    Zn        -
    -water    1 # kg

SOLUTION 7 # (Tavares, 2013) Salto de Pirapora/SP - PM04 out/10 (Tabela 7.1.3.1 - página
164)
# Below detection limits values included as zero.
    temp      21.2
    pe        -1.471 # Calculated with eh-to-pe.xls file
    pH        7.07
#   ORP       -85.9 mV
#   EC        755 µS/cm # Electrical conductivity
    redox     pe
    units     mg/l
    density   1
    O(0)      0.87
    Ba        1.48
```

```
#    Cd        -
    Na        10.1
    K         3.3
    Ca        67.37
    Mg        56.38
    Fe        1.84 # Dissolved Iron
#    Fe(2)     -
#    Fe(3)     -
    Mn        0.19
    Alkalinity 375.34 as Ca.5(CO3).5 # Total Alkalinity calculated as mgCaCO3/L
#    C         0.26
    S(6)      0.24
#    S(-2)     - # Sulfide (sulfite SO3(-2) is not included in phreeqc database and
implies in differences in Ionic Balance for some wells)
#    S(4)      - # Sulfite included by Paulo Alencar in wateq4f.dat database considering
discussions at http://phreeqcusers.org/index.php?topic=963.0
    Cl        4.51
    F         0.13
#    N(-3)     - # NH3 reported as N
    N(+3)     0.01 # Nitrite reported as N
    N(+5)     0.16 # Nitrate reported as N
#    N(0)      - # Total nitrogen
    P         0.02 # Phosphate reported as P
    Si        13.74
    Al        0.013
#    As        -
#    Ag        -
#    Br        -
#    B         -
#    Co        -
#    Pb        -
#    Cr        -
#    Cr(+6)    -
#    Cu        -
#    Mo        -
#    Ni        0.00051
#    Se(6)     - # Dissolved Selenium considered as selenate
    Sr        0.53
#    V         -
#    Zn        -
    -water    1 # kg

SOLUTION 8 # (Tavares, 2013) Salto de Pirapora/SP - PM19 out/10 (Tabela 7.1.3.1 - página
164)
# Below detection limits values included as zero.
    temp      25
    pe        3.135 # Calculated with eh-to-pe.xls file
    pH        5.65
#   ORP       185.5 mV
#   EC        2530 µS/cm # Electrical conductivity
    redox     pe
    units     mg/l
    density   1
    O(0)      1.16
    Ba        1.9
#    Cd        -
    Na        128
    K         5.9
    Ca        81.11
    Mg        160.83
    Fe        0.05 # Dissolved Iron
#    Fe(2)     -
#    Fe(3)     -
    Mn        1.14
    Alkalinity 40.03 as Ca.5(CO3).5 # Total Alkalinity calculated as mgCaCO3/L
#    C         -
    S(6)      15.58
#    S(-2)     - # Sulfide (sulfite SO3(-2) is not included in phreeqc database and
```

```
implies in differences in Ionic Balance for some wells)
#    S(4)      - # Sulfite included by Paulo Alencar in wateq4f.dat database considering
discussions at http://phreeqcusers.org/index.php?topic=963.0
    Cl        783.49
    F         0.13
#    N(-3)     - # NH3 reported as N
    N(+3)     0.09 # Nitrite reported as N
    N(+5)     37.85 # Nitrate reported as N
#    N(0)      - # Total nitrogen
    P         0.15 # Phosphate reported as P
    Si        8.6
    Al        0.014
#    As        -
#    Ag        -
#    Br        -
#    B         -
#    Co        0.04
#    Pb        0.001
#    Cr        -
#    Cr(+6)    -
#    Cu        -
#    Mo        -
#    Ni        0.55
#    Se(6)     - # Dissolved Selenium considered as selenate
    Sr        1.21
#    V         -
#    Zn        -
    -water    1 # kg

SOLUTION 9 # (Tavares, 2013) Salto de Pirapora/SP - PM24/45 out/10 (Tabela 7.1.3.1 -
página 164)
# Below detection limits values included as zero.
    temp      21.5
    pe        3.315 # Calculated with eh-to-pe.xls file
    pH        5.36
#   ORP       193.8 mV
#   EC        408 µS/cm # Electrical conductivity
    redox     pe
    units     mg/l
    density   1
    O(0)      1.29
    Ba        0.61
#    Cd        -
    Na        3.5
    K         3.1
    Ca        12.1
    Mg        28.19
    Fe        0.08 # Dissolved Iron
#    Fe(2)     -
#    Fe(3)     -
    Mn        0.13
    Alkalinity 25.02 as Ca.5(CO3).5 # Total Alkalinity calculated as mgCaCO3/L
#    C         -
    S(6)      0.49
#    S(-2)     - # Sulfide (sulfite SO3(-2) is not included in phreeqc database and
implies in differences in Ionic Balance for some wells)
#    S(4)      - # Sulfite included by Paulo Alencar in wateq4f.dat database considering
discussions at http://phreeqcusers.org/index.php?topic=963.0
    Cl        92.35
    F         0.14
#    N(-3)     - # NH3 reported as N
    N(+3)     0.16 # Nitrite reported as N
    N(+5)     3.14 # Nitrate reported as N
#    N(0)      - # Total nitrogen
    P         0.06 # Phosphate reported as P
    Si        8.07
    Al        0.028
#    As        -
```

```
#    Ag        -
#    Br        -
#    B         -
#    Co        0.0022
#    Pb        0.022
#    Cr        -
#    Cr(+6)    -
#    Cu        -
#    Mo        -
#    Ni        0.63
#    Se(6)     - # Dissolved Selenium considered as selenate
     Sr        0.31
#    V         -
#    Zn        -
     -water    1 # kg

SOLUTION 10 # (Tavares, 2013) Salto de Pirapora/SP - PM25 out/10 (Tabela 7.1.3.1 - página
164)
# Below detection limits values included as zero.
     temp      23.7
     pe        1.241 # Calculated with eh-to-pe.xls file
     pH        5.52
#    ORP       73.1 mV
#    EC        164.4 µS/cm # Electrical conductivity
     redox     pe
     units     mg/l
     density   1
     O(0)      0.88
     Ba        0.9
#    Cd        -
     Na        15
     K         1.1
     Ca        1.05
     Mg        0.97
     Fe        10.15 # Dissolved Iron
#    Fe(2)     -
#    Fe(3)     -
     Mn        3.44
     Alkalinity 35.03 as Ca.5(CO3).5 # Total Alkalinity calculated as mgCaCO3/L
#    C         -
     S(6)      1.99
#    S(-2)     - # Sulfide (sulfite SO3(-2) is not included in phreeqc database and
implies in differences in Ionic Balance for some wells)
#    S(4)      - # Sulfite included by Paulo Alencar in wateq4f.dat database considering
discussions at http://phreeqcusers.org/index.php?topic=963.0
     Cl        20.36
     F         0.08
#    N(-3)     - # NH3 reported as N
     N(+3)     0.05 # Nitrite reported as N
     N(+5)     0.15 # Nitrate reported as N
#    N(0)      - # Total nitrogen
     P         0.01 # Phosphate reported as P
     Si        3.4
     Al        0.019
#    As        -
#    Ag        -
#    Br        -
#    B         -
#    Co        0.014
#    Pb        0.018
#    Cr        -
#    Cr(+6)    -
#    Cu        -
#    Mo        -
#    Ni        0.0035
#    Se(6)     - # Dissolved Selenium considered as selenate
     Sr        0.1
#    V         -
```

```
#    Zn        -
    -water    1 # kg

SOLUTION 11 # (Tavares, 2013) Salto de Pirapora/SP - PM27 out/10 (Tabela 7.1.3.1 - página
164)
# Below detection limits values included as zero.
    temp      23.3
    pe        -1.312 # Calculated with eh-to-pe.xls file
    pH        6.52
#   ORP       -77.2 mV
#   EC        892 µS/cm # Electrical conductivity
    redox     pe
    units     mg/l
    density   1
    O(0)      0.75
    Ba        8.11
#    Cd        -
    Na        23
    K         15
    Ca        7.23
    Mg        5.2
    Fe        15.23 # Dissolved Iron
#    Fe(2)     -
#    Fe(3)     -
    Mn        9.24
    Alkalinity 285.26 as Ca.5(CO3).5 # Total Alkalinity calculated as mgCaCO3/L
#    C         0.06
    S(6)      0.06
#    S(-2)     - # Sulfide (sulfite SO3(-2) is not included in phreeqc database and
implies in differences in Ionic Balance for some wells)
#    S(4)      - # Sulfite included by Paulo Alencar in wateq4f.dat database considering
discussions at http://phreeqcusers.org/index.php?topic=963.0
    Cl        57.79
    F         0.53
#    N(-3)     - # NH3 reported as N
    N(+3)     0.03 # Nitrite reported as N
    N(+5)     0.15 # Nitrate reported as N
#    N(0)      - # Total nitrogen
    P         0.03 # Phosphate reported as P
    Si        2.19
    Al        0.035
#    As        -
#    Ag        -
#    Br        -
#    B         -
#    Co        0.13
#    Pb        0.00058
#    Cr        -
#    Cr(+6)    -
#    Cu        -
#    Mo        -
#    Ni        0.011
#    Se(6)     - # Dissolved Selenium considered as selenate
    Sr        0.2
#    V         -
#    Zn        -
    -water    1 # kg

SOLUTION 12 # (Sanches, 2015) Itaboraí/RJ - P-01  (06/13) jun/13
# Below detection limits values included as zero.
    temp      23.06
    pe        0.371 # Calculated with eh-to-pe.xls file
    pH        5.5
#   ORP       40 mV
#   EC        363 µS/cm # Electrical conductivity
    redox     pe
    units     mg/l
    density   1
```

```
#    O(0)      -
    Ba        0
#    Cd        -
    Na        52.3
    K         7
    Ca        18.5
    Mg        4.26
#    Fe        - # Dissolved Iron
#    Fe(2)     -
#    Fe(3)     -
#    Mn        -
    Alkalinity 24.59 as Ca.5(CO3).5 # Total Alkalinity calculated as mgCaCO3/L
#    C         -
    S(6)      73.1
#    S(-2)     - # Sulfide (sulfite SO3(-2) is not included in phreeqc database and
implies in differences in Ionic Balance for some wells)
#    S(4)      - # Sulfite included by Paulo Alencar in wateq4f.dat database considering
discussions at http://phreeqcusers.org/index.php?topic=963.0
    Cl        66.8
    F         0.01
#    N(-3)     - # NH3 reported as N
    N(+3)     0 # Nitrite reported as N
    N(+5)     35.01 # Nitrate reported as N
#    N(0)      - # Total nitrogen
    P         0.01 # Phosphate reported as P
#    Si        -
#    Al        -
#    As        -
#    Ag        -
    Br        0.5
#    B         -
#    Co        -
#    Pb        -
#    Cr        -
#    Cr(+6)    -
#    Cu        -
#    Mo        -
#    Ni        -
#    Se(6)     - # Dissolved Selenium considered as selenate
#    Sr        -
#    V         -
#    Zn        -
    -water    1 # kg

SOLUTION 13 # (Sanches, 2015) Itaboraí/RJ - P-02  (06/13) jun/13
# Below detection limits values included as zero.
    temp      24.78
    pe        0.447 # Calculated with eh-to-pe.xls file
    pH        6.5
#   ORP       6 mV
#   EC        418 µS/cm # Electrical conductivity
    redox     pe
    units     mg/l
    density   1
#    O(0)      -
    Ba        1.17
#    Cd        -
    Na        65.1
    K         5.3
    Ca        71
    Mg        5.41
#    Fe        - # Dissolved Iron
#    Fe(2)     -
#    Fe(3)     -
#    Mn        -
    Alkalinity 238.52 as Ca.5(CO3).5 # Total Alkalinity calculated as mgCaCO3/L
#    C         -
    S(6)      18.2
```

```
#    S(-2)      - # Sulfide (sulfite SO3(-2) is not included in phreeqc database and
implies in differences in Ionic Balance for some wells)
#    S(4)       - # Sulfite included by Paulo Alencar in wateq4f.dat database considering
discussions at http://phreeqcusers.org/index.php?topic=963.0
    Cl         73.8
    F          0.06
#    N(-3)      - # NH3 reported as N
    N(+3)      0 # Nitrite reported as N
    N(+5)      1.17 # Nitrate reported as N
#    N(0)       - # Total nitrogen
    P          0.06 # Phosphate reported as P
#    Si         -
#    Al         -
#    As         -
#    Ag         -
    Br         0.6
#    B          -
#    Co         -
#    Pb         -
#    Cr         -
#    Cr(+6)     -
#    Cu         -
#    Mo         -
#    Ni         -
#    Se(6)      - # Dissolved Selenium considered as selenate
#    Sr         -
#    V          -
#    Zn         -
    -water     1 # kg

SOLUTION 14 # (Sanches, 2015) Itaboraí/RJ - P-03  (06/13) jun/13
# Below detection limits values included as zero.
    temp       25.08
    pe         0.406 # Calculated with eh-to-pe.xls file
    pH         7.2
#   ORP        38 mV
#   EC         728 µS/cm # Electrical conductivity
    redox      pe
    units      mg/l
    density    1
#    O(0)       -
    Ba         0.62
#    Cd         -
    Na         141
    K          4.3
    Ca         49
    Mg         5.14
#    Fe         - # Dissolved Iron
#    Fe(2)      -
#    Fe(3)      -
#    Mn         -
    Alkalinity 150 as Ca.5(CO3).5 # Total Alkalinity calculated as mgCaCO3/L
#    C          -
    S(6)       52.1
#    S(-2)      - # Sulfide (sulfite SO3(-2) is not included in phreeqc database and
implies in differences in Ionic Balance for some wells)
#    S(4)       - # Sulfite included by Paulo Alencar in wateq4f.dat database considering
discussions at http://phreeqcusers.org/index.php?topic=963.0
    Cl         174
    F          0.07
#    N(-3)      - # NH3 reported as N
    N(+3)      0.06 # Nitrite reported as N
    N(+5)      3.26 # Nitrate reported as N
#    N(0)       - # Total nitrogen
    P          0.07 # Phosphate reported as P
#    Si         -
#    Al         -
#    As         -
```

```
#    Ag        -
    Br        0.71
#    B         -
#    Co        -
#    Pb        -
#    Cr        -
#    Cr(+6)    -
#    Cu        -
#    Mo        -
#    Ni        -
#    Se(6)     - # Dissolved Selenium considered as selenate
#    Sr        -
#    V         -
#    Zn        -
    -water    1 # kg

SOLUTION 15 # (Sanches, 2015) Itaboraí/RJ - P-04  (06/13) jun/13
# Below detection limits values included as zero.
    temp      25.89
    pe        0.454 # Calculated with eh-to-pe.xls file
    pH        5.9
#   ORP       14 mV
#   EC        3138 µS/cm # Electrical conductivity
    redox     pe
    units     mg/l
    density   1
#    O(0)      -
    Ba        1.37
#    Cd        -
    Na        193.5
    K         16.2
    Ca        337.9
    Mg        85.95
#    Fe        - # Dissolved Iron
#    Fe(2)     -
#    Fe(3)     -
#    Mn        -
    Alkalinity 220.49 as Ca.5(CO3).5 # Total Alkalinity calculated as mgCaCO3/L
#    C         -
    S(6)      55.6
#    S(-2)     - # Sulfide (sulfite SO3(-2) is not included in phreeqc database and
implies in differences in Ionic Balance for some wells)
#    S(4)      - # Sulfite included by Paulo Alencar in wateq4f.dat database considering
discussions at http://phreeqcusers.org/index.php?topic=963.0
    Cl        950
    F         0.02
#    N(-3)     - # NH3 reported as N
    N(+3)     0 # Nitrite reported as N
    N(+5)     1.46 # Nitrate reported as N
#    N(0)      - # Total nitrogen
    P         0.02 # Phosphate reported as P
#    Si        -
#    Al        -
#    As        -
#    Ag        -
    Br        3.38
#    B         -
#    Co        -
#    Pb        -
#    Cr        -
#    Cr(+6)    -
#    Cu        -
#    Mo        -
#    Ni        -
#    Se(6)     - # Dissolved Selenium considered as selenate
#    Sr        -
#    V         -
#    Zn        -
```

```
    -water    1 # kg

SOLUTION 16 # (Sanches, 2015) Itaboraí/RJ - P-05  (10/13) out/13
# Below detection limits values included as zero.
    temp      24.52
    pe        0.276 # Calculated with eh-to-pe.xls file
    pH        5.2
#   ORP       175 mV
#   EC        47 µS/cm # Electrical conductivity
    redox     pe
    units     mg/l
    density   1
#    O(0)      -
    Ba        2.81
    Cd        0.00092
    Na        13.4
    K         2.5
    Ca        9.1
    Mg        2.34
    Fe        0.85189 # Dissolved Iron
#    Fe(2)     -
#    Fe(3)     -
    Mn        0.0174
    Alkalinity 47.54 as Ca.5(CO3).5 # Total Alkalinity calculated as mgCaCO3/L
#    C         -
    S(6)      4.3
#    S(-2)     - # Sulfide (sulfite SO3(-2) is not included in phreeqc database and
implies in differences in Ionic Balance for some wells)
#    S(4)      - # Sulfite included by Paulo Alencar in wateq4f.dat database considering
discussions at http://phreeqcusers.org/index.php?topic=963.0
    Cl        9.6
    F         1.07
#    N(-3)     - # NH3 reported as N
    N(+3)     0 # Nitrite reported as N
    N(+5)     3.56 # Nitrate reported as N
#    N(0)      - # Total nitrogen
    P         0.008 # Phosphate reported as P
#    Si        -
    Al        0.01755
#    As        0
#    Ag        -
    Br        0
    B         0.1175
#    Co        -
    Pb        0.00084
#    Cr        0.002
#    Cr(+6)    -
    Cu        0.00918
#    Mo        0
#    Ni        0.0036
#    Se(6)     0 # Dissolved Selenium considered as selenate
#    Sr        -
#    V         0.00325
#    Zn        0.12199
    -water    1 # kg

SOLUTION 17 # (Sanches, 2015) Itaboraí/RJ - P-06  (10/13) out/13
# Below detection limits values included as zero.
    temp      24.48
    pe        0.145 # Calculated with eh-to-pe.xls file
    pH        4.2
#   ORP       576 mV
#   EC        313 µS/cm # Electrical conductivity
    redox     pe
    units     mg/l
    density   1
#    O(0)      -
    Ba        1.8
```

```
    Cd        0.0013
    Na        20.5
    K         8.2
    Ca        13.3
    Mg        7.55
    Fe        0.02407 # Dissolved Iron
#    Fe(2)     -
#    Fe(3)     -
    Mn        0.08004
    Alkalinity 27.87 as Ca.5(CO3).5 # Total Alkalinity calculated as mgCaCO3/L
#    C         -
    S(6)      2.7
#    S(-2)     - # Sulfide (sulfite SO3(-2) is not included in phreeqc database and
implies in differences in Ionic Balance for some wells)
#    S(4)      - # Sulfite included by Paulo Alencar in wateq4f.dat database considering
discussions at http://phreeqcusers.org/index.php?topic=963.0
    Cl        63
    F         1.19
#    N(-3)     - # NH3 reported as N
    N(+3)     0 # Nitrite reported as N
    N(+5)     28.54 # Nitrate reported as N
#    N(0)      - # Total nitrogen
    P         0.061 # Phosphate reported as P
#    Si        -
    Al        0.85748
#    As        0
#    Ag        -
    Br        0.34
    B         0.169
#    Co        -
    Pb        0.00296
#    Cr        0.00184
#    Cr(+6)    -
    Cu        0.00536
#    Mo        0
#    Ni        0.00419
#    Se(6)     0 # Dissolved Selenium considered as selenate
#    Sr        -
#    V         0.00325
    Zn        0.26114
    -water    1 # kg

SOLUTION 18 # (Sanches, 2015) Itaboraí/RJ - P-07  (10/13) out/13
# Below detection limits values included as zero.
    temp      25.8
    pe        0.269 # Calculated with eh-to-pe.xls file
    pH        6.5
#   ORP       211 mV
#   EC        289 µS/cm # Electrical conductivity
    redox     pe
    units     mg/l
    density   1
#    O(0)      -
    Ba        1.51
    Cd        0.00083
    Na        62.3
    K         3.2
    Ca        29.8
    Mg        6.74
    Fe        0.03211 # Dissolved Iron
#    Fe(2)     -
#    Fe(3)     -
    Mn        0.00646
    Alkalinity 215.57 as Ca.5(CO3).5 # Total Alkalinity calculated as mgCaCO3/L
#    C         -
    S(6)      2.9
#    S(-2)     - # Sulfide (sulfite SO3(-2) is not included in phreeqc database and
implies in differences in Ionic Balance for some wells)
```

```
#    S(4)      - # Sulfite included by Paulo Alencar in wateq4f.dat database considering
discussions at http://phreeqcusers.org/index.php?topic=963.0
    Cl        17.9
    F         1.24
#    N(-3)     - # NH3 reported as N
    N(+3)     0 # Nitrite reported as N
    N(+5)     0.46 # Nitrate reported as N
#    N(0)      - # Total nitrogen
    P         0.143 # Phosphate reported as P
#    Si        -
    Al        0.02902
#    As        0
#    Ag        -
    Br        0.44
    B         0.1404
#    Co        -
    Pb        0.00053
#    Cr        0.00234
#    Cr(+6)    -
    Cu        0.00266
#    Mo        0
#    Ni        0.00066
#    Se(6)     0 # Dissolved Selenium considered as selenate
#    Sr        -
#    V         0.00379
    Zn        0.15426
    -water    1 # kg

SOLUTION 19 # (Sanches, 2015) Itaboraí/RJ - P-08  (10/13) out/13
# Below detection limits values included as zero.
    temp      26.22
    pe        0.227 # Calculated with eh-to-pe.xls file
    pH        4.4
#   ORP       310 mV
#   EC        48 µS/cm # Electrical conductivity
    redox     pe
    units     mg/l
    density   1
#    O(0)      -
    Ba        0.8
    Cd        0.00088
    Na        13.3
    K         2.5
    Ca        8.6
    Mg        2.81
    Fe        0.03947 # Dissolved Iron
#    Fe(2)     -
#    Fe(3)     -
    Mn        0.05055
    Alkalinity 38.52 as Ca.5(CO3).5 # Total Alkalinity calculated as mgCaCO3/L
#    C         -
    S(6)      13
#    S(-2)     - # Sulfide (sulfite SO3(-2) is not included in phreeqc database and
implies in differences in Ionic Balance for some wells)
#    S(4)      - # Sulfite included by Paulo Alencar in wateq4f.dat database considering
discussions at http://phreeqcusers.org/index.php?topic=963.0
    Cl        9.2
    F         1.08
#    N(-3)     - # NH3 reported as N
    N(+3)     0.02 # Nitrite reported as N
    N(+5)     4.62 # Nitrate reported as N
#    N(0)      - # Total nitrogen
    P         0.003 # Phosphate reported as P
#    Si        -
    Al        0.05251
#    As        0
#    Ag        -
    Br        0.17
```

```
    B         0.1265
#    Co        -
    Pb        0.00016
#    Cr        0.00141
#    Cr(+6)    -
    Cu        0.00203
#    Mo        0
#    Ni        0.00028
#    Se(6)     0 # Dissolved Selenium considered as selenate
#    Sr        -
#    V         0.00328
    Zn        0.11026
    -water    1 # kg

SOLUTION 20 # (Sanches, 2015) Itaboraí/RJ - P-09  (10/13) out/13
# Below detection limits values included as zero.
    temp      24.26
    pe        0.28 # Calculated with eh-to-pe.xls file
    pH        6.1
#   ORP       163 mV
#   EC        62 µS/cm # Electrical conductivity
    redox     pe
    units     mg/l
    density   1
#    O(0)      -
    Ba        1.2
    Cd        0.00102
    Na        15.3
    K         2.8
    Ca        14.5
    Mg        3.73
    Fe        0.17229 # Dissolved Iron
#    Fe(2)     -
#    Fe(3)     -
    Mn        0.092
    Alkalinity 65.57 as Ca.5(CO3).5 # Total Alkalinity calculated as mgCaCO3/L
#    C         -
    S(6)      12.1
#    S(-2)     - # Sulfide (sulfite SO3(-2) is not included in phreeqc database and
implies in differences in Ionic Balance for some wells)
#    S(4)      - # Sulfite included by Paulo Alencar in wateq4f.dat database considering
discussions at http://phreeqcusers.org/index.php?topic=963.0
    Cl        9
    F         1.1
#    N(-3)     - # NH3 reported as N
    N(+3)     0 # Nitrite reported as N
    N(+5)     4.12 # Nitrate reported as N
#    N(0)      - # Total nitrogen
    P         0.056 # Phosphate reported as P
#    Si        -
    Al        0.12796
#    As        0
#    Ag        -
    Br        0.45
    B         0.132
#    Co        -
    Pb        0.00105
#    Cr        0.00173
#    Cr(+6)    -
    Cu        0.00447
#    Mo        0
#    Ni        0.00126
#    Se(6)     0 # Dissolved Selenium considered as selenate
#    Sr        -
#    V         0.00387
    Zn        0.09931
    -water    1 # kg
```

```
SOLUTION 21 # (Sanches, 2015) Itaboraí/RJ - P-10  (10/13) out/13
# Below detection limits values included as zero.
    temp      25.37
    pe        0.313 # Calculated with eh-to-pe.xls file
    pH        6.4
#   ORP       135 mV
#   EC        80 µS/cm # Electrical conductivity
    redox     pe
    units     mg/l
    density   1
#    O(0)      -
    Ba        1.79
    Cd        0.00061
    Na        18
    K         2
    Ca        14
    Mg        4
    Fe        0.00789 # Dissolved Iron
#    Fe(2)     -
#    Fe(3)     -
    Mn        0.00413
    Alkalinity 81.97 as Ca.5(CO3).5 # Total Alkalinity calculated as mgCaCO3/L
#    C         -
    S(6)      2
#    S(-2)     - # Sulfide (sulfite SO3(-2) is not included in phreeqc database and
implies in differences in Ionic Balance for some wells)
#    S(4)      - # Sulfite included by Paulo Alencar in wateq4f.dat database considering
discussions at http://phreeqcusers.org/index.php?topic=963.0
    Cl        4
    F         1.02
#    N(-3)     - # NH3 reported as N
    N(+3)     0 # Nitrite reported as N
    N(+5)     4.96 # Nitrate reported as N
#    N(0)      - # Total nitrogen
    P         0.003 # Phosphate reported as P
#    Si        -
    Al        0.02213
#    As        0
#    Ag        -
    Br        0.4
    B         0.124
#    Co        -
    Pb        0.00065
#    Cr        0.00247
#    Cr(+6)    -
    Cu        0.00205
#    Mo        0
#    Ni        0
#    Se(6)     0 # Dissolved Selenium considered as selenate
#    Sr        -
#    V         0.00357
    Zn        0.12593
    -water    1 # kg

SOLUTION 22 # (Sanches, 2015) Itaboraí/RJ - P-11  (10/13) out/13
# Below detection limits values included as zero.
    temp      24.83
    pe        0.437 # Calculated with eh-to-pe.xls file
    pH        6.9
#   ORP       13 mV
#   EC        318 µS/cm # Electrical conductivity
    redox     pe
    units     mg/l
    density   1
#    O(0)      -
    Ba        0.75
    Cd        0.00091
    Na        58
```

```
    K         4.6
    Ca        36.3
    Mg        7.42
    Fe        0.07531 # Dissolved Iron
#    Fe(2)     -
#    Fe(3)     -
    Mn        0.13665
    Alkalinity 245.9 as Ca.5(CO3).5 # Total Alkalinity calculated as mgCaCO3/L
#    C         -
    S(6)      3.6
#    S(-2)     - # Sulfide (sulfite SO3(-2) is not included in phreeqc database and
implies in differences in Ionic Balance for some wells)
#    S(4)      - # Sulfite included by Paulo Alencar in wateq4f.dat database considering
discussions at http://phreeqcusers.org/index.php?topic=963.0
    Cl        16
    F         1.22
#    N(-3)     - # NH3 reported as N
    N(+3)     0 # Nitrite reported as N
    N(+5)     3.21 # Nitrate reported as N
#    N(0)      - # Total nitrogen
    P         0.114 # Phosphate reported as P
#    Si        -
    Al        0.00621
#    As        0
#    Ag        -
    Br        0.44
    B         0.07915
#    Co        -
    Pb        0.00136
#    Cr        0.00208
#    Cr(+6)    -
    Cu        0.00194
#    Mo        0
#    Ni        0.00069
#    Se(6)     0 # Dissolved Selenium considered as selenate
#    Sr        -
#    V         0.00358
    Zn        0.00676
    -water    1 # kg

SOLUTION 23 # (Sanches, 2015) Itaboraí/RJ - P-12  (10/13) out/13
# Below detection limits values included as zero.
    temp      27.33
    pe        0.447 # Calculated with eh-to-pe.xls file
    pH        5.8
#   ORP       35 mV
#   EC        155 µS/cm # Electrical conductivity
    redox     pe
    units     mg/l
    density   1
#    O(0)      -
    Ba        2.52
    Cd        0.00065
    Na        21.3
    K         4
    Ca        17.6
    Mg        9.18
    Fe        0.46189 # Dissolved Iron
#    Fe(2)     -
#    Fe(3)     -
    Mn        0.03012
    Alkalinity 93.44 as Ca.5(CO3).5 # Total Alkalinity calculated as mgCaCO3/L
#    C         -
    S(6)      4.8
#    S(-2)     - # Sulfide (sulfite SO3(-2) is not included in phreeqc database and
implies in differences in Ionic Balance for some wells)
#    S(4)      - # Sulfite included by Paulo Alencar in wateq4f.dat database considering
discussions at http://phreeqcusers.org/index.php?topic=963.0
```

```
    Cl        18
    F         1.06
#    N(-3)     - # NH3 reported as N
    N(+3)     0 # Nitrite reported as N
    N(+5)     4.37 # Nitrate reported as N
#    N(0)      - # Total nitrogen
    P         0.029 # Phosphate reported as P
#    Si        -
    Al        0.00859
#    As        0
#    Ag        -
    Br        0.46
    B         0.1144
#    Co        -
    Pb        0.00451
#    Cr        0.00233
#    Cr(+6)    -
    Cu        0.00387
#    Mo        0
#    Ni        0.00094
#    Se(6)     0 # Dissolved Selenium considered as selenate
#    Sr        0
#    V         0.00366
    Zn        0.10656
    -water    1 # kg

SOLUTION 24 # (Sanches, 2015) Itaboraí/RJ - P-13  (10/13) out/13
# Below detection limits values included as zero.
    temp      26.74
    pe        0.404 # Calculated with eh-to-pe.xls file
    pH        8.4
#   ORP       60 mV
#   EC        1367 µS/cm # Electrical conductivity
    redox     pe
    units     mg/l
    density   1
#    O(0)      -
    Ba        1.98
    Cd        0.00083
    Na        239.2
    K         3.3
    Ca        20
    Mg        13.54
    Fe        0.03058 # Dissolved Iron
#    Fe(2)     -
#    Fe(3)     -
    Mn        0.00559
    Alkalinity 609.02 as Ca.5(CO3).5 # Total Alkalinity calculated as mgCaCO3/L
#    C         -
    S(6)      3.6
#    S(-2)     - # Sulfide (sulfite SO3(-2) is not included in phreeqc database and
implies in differences in Ionic Balance for some wells)
#    S(4)      - # Sulfite included by Paulo Alencar in wateq4f.dat database considering
discussions at http://phreeqcusers.org/index.php?topic=963.0
    Cl        37
    F         6.03
#    N(-3)     - # NH3 reported as N
    N(+3)     0 # Nitrite reported as N
    N(+5)     2.84 # Nitrate reported as N
#    N(0)      - # Total nitrogen
    P         0.012 # Phosphate reported as P
#    Si        -
    Al        0.06192
#    As        0
#    Ag        -
    Br        0.49
    B         0.6051
#    Co        -
```

```
    Pb        0.00108
#    Cr        0.00156
#    Cr(+6)    -
    Cu        0.00248
#    Mo        0.00683
#    Ni        0.00161
#    Se(6)     0 # Dissolved Selenium considered as selenate
#    Sr        -
#    V         0.00337
    Zn        0.13158
    -water    1 # kg

SOLUTION 25 # (Sanches, 2015) Itaboraí/RJ - P-14  (10/13) out/13
# Below detection limits values included as zero.
    temp      24.93
    pe        0.441 # Calculated with eh-to-pe.xls file
    pH        7.5
#   ORP       12 mV
#   EC        586 µS/cm # Electrical conductivity
    redox     pe
    units     mg/l
    density   1
#    O(0)      -
    Ba        0.98
    Cd        0.00077
    Na        50.8
    K         5.4
    Ca        54.1
    Mg        14.24
    Fe        0.04925 # Dissolved Iron
#    Fe(2)     -
#    Fe(3)     -
    Mn        0.06439
    Alkalinity 202.46 as Ca.5(CO3).5 # Total Alkalinity calculated as mgCaCO3/L
#    C         -
    S(6)      17.2
#    S(-2)     - # Sulfide (sulfite SO3(-2) is not included in phreeqc database and
implies in differences in Ionic Balance for some wells)
#    S(4)      - # Sulfite included by Paulo Alencar in wateq4f.dat database considering
discussions at http://phreeqcusers.org/index.php?topic=963.0
    Cl        60.4
    F         1.05
#    N(-3)     - # NH3 reported as N
    N(+3)     0 # Nitrite reported as N
    N(+5)     5.87 # Nitrate reported as N
#    N(0)      - # Total nitrogen
    P         0.102 # Phosphate reported as P
#    Si        -
    Al        0.04881
#    As        0
#    Ag        -
    Br        0.54
    B         0.1343
#    Co        -
    Pb        0.00052
#    Cr        0.00306
#    Cr(+6)    -
    Cu        0.00138
#    Mo        0.00314
#    Ni        0
#    Se(6)     0 # Dissolved Selenium considered as selenate
#    Sr        -
#    V         0.00408
    Zn        0.10808
    -water    1 # kg

SOLUTION 26 # (Sanches, 2015) Itaboraí/RJ - P-15  (10/13) out/13
# Below detection limits values included as zero.
```

```
    temp      25.54
    pe        0.343 # Calculated with eh-to-pe.xls file
    pH        7.2
#   ORP       102 mV
#   EC        446 µS/cm # Electrical conductivity
    redox     pe
    units     mg/l
    density   1
#    O(0)      -
    Ba        0
    Cd        0.00071
    Na        29.6
    K         3.1
    Ca        42.8
    Mg        27.4
    Fe        0.17304 # Dissolved Iron
#    Fe(2)     -
#    Fe(3)     -
    Mn        0.11577
    Alkalinity 236.07 as Ca.5(CO3).5 # Total Alkalinity calculated as mgCaCO3/L
#    C         -
    S(6)      6.9
#    S(-2)     - # Sulfide (sulfite SO3(-2) is not included in phreeqc database and
implies in differences in Ionic Balance for some wells)
#    S(4)      - # Sulfite included by Paulo Alencar in wateq4f.dat database considering
discussions at http://phreeqcusers.org/index.php?topic=963.0
    Cl        33.2
    F         2
#    N(-3)     - # NH3 reported as N
    N(+3)     0.32 # Nitrite reported as N
    N(+5)     5.84 # Nitrate reported as N
#    N(0)      - # Total nitrogen
    P         0.087 # Phosphate reported as P
#    Si        -
    Al        0.02665
#    As        0
#    Ag        -
    Br        0.5
    B         0.1309
#    Co        -
    Pb        0.00064
#    Cr        0.00244
#    Cr(+6)    -
    Cu        0.00169
#    Mo        0.00135
#    Ni        0.00067
#    Se(6)     0 # Dissolved Selenium considered as selenate
#    Sr        -
#    V         0.00318
    Zn        0.12136
    -water    1 # kg

SOLUTION 27 # (Sanches, 2015) Itaboraí/RJ - P-16  (10/13) out/13
# Below detection limits values included as zero.
    temp      24.63
    pe        0.223 # Calculated with eh-to-pe.xls file
    pH        4.6
#   ORP       283 mV
#   EC        125 µS/cm # Electrical conductivity
    redox     pe
    units     mg/l
    density   1
#    O(0)      -
    Ba        1.61
    Cd        0.00098
    Na        24.1
    K         7.5
    Ca        14.1
```

```
    Mg        16.74
    Fe        0.02525 # Dissolved Iron
#    Fe(2)     -
#    Fe(3)     -
    Mn        0.06763
    Alkalinity 118.85 as Ca.5(CO3).5 # Total Alkalinity calculated as mgCaCO3/L
#    C         -
    S(6)      4.9
#    S(-2)     - # Sulfide (sulfite SO3(-2) is not included in phreeqc database and
implies in differences in Ionic Balance for some wells)
#    S(4)      - # Sulfite included by Paulo Alencar in wateq4f.dat database considering
discussions at http://phreeqcusers.org/index.php?topic=963.0
    Cl        29.7
    F         1.16
#    N(-3)     - # NH3 reported as N
    N(+3)     0.02 # Nitrite reported as N
    N(+5)     15.22 # Nitrate reported as N
#    N(0)      - # Total nitrogen
    P         0.003 # Phosphate reported as P
#    Si        -
    Al        0.04199
#    As        0
#    Ag        -
    Br        0.48
    B         0.1362
#    Co        -
    Pb        0.00046
#    Cr        0.0021
#    Cr(+6)    -
    Cu        0.00608
#    Mo        0
#    Ni        0.0019
#    Se(6)     0 # Dissolved Selenium considered as selenate
#    Sr        -
#    V         0.00335
    Zn        0.15529
    -water    1 # kg

SOLUTION 28 # (Sanches, 2015) Itaboraí/RJ - P-17  (10/13) out/13
# Below detection limits values included as zero.
    temp      25.06
    pe        0.253 # Calculated with eh-to-pe.xls file
    pH        5
#   ORP       227 mV
#   EC        67 µS/cm # Electrical conductivity
    redox     pe
    units     mg/l
    density   1
#    O(0)      -
    Ba        2.31
    Cd        0.00103
    Na        16.5
    K         4.5
    Ca        20.3
    Mg        12.12
    Fe        0.03198 # Dissolved Iron
#    Fe(2)     -
#    Fe(3)     -
    Mn        0.0118
    Alkalinity 103.28 as Ca.5(CO3).5 # Total Alkalinity calculated as mgCaCO3/L
#    C         -
    S(6)      3.5
#    S(-2)     - # Sulfide (sulfite SO3(-2) is not included in phreeqc database and
implies in differences in Ionic Balance for some wells)
#    S(4)      - # Sulfite included by Paulo Alencar in wateq4f.dat database considering
discussions at http://phreeqcusers.org/index.php?topic=963.0
    Cl        16.6
    F         1.09
```

```
#    N(-3)      - # NH3 reported as N
     N(+3)      0.01 # Nitrite reported as N
     N(+5)      9.57 # Nitrate reported as N
#    N(0)       - # Total nitrogen
     P          0.009 # Phosphate reported as P
#    Si         -
     Al         0.02567
#    As         0
#    Ag         -
     Br         0.45
     B          0.1363
#    Co         -
     Pb         0.00071
#    Cr         0.00281
#    Cr(+6)     -
     Cu         0.00263
#    Mo         0
#    Ni         0.00142
#    Se(6)      0 # Dissolved Selenium considered as selenate
#    Sr         -
#    V          0.00307
     Zn         0.1184
     -water     1 # kg

SOLUTION 29 # (Gomes, 2012) Itaboraí/RJ - P-01A  (08/09) ago/09
# Below detection limits values included as zero.
     temp       24.94
     pe         -1.995 # Calculated with eh-to-pe.xls file
     pH         8
#    ORP        -118 mV
#    EC         366 µS/cm # Electrical conductivity
     redox      pe
     units      mg/l
     density    1
#    O(0)       -
     Ba         1.05
     Cd         0.00073
     Na         76.4
     K          2.4
     Ca         6.4
     Mg         0.87
     Fe         0.11 # Dissolved Iron
#    Fe(2)      -
#    Fe(3)      -
     Mn         0.09
     Alkalinity 187.7 as Ca.5(CO3).5 # Total Alkalinity calculated as mgCaCO3/L
#    C          -
     S(6)       0.8
#    S(-2)      - # Sulfide (sulfite SO3(-2) is not included in phreeqc database and
implies in differences in Ionic Balance for some wells)
#    S(4)       - # Sulfite included by Paulo Alencar in wateq4f.dat database considering
discussions at http://phreeqcusers.org/index.php?topic=963.0
     Cl         3.7
     F          0.28
     N(-3)      0.006 # NH3 reported as N
     N(+3)      0.004 # Nitrite reported as N
     N(+5)      0.051 # Nitrate reported as N
#    N(0)       - # Total nitrogen
     P          0.068 # Phosphate reported as P
     Si         30.4
     Al         0.00849
#    As         0.00049
#    Ag         0
     Br         -
     B          0.0576
#    Co         0
     Pb         0.00363
#    Cr         0.00057
```

```
#    Cr(+6)    -
    Cu        0.00551
#    Mo        0.00408
#    Ni        0.00673
#    Se(6)     - # Dissolved Selenium considered as selenate
#    Sr        -
#    V         -
    Zn        0.1382
    -water    1 # kg

SOLUTION 30 # (Gomes, 2012) Itaboraí/RJ - P-01B  (08/09) ago/09
# Below detection limits values included as zero.
    temp      24.81
    pe        -2.317 # Calculated with eh-to-pe.xls file
    pH        6
#   ORP       -137 mV
#   EC        183 µS/cm # Electrical conductivity
    redox     pe
    units     mg/l
    density   1
#    O(0)      -
    Ba        0.37
    Cd        0.00066
    Na        48.4
    K         4.2
    Ca        5.6
    Mg        1.22
    Fe        0.73 # Dissolved Iron
#    Fe(2)     -
#    Fe(3)     -
    Mn        0.14
    Alkalinity 128.69 as Ca.5(CO3).5 # Total Alkalinity calculated as mgCaCO3/L
#    C         -
    S(6)      20
#    S(-2)     - # Sulfide (sulfite SO3(-2) is not included in phreeqc database and
implies in differences in Ionic Balance for some wells)
#    S(4)      - # Sulfite included by Paulo Alencar in wateq4f.dat database considering
discussions at http://phreeqcusers.org/index.php?topic=963.0
#    Cl        -
    F         0.21
    N(-3)     0.01 # NH3 reported as N
    N(+3)     0.005 # Nitrite reported as N
    N(+5)     0.083 # Nitrate reported as N
#    N(0)      - # Total nitrogen
    P         0.443 # Phosphate reported as P
    Si        71.8
    Al        0.00672
#    As        0.00019
#    Ag        0
    Br        -
    B         0.023
#    Co        0
    Pb        0.00147
#    Cr        0
#    Cr(+6)    -
    Cu        0.00093
#    Mo        0.00054
#    Ni        0
#    Se(6)     - # Dissolved Selenium considered as selenate
#    Sr        -
#    V         -
    Zn        0.103
    -water    1 # kg

SOLUTION 31 # (Gomes, 2012) Itaboraí/RJ - P-01C  (08/09) ago/09
# Below detection limits values included as zero.
    temp      24.74
    pe        -2.047 # Calculated with eh-to-pe.xls file
```

```
    pH        7
#   ORP       -121 mV
#   EC        2550 µS/cm # Electrical conductivity
    redox     pe
    units     mg/l
    density   1
#    O(0)      -
    Ba        1.76
    Cd        0.00069
    Na        144
    K         18.8
    Ca        181
    Mg        19.03
    Fe        23.56 # Dissolved Iron
#    Fe(2)     -
#    Fe(3)     -
    Mn        4.54
    Alkalinity 144.26 as Ca.5(CO3).5 # Total Alkalinity calculated as mgCaCO3/L
#    C         -
#    S(6)      -
#    S(-2)     - # Sulfide (sulfite SO3(-2) is not included in phreeqc database and
implies in differences in Ionic Balance for some wells)
#    S(4)      - # Sulfite included by Paulo Alencar in wateq4f.dat database considering
discussions at http://phreeqcusers.org/index.php?topic=963.0
    Cl        626
#    F         -
    N(-3)     0.076 # NH3 reported as N
    N(+3)     0.015 # Nitrite reported as N
    N(+5)     0.058 # Nitrate reported as N
#    N(0)      - # Total nitrogen
    P         0.065 # Phosphate reported as P
    Si        70
    Al        0.00151
#    As        0.0049
#    Ag        0
    Br        -
    B         0.0242
#    Co        0.00355
    Pb        0.00243
#    Cr        0
#    Cr(+6)    -
    Cu        0.0165
#    Mo        0.00077
#    Ni        0.00337
#    Se(6)     - # Dissolved Selenium considered as selenate
#    Sr        -
#    V         -
    Zn        0.0962
    -water    1 # kg

SOLUTION 32 # (Gomes, 2012) Itaboraí/RJ - P-02A  (08/09) ago/09
# Below detection limits values included as zero.
    temp      25.78
    pe        1.113 # Calculated with eh-to-pe.xls file
    pH        7.2
#   ORP       66 mV
#   EC        376 µS/cm # Electrical conductivity
    redox     pe
    units     mg/l
    density   1
#    O(0)      -
    Ba        0.58
    Cd        0.00068
    Na        9.1
    K         5.9
    Ca        38.1
    Mg        3.72
    Fe        0.02 # Dissolved Iron
```

```
#    Fe(2)      -
#    Fe(3)      -
    Mn         0.02
    Alkalinity 149.18 as Ca.5(CO3).5 # Total Alkalinity calculated as mgCaCO3/L
#    C          -
    S(6)       4
#    S(-2)      - # Sulfide (sulfite SO3(-2) is not included in phreeqc database and
implies in differences in Ionic Balance for some wells)
#    S(4)       - # Sulfite included by Paulo Alencar in wateq4f.dat database considering
discussions at http://phreeqcusers.org/index.php?topic=963.0
    Cl         5.7
    F          0.4
    N(-3)      0.003 # NH3 reported as N
    N(+3)      0.005 # Nitrite reported as N
    N(+5)      0.054 # Nitrate reported as N
#    N(0)       - # Total nitrogen
    P          0.055 # Phosphate reported as P
    Si         28.1
    Al         0.00508
#    As         0
#    Ag         0
    Br         -
    B          0.0222
#    Co         0
    Pb         0.00187
#    Cr         0
#    Cr(+6)     -
    Cu         0.0726
#    Mo         0.00195
#    Ni         0.00095
#    Se(6)      - # Dissolved Selenium considered as selenate
#    Sr         -
#    V          -
    Zn         0.0985
    -water     1 # kg

SOLUTION 33 # (Gomes, 2012) Itaboraí/RJ - P-02B  (08/09) ago/09
# Below detection limits values included as zero.
    temp       25.95
    pe         1.803 # Calculated with eh-to-pe.xls file
    pH         6
#   ORP        107 mV
#   EC         90 µS/cm # Electrical conductivity
    redox      pe
    units      mg/l
    density    1
#    O(0)       -
    Ba         0.08
    Cd         0.00079
    Na         4.2
    K          2.2
    Ca         5.2
    Mg         1.35
    Fe         0.02 # Dissolved Iron
#    Fe(2)      -
#    Fe(3)      -
    Mn         0.06
    Alkalinity 24.59 as Ca.5(CO3).5 # Total Alkalinity calculated as mgCaCO3/L
#    C          -
    S(6)       0
#    S(-2)      - # Sulfide (sulfite SO3(-2) is not included in phreeqc database and
implies in differences in Ionic Balance for some wells)
#    S(4)       - # Sulfite included by Paulo Alencar in wateq4f.dat database considering
discussions at http://phreeqcusers.org/index.php?topic=963.0
    Cl         6.8
    F          0.09
    N(-3)      0.007 # NH3 reported as N
    N(+3)      0.005 # Nitrite reported as N
```

```
    N(+5)     0.329 # Nitrate reported as N
#    N(0)      - # Total nitrogen
    P         0.016 # Phosphate reported as P
    Si        9.4
    Al        0.01108
#    As        0
#    Ag        0
    Br        -
    B         0.0078
#    Co        0
    Pb        0.0062
#    Cr        0
#    Cr(+6)    -
    Cu        0.01091
#    Mo        0.00064
#    Ni        0.0037
#    Se(6)     - # Dissolved Selenium considered as selenate
#    Sr        -
#    V         -
    Zn        0.0367
    -water    1 # kg

SOLUTION 34 # (Gomes, 2012) Itaboraí/RJ - P-02C  (08/09) ago/09
# Below detection limits values included as zero.
    temp      26.24
    pe        1.481 # Calculated with eh-to-pe.xls file
    pH        6.7
#   ORP       88 mV
#   EC        197 µS/cm # Electrical conductivity
    redox     pe
    units     mg/l
    density   1
#    O(0)      -
    Ba        0.17
    Cd        0.00099
    Na        18.4
    K         5.2
    Ca        7.3
    Mg        2.08
    Fe        0.01 # Dissolved Iron
#    Fe(2)     -
#    Fe(3)     -
    Mn        0.29
    Alkalinity 65.57 as Ca.5(CO3).5 # Total Alkalinity calculated as mgCaCO3/L
#    C         -
    S(6)      0
#    S(-2)     - # Sulfide (sulfite SO3(-2) is not included in phreeqc database and
implies in differences in Ionic Balance for some wells)
#    S(4)      - # Sulfite included by Paulo Alencar in wateq4f.dat database considering
discussions at http://phreeqcusers.org/index.php?topic=963.0
    Cl        3.8
    F         0.37
    N(-3)     0.004 # NH3 reported as N
    N(+3)     0.004 # Nitrite reported as N
    N(+5)     0.044 # Nitrate reported as N
#    N(0)      - # Total nitrogen
    P         0.059 # Phosphate reported as P
    Si        5.2
    Al        0.00818
#    As        0
#    Ag        0
    Br        -
    B         0.0105
#    Co        0.00093
    Pb        0.00576
#    Cr        0
#    Cr(+6)    -
    Cu        0.06238
```

```
#    Mo        0.00159
#    Ni        0.00946
#    Se(6)     - # Dissolved Selenium considered as selenate
#    Sr        -
#    V         -
    Zn        0.0765
    -water    1 # kg

SOLUTION 35 # (Gomes, 2012) Itaboraí/RJ - P-03A  (08/09) ago/09
# Below detection limits values included as zero.
    temp      25.24
    pe        -2.01 # Calculated with eh-to-pe.xls file
    pH        8.8
#   ORP       -119 mV
#   EC        375 µS/cm # Electrical conductivity
    redox     pe
    units     mg/l
    density   1
#    O(0)      -
    Ba        0.43
    Cd        0.00094
    Na        3.2
    K         1.6
    Ca        4.9
    Mg        0.79
    Fe        0.09 # Dissolved Iron
#    Fe(2)     -
#    Fe(3)     -
    Mn        0.3
    Alkalinity 268.85 as Ca.5(CO3).5 # Total Alkalinity calculated as mgCaCO3/L
#    C         -
#    S(6)      -
#    S(-2)     - # Sulfide (sulfite SO3(-2) is not included in phreeqc database and
implies in differences in Ionic Balance for some wells)
#    S(4)      - # Sulfite included by Paulo Alencar in wateq4f.dat database considering
discussions at http://phreeqcusers.org/index.php?topic=963.0
#    Cl        -
#    F         -
    N(-3)     0.011 # NH3 reported as N
    N(+3)     0.004 # Nitrite reported as N
    N(+5)     0.021 # Nitrate reported as N
#    N(0)      - # Total nitrogen
    P         0.127 # Phosphate reported as P
    Si        19.5
    Al        0.01562
#    As        0.00041
#    Ag        0
    Br        -
    B         0.0266
#    Co        0
    Pb        0.00166
#    Cr        0
#    Cr(+6)    -
    Cu        0.00088
#    Mo        0.1432
#    Ni        0
#    Se(6)     - # Dissolved Selenium considered as selenate
#    Sr        -
#    V         -
    Zn        0.0199
    -water    1 # kg

SOLUTION 36 # (Gomes, 2012) Itaboraí/RJ - P-03B  (08/09) ago/09
# Below detection limits values included as zero.
    temp      25.4
    pe        -0.422 # Calculated with eh-to-pe.xls file
    pH        8.6
#   ORP       -25 mV
```

```
#   EC        373 µS/cm # Electrical conductivity
    redox     pe
    units     mg/l
    density   1
#    O(0)      -
    Ba        0.19
    Cd        0.00088
    Na        90.2
    K         1.1
    Ca        4.1
    Mg        0.88
    Fe        0.02 # Dissolved Iron
#    Fe(2)     -
#    Fe(3)     -
    Mn        0.59
    Alkalinity 196.72 as Ca.5(CO3).5 # Total Alkalinity calculated as mgCaCO3/L
#    C         -
    S(6)      5.2
#    S(-2)     - # Sulfide (sulfite SO3(-2) is not included in phreeqc database and
implies in differences in Ionic Balance for some wells)
#    S(4)      - # Sulfite included by Paulo Alencar in wateq4f.dat database considering
discussions at http://phreeqcusers.org/index.php?topic=963.0
    Cl        7.8
    F         1.82
    N(-3)     0.007 # NH3 reported as N
    N(+3)     0.006 # Nitrite reported as N
    N(+5)     0.061 # Nitrate reported as N
#    N(0)      - # Total nitrogen
    P         0.095 # Phosphate reported as P
    Si        18.9
    Al        0.04564
#    As        0.00051
#    Ag        0
    Br        -
    B         0.0141
#    Co        0.00061
    Pb        0.00167
#    Cr        0
#    Cr(+6)    -
    Cu        0.00211
#    Mo        0.1104
#    Ni        0
#    Se(6)     - # Dissolved Selenium considered as selenate
#    Sr        -
#    V         -
    Zn        0.012
    -water    1 # kg

SOLUTION 37 # (Gomes, 2012) Itaboraí/RJ - P-04A  (08/09) ago/09
# Below detection limits values included as zero.
    temp      25.56
    pe        -2.682 # Calculated with eh-to-pe.xls file
    pH        7.7
#   ORP       -159 mV
#   EC        1104 µS/cm # Electrical conductivity
    redox     pe
    units     mg/l
    density   1
#    O(0)      -
    Ba        0.26
    Cd        0.00069
    Na        33.6
    K         8
    Ca        16.1
    Mg        6.65
    Fe        1.52 # Dissolved Iron
#    Fe(2)     -
#    Fe(3)     -
```

```
    Mn        1.35
    Alkalinity 40.98 as Ca.5(CO3).5 # Total Alkalinity calculated as mgCaCO3/L
#    C         -
    S(6)      22.5
#    S(-2)     - # Sulfide (sulfite SO3(-2) is not included in phreeqc database and
implies in differences in Ionic Balance for some wells)
#    S(4)      - # Sulfite included by Paulo Alencar in wateq4f.dat database considering
discussions at http://phreeqcusers.org/index.php?topic=963.0
    Cl        122
    F         6.14
    N(-3)     0.049 # NH3 reported as N
    N(+3)     0.007 # Nitrite reported as N
    N(+5)     0.018 # Nitrate reported as N
#    N(0)      - # Total nitrogen
    P         0.004 # Phosphate reported as P
    Si        37.5
    Al        0.00115
#    As        0.00093
#    Ag        0
    Br        -
    B         0.0122
#    Co        0.00264
    Pb        0.00317
#    Cr        0
#    Cr(+6)    -
    Cu        0.00336
#    Mo        0.00203
#    Ni        0.00112
#    Se(6)     - # Dissolved Selenium considered as selenate
#    Sr        -
#    V         -
    Zn        0.0098
    -water    1 # kg

SOLUTION 38 # (Gomes, 2012) Itaboraí/RJ - P-04B  (08/09) ago/09
# Below detection limits values included as zero.
    temp      25.6
    pe        -1.839 # Calculated with eh-to-pe.xls file
    pH        6.8
#   ORP       -109 mV
#   EC        900 µS/cm # Electrical conductivity
    redox     pe
    units     mg/l
    density   1
#    O(0)      -
    Ba        0.22
    Cd        0.00068
    Na        97
    K         6
    Ca        19
    Mg        8
    Fe        0.02 # Dissolved Iron
#    Fe(2)     -
#    Fe(3)     -
    Mn        0.48
    Alkalinity 55.74 as Ca.5(CO3).5 # Total Alkalinity calculated as mgCaCO3/L
#    C         -
    S(6)      15
#    S(-2)     - # Sulfide (sulfite SO3(-2) is not included in phreeqc database and
implies in differences in Ionic Balance for some wells)
#    S(4)      - # Sulfite included by Paulo Alencar in wateq4f.dat database considering
discussions at http://phreeqcusers.org/index.php?topic=963.0
    Cl        158
    F         0.37
    N(-3)     0.009 # NH3 reported as N
    N(+3)     0.004 # Nitrite reported as N
    N(+5)     0.023 # Nitrate reported as N
#    N(0)      - # Total nitrogen
```

```
    P         0.03 # Phosphate reported as P
    Si        22.5
    Al        0.0021
#    As        0.00064
#    Ag        0
    Br        -
    B         0.0317
#    Co        0.00031
    Pb        0.00337
#    Cr        0
#    Cr(+6)    -
    Cu        0.00317
#    Mo        0.00803
#    Ni        0
#    Se(6)     - # Dissolved Selenium considered as selenate
#    Sr        -
#    V         -
    Zn        0.0058
    -water    1 # kg

SOLUTION 39 # (Gomes, 2012) Itaboraí/RJ - P-05  (08/09) ago/09
# Below detection limits values included as zero.
#    temp      -
#    pe        - # Calculated with eh-to-pe.xls file
#    pH        -
#   ORP       - mV
#   EC        - µS/cm # Electrical conductivity
#    redox     pe
    units     mg/l
    density   1
#    O(0)      -
    Ba        0.07
    Cd        0.00067
#    Na        -
#    K         -
#    Ca        -
#    Mg        -
    Fe        0.35 # Dissolved Iron
#    Fe(2)     -
#    Fe(3)     -
    Mn        0.36
#    Alkalinity - as Ca.5(CO3).5 # Total Alkalinity calculated as mgCaCO3/L
#    C         -
#    S(6)      -
#    S(-2)     - # Sulfide (sulfite SO3(-2) is not included in phreeqc database and
implies in differences in Ionic Balance for some wells)
#    S(4)      - # Sulfite included by Paulo Alencar in wateq4f.dat database considering
discussions at http://phreeqcusers.org/index.php?topic=963.0
#    Cl        -
    F         0.65
    N(-3)     0.161 # NH3 reported as N
    N(+3)     0.014 # Nitrite reported as N
    N(+5)     0.014 # Nitrate reported as N
#    N(0)      - # Total nitrogen
    P         0.048 # Phosphate reported as P
    Si        14.5
    Al        0.00803
#    As        0.00845
#    Ag        0
    Br        -
    B         0.7341
#    Co        0.00001
    Pb        0.00233
#    Cr        0
#    Cr(+6)    -
    Cu        0.00474
#    Mo        0.00367
#    Ni        0.0018
```

```
#    Se(6)     - # Dissolved Selenium considered as selenate
#    Sr        -
#    V         -
    Zn        0.0119
    -water    1 # kg

SOLUTION 40 # (Marcolan, 2009) Urânia/SP - PM-1  (PM1-BX-1) set/07
# Below detection limits values included as zero.
    temp      26.2
    pe        7.037 # Calculated with eh-to-pe.xls file
    pH        7.47
#   ORP       418 mV
#   EC        413 µS/cm # Electrical conductivity
    redox     pe
    units     mg/l
    density   1
    O(0)      0.8
    Ba        0.419
#    Cd        -
    Na        8.4
    K         6.4
    Ca        44
    Mg        21
    Fe        0 # Dissolved Iron
#    Fe(2)     -
#    Fe(3)     -
    Mn        0
    Alkalinity 165.05 as Ca.5(CO3).5 # Total Alkalinity reported as mgCaCO3/L
#    C         0.35
    S(6)      0.27
#    S(-2)     - # Sulfide (sulfite SO3(-2) is not included in phreeqc database and
implies in differences in Ionic Balance for some wells)
#    S(4)      - # Sulfite included by Paulo Alencar in wateq4f.dat database considering
discussions at http://phreeqcusers.org/index.php?topic=963.0
    Cl        8.2
    F         0.28
    N(-3)     0 # NH3 reported as N
    N(+3)     0 # Nitrite reported as N
    N(+5)     40 # Nitrate reported as N
#    N(0)      - # Total nitrogen
    P         0 # Phosphate reported as P
    Si        65.6
    Al        0
#    As        -
#    Ag        -
    Br        0
#    B         -
#    Co        -
#    Pb        -
#    Cr        0.009
#    Cr(+6)    -
    Cu        0
#    Mo        -
#    Ni        0
#    Se(6)     - # Dissolved Selenium considered as selenate
    Sr        0.55
#    V         -
    Zn        0.01
    -water    1 # kg

SOLUTION 41 # (Marcolan, 2009) Urânia/SP - PM-2  (PM-2-24h) set/07
# Below detection limits values included as zero.
    temp      26.9
    pe        6.483 # Calculated with eh-to-pe.xls file
    pH        9.17
#   ORP       386 mV
#   EC        196 µS/cm # Electrical conductivity
    redox     pe
```

```
    units     mg/l
    density   1
    O(0)      3.3
    Ba        0.017
#    Cd        -
    Na        45
    K         3.6
    Ca        1.9
    Mg        0.2
    Fe        0.003 # Dissolved Iron
#    Fe(2)     -
#    Fe(3)     -
    Mn        0
    Alkalinity 97.91 as Ca.5(CO3).5 # Total Alkalinity reported as mgCaCO3/L
#    C         0.73
    S(6)      1.7
#    S(-2)     - # Sulfide (sulfite SO3(-2) is not included in phreeqc database and
implies in differences in Ionic Balance for some wells)
#    S(4)      - # Sulfite included by Paulo Alencar in wateq4f.dat database considering
discussions at http://phreeqcusers.org/index.php?topic=963.0
    Cl        1.2
    F         0.32
    N(-3)     0 # NH3 reported as N
    N(+3)     0 # Nitrite reported as N
    N(+5)     0.23 # Nitrate reported as N
#    N(0)      - # Total nitrogen
    P         0.24 # Phosphate reported as P
    Si        17.5
    Al        0.05
#    As        -
#    Ag        -
    Br        0
#    B         -
#    Co        -
#    Pb        -
#    Cr        0.139
#    Cr(+6)    -
    Cu        0
#    Mo        -
#    Ni        0
#    Se(6)     - # Dissolved Selenium considered as selenate
    Sr        0.09
#    V         -
    Zn        0.01
    -water    1 # kg

SOLUTION 42 # (Marcolan, 2009) Urânia/SP - PM-3A  (PM3A-BX-2) set/07
# Below detection limits values included as zero.
    temp      30.5
    pe        8.149 # Calculated with eh-to-pe.xls file
    pH        6.33
#   ORP       491 mV
#   EC        162.5 µS/cm # Electrical conductivity
    redox     pe
    units     mg/l
    density   1
    O(0)      4.2
    Ba        0.217
#    Cd        -
    Na        9.2
    K         4.3
    Ca        15
    Mg        5.7
    Fe        0 # Dissolved Iron
#    Fe(2)     -
#    Fe(3)     -
    Mn        0.02
    Alkalinity 65.19 as Ca.5(CO3).5 # Total Alkalinity reported as mgCaCO3/L
```

```
#    C         0.01
     S(6)      0.28
#    S(-2)      - # Sulfide (sulfite SO3(-2) is not included in phreeqc database and
implies in differences in Ionic Balance for some wells)
#    S(4)       - # Sulfite included by Paulo Alencar in wateq4f.dat database considering
discussions at http://phreeqcusers.org/index.php?topic=963.0
     Cl        3
     F         0.14
     N(-3)     0 # NH3 reported as N
     N(+3)     0 # Nitrite reported as N
     N(+5)     11 # Nitrate reported as N
#    N(0)       - # Total nitrogen
     P         0.1 # Phosphate reported as P
     Si        26.3
     Al        0
#    As         -
#    Ag         -
     Br        0
#    B          -
#    Co         -
#    Pb         -
#    Cr         0.011
#    Cr(+6)     -
     Cu        0
#    Mo         -
#    Ni         0.002
#    Se(6)      - # Dissolved Selenium considered as selenate
     Sr        0.12
#    V          -
     Zn        0.04
     -water    1 # kg

SOLUTION 43 # (Marcolan, 2009) Urânia/SP - PM-3B  (PM3B-BX-2) set/07
# Below detection limits values included as zero.
     temp      30.4
     pe        7.653 # Calculated with eh-to-pe.xls file
     pH        7.77
#    ORP       461 mV
#    EC        236 µS/cm # Electrical conductivity
     redox     pe
     units     mg/l
     density   1
     O(0)      2.4
     Ba        0.116
#    Cd         -
     Na        8.4
     K         4.3
     Ca        23
     Mg        13
     Fe        0 # Dissolved Iron
#    Fe(2)      -
#    Fe(3)      -
     Mn        0.01
     Alkalinity 121.69 as Ca.5(CO3).5 # Total Alkalinity reported as mgCaCO3/L
#    C          -
     S(6)      0.11
#    S(-2)      - # Sulfide (sulfite SO3(-2) is not included in phreeqc database and
implies in differences in Ionic Balance for some wells)
#    S(4)       - # Sulfite included by Paulo Alencar in wateq4f.dat database considering
discussions at http://phreeqcusers.org/index.php?topic=963.0
     Cl        0.25
     F         0.17
     N(-3)     0 # NH3 reported as N
     N(+3)     0 # Nitrite reported as N
     N(+5)     0.06 # Nitrate reported as N
#    N(0)       - # Total nitrogen
     P         0.012 # Phosphate reported as P
     Si        62.6
```

```
    Al        0.01
#    As        -
#    Ag        -
    Br        0
#    B         -
#    Co        -
#    Pb        -
#    Cr        0.078
#    Cr(+6)    -
    Cu        0
#    Mo        -
#    Ni        0
#    Se(6)     - # Dissolved Selenium considered as selenate
    Sr        0.83
#    V         -
    Zn        0.01
    -water    1 # kg

SOLUTION 44 # (Marcolan, 2009) Urânia/SP - PM-3C  (PM3C-BX) set/07
# Below detection limits values included as zero.
    temp      28.1
    pe        4.349 # Calculated with eh-to-pe.xls file
    pH        11.13
#   ORP       260 mV
#   EC        599 µS/cm # Electrical conductivity
    redox     pe
    units     mg/l
    density   1
    O(0)      1
    Ba        0.055
#    Cd        -
    Na        23
    K         10.7
    Ca        39
    Mg        0
    Fe        0 # Dissolved Iron
#    Fe(2)     -
#    Fe(3)     -
    Mn        0
    Alkalinity 139.88 as Ca.5(CO3).5 # Total Alkalinity reported as mgCaCO3/L (18.16 as
HCO3-)
    C         74.84
    S(6)      14
#    S(-2)     - # Sulfide (sulfite SO3(-2) is not included in phreeqc database and
implies in differences in Ionic Balance for some wells)
#    S(4)      - # Sulfite included by Paulo Alencar in wateq4f.dat database considering
discussions at http://phreeqcusers.org/index.php?topic=963.0
    Cl        3.3
    F         0.44
    N(-3)     0 # NH3 reported as N
    N(+3)     0.23 # Nitrite reported as N
    N(+5)     0.25 # Nitrate reported as N
#    N(0)      - # Total nitrogen
    P         0.05 # Phosphate reported as P
    Si        10.1
    Al        2.01
#    As        -
#    Ag        -
    Br        0
#    B         -
#    Co        -
#    Pb        -
#    Cr        0.023
#    Cr(+6)    -
    Cu        0
#    Mo        -
#    Ni        0.001
#    Se(6)     - # Dissolved Selenium considered as selenate
```

```
    Sr        0.9
#    V         -
    Zn        0
    -water    1 # kg

#SOLUTION x # (Marcolan, 2009) Urânia/SP - PM-x  (PMx) set/07
## Below detection limits values included as zero.
#    temp      x
#    pe        x # Calculated with eh-to-pe.xls file
#    pH        x
##   ORP       x mV
##   EC        x µS/cm # Electrical conductivity
#    redox     pe
#    units     mg/l
#    density   1
#    O(0)      x
#    Ba        0.
##    Cd        -
#    Na        x
#    K         x
#    Ca        x
#    Mg        x
#    Fe        0 # Dissolved Iron
##    Fe(2)     -
##    Fe(3)     -
#    Mn        0.
#    Alkalinity x as Ca.5(CO3).5 # Total Alkalinity reported as mgCaCO3/L
##    C         -
#    S(6)      x
##    S(-2)     - # Sulfide (sulfite SO3(-2) is not included in phreeqc database and
implies in differences in Ionic Balance for some wells)
##    S(4)      - # Sulfite included by Paulo Alencar in wateq4f.dat database considering
discussions at http://phreeqcusers.org/index.php?topic=963.0
#    Cl        x
#    F         x
#    N(-3)     0. # NH3 reported as N
#    N(+3)     0. # Nitrite reported as N
#    N(+5)     0. # Nitrate reported as N
##    N(0)      - # Total nitrogen
#    P         0. # Phosphate reported as P
#    Si        x
#    Al        0.
##    As        -
##    Ag        -
#    Br        0
##    B         -
##    Co        -
##    Pb        -
##    Cr        0.
##    Cr(+6)    -
#    Cu        0
##    Mo        -
##    Ni        0.
##    Se(6)     - # Dissolved Selenium considered as selenate
#    Sr        0.
##    V         -
#    Zn        0.0
#    -water    1 # kg

PRINT; -alkalinity true

SELECTED_OUTPUT
 -file Monografia_PAP_phreeqc_PAP_lnll.txt
 -reset true
 -pH
 -pe
 -alkalinity
 -charge_balance
```

```
 -Percent_error
 -totals Ba Cd S(6) Cl
 -molalities Ba+2 BaCO3 BaSO4 BaHCO3+ BaOH+ BaCl+ BaNO3+ Cd+2 CdHCO3+ CdCO3 CdCl+ CdSO4
# -molalities BaSO4
 -saturation_indices Barite Witherite BaCl2 BaCl2:2H2O BaCl2:H2O BaS Greenockite Cd(OH)2
Otavite CdSO4
# -totals Cd
# -molalities Cd+2
# -molalities CdCO3
# -saturation_indices Otavite
# -calculate_values SC_TF
# -calculate_values SC_T25
# -calculate_values DS
```

```
   Input file: C:\Users\Paulo\Desktop\Mono_MBA_GAC_USP\Referencias\3 - Metodologia\3-1 -
Modelo hidrogeoquimico\Monografia_PAP_phreeqc_PAP_lnll.pqi
  Output file: C:\Users\Paulo\Desktop\Mono_MBA_GAC_USP\Referencias\3 - Metodologia\3-1 -
Modelo hidrogeoquimico\Monografia_PAP_phreeqc_PAP_lnll.pqo
Database file: C:\Program Files (x86)\USGS\Phreeqc Interactive 3.6.2-15100\database
\phreeqc_PAP_lnll.dat

------------------
Reading data base.
------------------

      SOLUTION_MASTER_SPECIES
      SOLUTION_SPECIES
      PHASES
      EXCHANGE_MASTER_SPECIES
      EXCHANGE_SPECIES
      SURFACE_MASTER_SPECIES
      SURFACE_SPECIES
      RATES
      END
-----------------------------------
Reading input data for simulation 1.
-----------------------------------

      DATABASE C:\Program Files (x86)\USGS\Phreeqc Interactive 3.6.2-15100\database
\phreeqc_PAP_lnll.dat
      SOLUTION 1 # (Tavares, 2013) Gália/SP - G PM-03 jul/10 (Tabela 7.1.2.1 - página 154)
          temp      23.8
          pe        4.883 # Calculated with eh-to-pe.xls file
          pH        7.04
          redox     pe
          units     mg/l
          density   1
          Ba        0.28
          Na        2.7
          K         2.3
          Ca        63.09
          Mg        16.16
          Fe        0 # Dissolved Iron
          Mn        0.03
          Alkalinity 180.17 as Ca.5(CO3).5 # Total Alkalinity calculated as mgCaCO3/L
          S(6)      4.43
          Cl        4.58
          F         0.07
          N(+3)     0.02 # Nitrite reported as N
          N(+5)     16.13 # Nitrate reported as N
          P         0.05 # Phosphate reported as P
          Si        14.37
          Al        0
          Sr        0.53
          water    1 # kg
      SOLUTION 2 # (Tavares, 2013) Gália/SP - G PM-02 jul/10 (Tabela 7.1.2.1 - página 154)
          temp      27
          pe        4.473 # Calculated with eh-to-pe.xls file
          pH        8.86
          redox     pe
          units     mg/l
          density   1
          Ba        1.54
          Na        4.7
          K         5.7
          Ca        21.08
          Mg        18.48
          Fe        0 # Dissolved Iron
          Mn        0.03
          Alkalinity 131.66 as Ca.5(CO3).5 # Total Alkalinity calculated as mgCaCO3/L
          S(6)      1.29
          Cl        2.85
```

```
        F         0.08
        N(+3)     0.009 # Nitrite reported as N
        N(+5)     1.25 # Nitrate reported as N
        P         0.04 # Phosphate reported as P
        Si        11.58
        Al        0
        Sr        0.58
        water    1 # kg
    SOLUTION 3 # (Tavares, 2013) Gália/SP - G PM-01 jul/10 (Tabela 7.1.2.1 - página 154)
        temp      24.1
        pe        6.553 # Calculated with eh-to-pe.xls file
        pH        9.37
        redox     pe
        units     mg/l
        density   1
        Ba        0.34
        Na        21.6
        K         16.8
        Ca        7.42
        Mg        7.29
        Fe        0 # Dissolved Iron
        Mn        0.03
        Alkalinity 86.52 as Ca.5(CO3).5 # Total Alkalinity calculated as mgCaCO3/L
        S(6)      7.78
        Cl        13.45
        F         0.12
        N(+3)     0.02 # Nitrite reported as N
        N(+5)     7.97 # Nitrate reported as N
        P         0.06 # Phosphate reported as P
        Si        5.27
        Al        0
        Sr        1.46
        water    1 # kg
    SOLUTION 4 # (Tavares, 2013) Salto de Pirapora/SP - PM01 out/10 (Tabela 7.1.3.1 -
página 164)
        temp      22.5
        pe        5.386 # Calculated with eh-to-pe.xls file
        pH        5.58
        redox     pe
        units     mg/l
        density   1
        O(0)      4.72
        Ba        0.07
        Na        0.5
        K         0.2
        Ca        0.56
        Mg        0.05
        Fe        0.09 # Dissolved Iron
        Mn        0.01
        Alkalinity 15.02 as Ca.5(CO3).5 # Total Alkalinity calculated as mgCaCO3/L
        S(6)      0.08
        Cl        0.23
        F         0.04
        N(+5)     0.23 # Nitrate reported as N
        P         0.03 # Phosphate reported as P
        Si        0.35
        Al        0.02
        Sr        0.15
        water    1 # kg
    SOLUTION 5 # (Tavares, 2013) Salto de Pirapora/SP - PM07 out/10 (Tabela 7.1.3.1 -
página 164)
        temp      23.4
        pe        1.592 # Calculated with eh-to-pe.xls file
        pH        5.32
        redox     pe
        units     mg/l
        density   1
        O(0)      0.63
```

```
        Ba        0.22
        Na        17
        K         2.1
        Ca        1.2
        Mg        1.06
        Fe        2.01 # Dissolved Iron
        Mn        0.05
        Alkalinity 10.01 as Ca.5(CO3).5 # Total Alkalinity calculated as mgCaCO3/L
        S(6)      0.31
        Cl        24.62
        F         0.06
        N(+3)     0.07 # Nitrite reported as N
        N(+5)     0.05 # Nitrate reported as N
        P         0.02 # Phosphate reported as P
        Si        6.08
        Al        0.025
        Sr        0.22
        water    1 # kg
    SOLUTION 6 # (Tavares, 2013) Salto de Pirapora/SP - PM03 out/10 (Tabela 7.1.3.1 -
página 164)
        temp      22.7
        pe        1.724 # Calculated with eh-to-pe.xls file
        pH        5.21
        redox     pe
        units     mg/l
        density   1
        O(0)      0.58
        Ba        0.74
        Na        26
        K         5.6
        Ca        4.94
        Mg        6.4
        Fe        0.11 # Dissolved Iron
        Mn        0.56
        Alkalinity 7.51 as Ca.5(CO3).5 # Total Alkalinity calculated as mgCaCO3/L
        S(6)      3.26
        Cl        81.53
        F         0.08
        N(+3)     0.16 # Nitrite reported as N
        N(+5)     4.03 # Nitrate reported as N
        P         0.04 # Phosphate reported as P
        Si        6.98
        Al        0.067
        Sr        0.5
        water    1 # kg
    SOLUTION 7 # (Tavares, 2013) Salto de Pirapora/SP - PM04 out/10 (Tabela 7.1.3.1 -
página 164)
        temp      21.2
        pe        -1.471 # Calculated with eh-to-pe.xls file
        pH        7.07
        redox     pe
        units     mg/l
        density   1
        O(0)      0.87
        Ba        1.48
        Na        10.1
        K         3.3
        Ca        67.37
        Mg        56.38
        Fe        1.84 # Dissolved Iron
        Mn        0.19
        Alkalinity 375.34 as Ca.5(CO3).5 # Total Alkalinity calculated as mgCaCO3/L
        S(6)      0.24
        Cl        4.51
        F         0.13
        N(+3)     0.01 # Nitrite reported as N
        N(+5)     0.16 # Nitrate reported as N
        P         0.02 # Phosphate reported as P
```

```
          Si        13.74
          Al        0.013
          Sr        0.53
          water     1 # kg
      SOLUTION 8 # (Tavares, 2013) Salto de Pirapora/SP - PM19 out/10 (Tabela 7.1.3.1 -
página 164)
          temp      25
          pe        3.135 # Calculated with eh-to-pe.xls file
          pH        5.65
          redox     pe
          units     mg/l
          density   1
          O(0)      1.16
          Ba        1.9
          Na        128
          K         5.9
          Ca        81.11
          Mg        160.83
          Fe        0.05 # Dissolved Iron
          Mn        1.14
          Alkalinity 40.03 as Ca.5(CO3).5 # Total Alkalinity calculated as mgCaCO3/L
          S(6)      15.58
          Cl        783.49
          F         0.13
          N(+3)     0.09 # Nitrite reported as N
          N(+5)     37.85 # Nitrate reported as N
          P         0.15 # Phosphate reported as P
          Si        8.6
          Al        0.014
          Sr        1.21
          water     1 # kg
      SOLUTION 9 # (Tavares, 2013) Salto de Pirapora/SP - PM24/45 out/10 (Tabela 7.1.3.1 -
página 164)
          temp      21.5
          pe        3.315 # Calculated with eh-to-pe.xls file
          pH        5.36
          redox     pe
          units     mg/l
          density   1
          O(0)      1.29
          Ba        0.61
          Na        3.5
          K         3.1
          Ca        12.1
          Mg        28.19
          Fe        0.08 # Dissolved Iron
          Mn        0.13
          Alkalinity 25.02 as Ca.5(CO3).5 # Total Alkalinity calculated as mgCaCO3/L
          S(6)      0.49
          Cl        92.35
          F         0.14
          N(+3)     0.16 # Nitrite reported as N
          N(+5)     3.14 # Nitrate reported as N
          P         0.06 # Phosphate reported as P
          Si        8.07
          Al        0.028
          Sr        0.31
          water     1 # kg
      SOLUTION 10 # (Tavares, 2013) Salto de Pirapora/SP - PM25 out/10 (Tabela 7.1.3.1 -
página 164)
          temp      23.7
          pe        1.241 # Calculated with eh-to-pe.xls file
          pH        5.52
          redox     pe
          units     mg/l
          density   1
          O(0)      0.88
          Ba        0.9
```

```
        Na        15
        K         1.1
        Ca        1.05
        Mg        0.97
        Fe        10.15 # Dissolved Iron
        Mn        3.44
        Alkalinity 35.03 as Ca.5(CO3).5 # Total Alkalinity calculated as mgCaCO3/L
        S(6)      1.99
        Cl        20.36
        F         0.08
        N(+3)     0.05 # Nitrite reported as N
        N(+5)     0.15 # Nitrate reported as N
        P         0.01 # Phosphate reported as P
        Si        3.4
        Al        0.019
        Sr        0.1
        water    1 # kg
    SOLUTION 11 # (Tavares, 2013) Salto de Pirapora/SP - PM27 out/10 (Tabela 7.1.3.1 -
página 164)
        temp      23.3
        pe        -1.312 # Calculated with eh-to-pe.xls file
        pH        6.52
        redox     pe
        units     mg/l
        density   1
        O(0)      0.75
        Ba        8.11
        Na        23
        K         15
        Ca        7.23
        Mg        5.2
        Fe        15.23 # Dissolved Iron
        Mn        9.24
        Alkalinity 285.26 as Ca.5(CO3).5 # Total Alkalinity calculated as mgCaCO3/L
        S(6)      0.06
        Cl        57.79
        F         0.53
        N(+3)     0.03 # Nitrite reported as N
        N(+5)     0.15 # Nitrate reported as N
        P         0.03 # Phosphate reported as P
        Si        2.19
        Al        0.035
        Sr        0.2
        water    1 # kg
    SOLUTION 12 # (Sanches, 2015) Itaboraí/RJ - P-01  (06/13) jun/13
        temp      23.06
        pe        0.371 # Calculated with eh-to-pe.xls file
        pH        5.5
        redox     pe
        units     mg/l
        density   1
        Ba        0
        Na        52.3
        K         7
        Ca        18.5
        Mg        4.26
        Alkalinity 24.59 as Ca.5(CO3).5 # Total Alkalinity calculated as mgCaCO3/L
        S(6)      73.1
        Cl        66.8
        F         0.01
        N(+3)     0 # Nitrite reported as N
        N(+5)     35.01 # Nitrate reported as N
        P         0.01 # Phosphate reported as P
        Br        0.5
        water    1 # kg
    SOLUTION 13 # (Sanches, 2015) Itaboraí/RJ - P-02  (06/13) jun/13
        temp      24.78
        pe        0.447 # Calculated with eh-to-pe.xls file
```

```
    pH        6.5
    redox     pe
    units     mg/l
    density   1
    Ba        1.17
    Na        65.1
    K         5.3
    Ca        71
    Mg        5.41
    Alkalinity 238.52 as Ca.5(CO3).5 # Total Alkalinity calculated as mgCaCO3/L
    S(6)      18.2
    Cl        73.8
    F         0.06
    N(+3)     0 # Nitrite reported as N
    N(+5)     1.17 # Nitrate reported as N
    P         0.06 # Phosphate reported as P
    Br        0.6
    water    1 # kg
SOLUTION 14 # (Sanches, 2015) Itaboraí/RJ - P-03  (06/13) jun/13
    temp      25.08
    pe        0.406 # Calculated with eh-to-pe.xls file
    pH        7.2
    redox     pe
    units     mg/l
    density   1
    Ba        0.62
    Na        141
    K         4.3
    Ca        49
    Mg        5.14
    Alkalinity 150 as Ca.5(CO3).5 # Total Alkalinity calculated as mgCaCO3/L
    S(6)      52.1
    Cl        174
    F         0.07
    N(+3)     0.06 # Nitrite reported as N
    N(+5)     3.26 # Nitrate reported as N
    P         0.07 # Phosphate reported as P
    Br        0.71
    water    1 # kg
SOLUTION 15 # (Sanches, 2015) Itaboraí/RJ - P-04  (06/13) jun/13
    temp      25.89
    pe        0.454 # Calculated with eh-to-pe.xls file
    pH        5.9
    redox     pe
    units     mg/l
    density   1
    Ba        1.37
    Na        193.5
    K         16.2
    Ca        337.9
    Mg        85.95
    Alkalinity 220.49 as Ca.5(CO3).5 # Total Alkalinity calculated as mgCaCO3/L
    S(6)      55.6
    Cl        950
    F         0.02
    N(+3)     0 # Nitrite reported as N
    N(+5)     1.46 # Nitrate reported as N
    P         0.02 # Phosphate reported as P
    Br        3.38
    water    1 # kg
SOLUTION 16 # (Sanches, 2015) Itaboraí/RJ - P-05  (10/13) out/13
    temp      24.52
    pe        0.276 # Calculated with eh-to-pe.xls file
    pH        5.2
    redox     pe
    units     mg/l
    density   1
    Ba        2.81
```

```
    Cd        0.00092
    Na        13.4
    K         2.5
    Ca        9.1
    Mg        2.34
    Fe        0.85189 # Dissolved Iron
    Mn        0.0174
    Alkalinity 47.54 as Ca.5(CO3).5 # Total Alkalinity calculated as mgCaCO3/L
    S(6)      4.3
    Cl        9.6
    F         1.07
    N(+3)     0 # Nitrite reported as N
    N(+5)     3.56 # Nitrate reported as N
    P         0.008 # Phosphate reported as P
    Al        0.01755
    Br        0
    B         0.1175
    Pb        0.00084
    Cu        0.00918
    water    1 # kg
SOLUTION 17 # (Sanches, 2015) Itaboraí/RJ - P-06  (10/13) out/13
    temp      24.48
    pe        0.145 # Calculated with eh-to-pe.xls file
    pH        4.2
    redox     pe
    units     mg/l
    density   1
    Ba        1.8
    Cd        0.0013
    Na        20.5
    K         8.2
    Ca        13.3
    Mg        7.55
    Fe        0.02407 # Dissolved Iron
    Mn        0.08004
    Alkalinity 27.87 as Ca.5(CO3).5 # Total Alkalinity calculated as mgCaCO3/L
    S(6)      2.7
    Cl        63
    F         1.19
    N(+3)     0 # Nitrite reported as N
    N(+5)     28.54 # Nitrate reported as N
    P         0.061 # Phosphate reported as P
    Al        0.85748
    Br        0.34
    B         0.169
    Pb        0.00296
    Cu        0.00536
    Zn        0.26114
    water    1 # kg
SOLUTION 18 # (Sanches, 2015) Itaboraí/RJ - P-07  (10/13) out/13
    temp      25.8
    pe        0.269 # Calculated with eh-to-pe.xls file
    pH        6.5
    redox     pe
    units     mg/l
    density   1
    Ba        1.51
    Cd        0.00083
    Na        62.3
    K         3.2
    Ca        29.8
    Mg        6.74
    Fe        0.03211 # Dissolved Iron
    Mn        0.00646
    Alkalinity 215.57 as Ca.5(CO3).5 # Total Alkalinity calculated as mgCaCO3/L
    S(6)      2.9
    Cl        17.9
    F         1.24
```

```
    N(+3)     0 # Nitrite reported as N
    N(+5)     0.46 # Nitrate reported as N
    P         0.143 # Phosphate reported as P
    Al        0.02902
    Br        0.44
    B         0.1404
    Pb        0.00053
    Cu        0.00266
    Zn        0.15426
    water    1 # kg
SOLUTION 19 # (Sanches, 2015) Itaboraí/RJ - P-08  (10/13) out/13
    temp      26.22
    pe        0.227 # Calculated with eh-to-pe.xls file
    pH        4.4
    redox     pe
    units     mg/l
    density   1
    Ba        0.8
    Cd        0.00088
    Na        13.3
    K         2.5
    Ca        8.6
    Mg        2.81
    Fe        0.03947 # Dissolved Iron
    Mn        0.05055
    Alkalinity 38.52 as Ca.5(CO3).5 # Total Alkalinity calculated as mgCaCO3/L
    S(6)      13
    Cl        9.2
    F         1.08
    N(+3)     0.02 # Nitrite reported as N
    N(+5)     4.62 # Nitrate reported as N
    P         0.003 # Phosphate reported as P
    Al        0.05251
    Br        0.17
    B         0.1265
    Pb        0.00016
    Cu        0.00203
    Zn        0.11026
    water    1 # kg
SOLUTION 20 # (Sanches, 2015) Itaboraí/RJ - P-09  (10/13) out/13
    temp      24.26
    pe        0.28 # Calculated with eh-to-pe.xls file
    pH        6.1
    redox     pe
    units     mg/l
    density   1
    Ba        1.2
    Cd        0.00102
    Na        15.3
    K         2.8
    Ca        14.5
    Mg        3.73
    Fe        0.17229 # Dissolved Iron
    Mn        0.092
    Alkalinity 65.57 as Ca.5(CO3).5 # Total Alkalinity calculated as mgCaCO3/L
    S(6)      12.1
    Cl        9
    F         1.1
    N(+3)     0 # Nitrite reported as N
    N(+5)     4.12 # Nitrate reported as N
    P         0.056 # Phosphate reported as P
    Al        0.12796
    Br        0.45
    B         0.132
    Pb        0.00105
    Cu        0.00447
    Zn        0.09931
    water    1 # kg
```

```
SOLUTION 21 # (Sanches, 2015) Itaboraí/RJ - P-10  (10/13) out/13
    temp      25.37
    pe        0.313 # Calculated with eh-to-pe.xls file
    pH        6.4
    redox     pe
    units     mg/l
    density   1
    Ba        1.79
    Cd        0.00061
    Na        18
    K         2
    Ca        14
    Mg        4
    Fe        0.00789 # Dissolved Iron
    Mn        0.00413
    Alkalinity 81.97 as Ca.5(CO3).5 # Total Alkalinity calculated as mgCaCO3/L
    S(6)      2
    Cl        4
    F         1.02
    N(+3)     0 # Nitrite reported as N
    N(+5)     4.96 # Nitrate reported as N
    P         0.003 # Phosphate reported as P
    Al        0.02213
    Br        0.4
    B         0.124
    Pb        0.00065
    Cu        0.00205
    Zn        0.12593
    water    1 # kg
SOLUTION 22 # (Sanches, 2015) Itaboraí/RJ - P-11  (10/13) out/13
    temp      24.83
    pe        0.437 # Calculated with eh-to-pe.xls file
    pH        6.9
    redox     pe
    units     mg/l
    density   1
    Ba        0.75
    Cd        0.00091
    Na        58
    K         4.6
    Ca        36.3
    Mg        7.42
    Fe        0.07531 # Dissolved Iron
    Mn        0.13665
    Alkalinity 245.9 as Ca.5(CO3).5 # Total Alkalinity calculated as mgCaCO3/L
    S(6)      3.6
    Cl        16
    F         1.22
    N(+3)     0 # Nitrite reported as N
    N(+5)     3.21 # Nitrate reported as N
    P         0.114 # Phosphate reported as P
    Al        0.00621
    Br        0.44
    B         0.07915
    Pb        0.00136
    Cu        0.00194
    Zn        0.00676
    water    1 # kg
SOLUTION 23 # (Sanches, 2015) Itaboraí/RJ - P-12  (10/13) out/13
    temp      27.33
    pe        0.447 # Calculated with eh-to-pe.xls file
    pH        5.8
    redox     pe
    units     mg/l
    density   1
    Ba        2.52
    Cd        0.00065
    Na        21.3
```

```
    K         4
    Ca        17.6
    Mg        9.18
    Fe        0.46189 # Dissolved Iron
    Mn        0.03012
    Alkalinity 93.44 as Ca.5(CO3).5 # Total Alkalinity calculated as mgCaCO3/L
    S(6)      4.8
    Cl        18
    F         1.06
    N(+3)     0 # Nitrite reported as N
    N(+5)     4.37 # Nitrate reported as N
    P         0.029 # Phosphate reported as P
    Al        0.00859
    Br        0.46
    B         0.1144
    Pb        0.00451
    Cu        0.00387
    Zn        0.10656
    water    1 # kg
SOLUTION 24 # (Sanches, 2015) Itaboraí/RJ - P-13  (10/13) out/13
    temp      26.74
    pe        0.404 # Calculated with eh-to-pe.xls file
    pH        8.4
    redox     pe
    units     mg/l
    density   1
    Ba        1.98
    Cd        0.00083
    Na        239.2
    K         3.3
    Ca        20
    Mg        13.54
    Fe        0.03058 # Dissolved Iron
    Mn        0.00559
    Alkalinity 609.02 as Ca.5(CO3).5 # Total Alkalinity calculated as mgCaCO3/L
    S(6)      3.6
    Cl        37
    F         6.03
    N(+3)     0 # Nitrite reported as N
    N(+5)     2.84 # Nitrate reported as N
    P         0.012 # Phosphate reported as P
    Al        0.06192
    Br        0.49
    B         0.6051
    Pb        0.00108
    Cu        0.00248
    Zn        0.13158
    water    1 # kg
SOLUTION 25 # (Sanches, 2015) Itaboraí/RJ - P-14  (10/13) out/13
    temp      24.93
    pe        0.441 # Calculated with eh-to-pe.xls file
    pH        7.5
    redox     pe
    units     mg/l
    density   1
    Ba        0.98
    Cd        0.00077
    Na        50.8
    K         5.4
    Ca        54.1
    Mg        14.24
    Fe        0.04925 # Dissolved Iron
    Mn        0.06439
    Alkalinity 202.46 as Ca.5(CO3).5 # Total Alkalinity calculated as mgCaCO3/L
    S(6)      17.2
    Cl        60.4
    F         1.05
    N(+3)     0 # Nitrite reported as N
```

```
    N(+5)     5.87 # Nitrate reported as N
    P         0.102 # Phosphate reported as P
    Al        0.04881
    Br        0.54
    B         0.1343
    Pb        0.00052
    Cu        0.00138
    Zn        0.10808
    water    1 # kg
SOLUTION 26 # (Sanches, 2015) Itaboraí/RJ - P-15  (10/13) out/13
    temp      25.54
    pe        0.343 # Calculated with eh-to-pe.xls file
    pH        7.2
    redox     pe
    units     mg/l
    density   1
    Ba        0
    Cd        0.00071
    Na        29.6
    K         3.1
    Ca        42.8
    Mg        27.4
    Fe        0.17304 # Dissolved Iron
    Mn        0.11577
    Alkalinity 236.07 as Ca.5(CO3).5 # Total Alkalinity calculated as mgCaCO3/L
    S(6)      6.9
    Cl        33.2
    F         2
    N(+3)     0.32 # Nitrite reported as N
    N(+5)     5.84 # Nitrate reported as N
    P         0.087 # Phosphate reported as P
    Al        0.02665
    Br        0.5
    B         0.1309
    Pb        0.00064
    Cu        0.00169
    Zn        0.12136
    water    1 # kg
SOLUTION 27 # (Sanches, 2015) Itaboraí/RJ - P-16  (10/13) out/13
    temp      24.63
    pe        0.223 # Calculated with eh-to-pe.xls file
    pH        4.6
    redox     pe
    units     mg/l
    density   1
    Ba        1.61
    Cd        0.00098
    Na        24.1
    K         7.5
    Ca        14.1
    Mg        16.74
    Fe        0.02525 # Dissolved Iron
    Mn        0.06763
    Alkalinity 118.85 as Ca.5(CO3).5 # Total Alkalinity calculated as mgCaCO3/L
    S(6)      4.9
    Cl        29.7
    F         1.16
    N(+3)     0.02 # Nitrite reported as N
    N(+5)     15.22 # Nitrate reported as N
    P         0.003 # Phosphate reported as P
    Al        0.04199
    Br        0.48
    B         0.1362
    Pb        0.00046
    Cu        0.00608
    Zn        0.15529
    water    1 # kg
SOLUTION 28 # (Sanches, 2015) Itaboraí/RJ - P-17  (10/13) out/13
```

```
    temp      25.06
    pe        0.253 # Calculated with eh-to-pe.xls file
    pH        5
    redox     pe
    units     mg/l
    density   1
    Ba        2.31
    Cd        0.00103
    Na        16.5
    K         4.5
    Ca        20.3
    Mg        12.12
    Fe        0.03198 # Dissolved Iron
    Mn        0.0118
    Alkalinity 103.28 as Ca.5(CO3).5 # Total Alkalinity calculated as mgCaCO3/L
    S(6)      3.5
    Cl        16.6
    F         1.09
    N(+3)     0.01 # Nitrite reported as N
    N(+5)     9.57 # Nitrate reported as N
    P         0.009 # Phosphate reported as P
    Al        0.02567
    Br        0.45
    B         0.1363
    Pb        0.00071
    Cu        0.00263
    Zn        0.1184
    water    1 # kg
SOLUTION 29 # (Gomes, 2012) Itaboraí/RJ - P-01A  (08/09) ago/09
    temp      24.94
    pe        -1.995 # Calculated with eh-to-pe.xls file
    pH        8
    redox     pe
    units     mg/l
    density   1
    Ba        1.05
    Cd        0.00073
    Na        76.4
    K         2.4
    Ca        6.4
    Mg        0.87
    Fe        0.11 # Dissolved Iron
    Mn        0.09
    Alkalinity 187.7 as Ca.5(CO3).5 # Total Alkalinity calculated as mgCaCO3/L
    S(6)      0.8
    Cl        3.7
    F         0.28
    N(-3)     0.006 # NH3 reported as N
    N(+3)     0.004 # Nitrite reported as N
    N(+5)     0.051 # Nitrate reported as N
    P         0.068 # Phosphate reported as P
    Si        30.4
    Al        0.00849
    Br        -
    B         0.0576
    Pb        0.00363
    Cu        0.00551
    Zn        0.1382
    water    1 # kg
SOLUTION 30 # (Gomes, 2012) Itaboraí/RJ - P-01B  (08/09) ago/09
    temp      24.81
    pe        -2.317 # Calculated with eh-to-pe.xls file
    pH        6
    redox     pe
    units     mg/l
    density   1
    Ba        0.37
    Cd        0.00066
```

```
    Na        48.4
    K         4.2
    Ca        5.6
    Mg        1.22
    Fe        0.73 # Dissolved Iron
    Mn        0.14
    Alkalinity 128.69 as Ca.5(CO3).5 # Total Alkalinity calculated as mgCaCO3/L
    S(6)      20
    F         0.21
    N(-3)     0.01 # NH3 reported as N
    N(+3)     0.005 # Nitrite reported as N
    N(+5)     0.083 # Nitrate reported as N
    P         0.443 # Phosphate reported as P
    Si        71.8
    Al        0.00672
    Br        -
    B         0.023
    Pb        0.00147
    Cu        0.00093
    Zn        0.103
    water    1 # kg
SOLUTION 31 # (Gomes, 2012) Itaboraí/RJ - P-01C  (08/09) ago/09
    temp      24.74
    pe        -2.047 # Calculated with eh-to-pe.xls file
    pH        7
    redox     pe
    units     mg/l
    density   1
    Ba        1.76
    Cd        0.00069
    Na        144
    K         18.8
    Ca        181
    Mg        19.03
    Fe        23.56 # Dissolved Iron
    Mn        4.54
    Alkalinity 144.26 as Ca.5(CO3).5 # Total Alkalinity calculated as mgCaCO3/L
    Cl        626
    N(-3)     0.076 # NH3 reported as N
    N(+3)     0.015 # Nitrite reported as N
    N(+5)     0.058 # Nitrate reported as N
    P         0.065 # Phosphate reported as P
    Si        70
    Al        0.00151
    Br        -
    B         0.0242
    Pb        0.00243
    Cu        0.0165
    Zn        0.0962
    water    1 # kg
SOLUTION 32 # (Gomes, 2012) Itaboraí/RJ - P-02A  (08/09) ago/09
    temp      25.78
    pe        1.113 # Calculated with eh-to-pe.xls file
    pH        7.2
    redox     pe
    units     mg/l
    density   1
    Ba        0.58
    Cd        0.00068
    Na        9.1
    K         5.9
    Ca        38.1
    Mg        3.72
    Fe        0.02 # Dissolved Iron
    Mn        0.02
    Alkalinity 149.18 as Ca.5(CO3).5 # Total Alkalinity calculated as mgCaCO3/L
    S(6)      4
    Cl        5.7
```

```
    F         0.4
    N(-3)     0.003 # NH3 reported as N
    N(+3)     0.005 # Nitrite reported as N
    N(+5)     0.054 # Nitrate reported as N
    P         0.055 # Phosphate reported as P
    Si        28.1
    Al        0.00508
    Br        -
    B         0.0222
    Pb        0.00187
    Cu        0.0726
    Zn        0.0985
    water    1 # kg
SOLUTION 33 # (Gomes, 2012) Itaboraí/RJ - P-02B  (08/09) ago/09
    temp      25.95
    pe        1.803 # Calculated with eh-to-pe.xls file
    pH        6
    redox     pe
    units     mg/l
    density   1
    Ba        0.08
    Cd        0.00079
    Na        4.2
    K         2.2
    Ca        5.2
    Mg        1.35
    Fe        0.02 # Dissolved Iron
    Mn        0.06
    Alkalinity 24.59 as Ca.5(CO3).5 # Total Alkalinity calculated as mgCaCO3/L
    S(6)      0
    Cl        6.8
    F         0.09
    N(-3)     0.007 # NH3 reported as N
    N(+3)     0.005 # Nitrite reported as N
    N(+5)     0.329 # Nitrate reported as N
    P         0.016 # Phosphate reported as P
    Si        9.4
    Al        0.01108
    Br        -
    B         0.0078
    Pb        0.0062
    Cu        0.01091
    Zn        0.0367
    water    1 # kg
SOLUTION 34 # (Gomes, 2012) Itaboraí/RJ - P-02C  (08/09) ago/09
    temp      26.24
    pe        1.481 # Calculated with eh-to-pe.xls file
    pH        6.7
    redox     pe
    units     mg/l
    density   1
    Ba        0.17
    Cd        0.00099
    Na        18.4
    K         5.2
    Ca        7.3
    Mg        2.08
    Fe        0.01 # Dissolved Iron
    Mn        0.29
    Alkalinity 65.57 as Ca.5(CO3).5 # Total Alkalinity calculated as mgCaCO3/L
    S(6)      0
    Cl        3.8
    F         0.37
    N(-3)     0.004 # NH3 reported as N
    N(+3)     0.004 # Nitrite reported as N
    N(+5)     0.044 # Nitrate reported as N
    P         0.059 # Phosphate reported as P
    Si        5.2
```

```
    Al        0.00818
    Br        -
    B         0.0105
    Pb        0.00576
    Cu        0.06238
    Zn        0.0765
    water    1 # kg
SOLUTION 35 # (Gomes, 2012) Itaboraí/RJ - P-03A  (08/09) ago/09
    temp      25.24
    pe        -2.01 # Calculated with eh-to-pe.xls file
    pH        8.8
    redox     pe
    units     mg/l
    density   1
    Ba        0.43
    Cd        0.00094
    Na        3.2
    K         1.6
    Ca        4.9
    Mg        0.79
    Fe        0.09 # Dissolved Iron
    Mn        0.3
    Alkalinity 268.85 as Ca.5(CO3).5 # Total Alkalinity calculated as mgCaCO3/L
    N(-3)     0.011 # NH3 reported as N
    N(+3)     0.004 # Nitrite reported as N
    N(+5)     0.021 # Nitrate reported as N
    P         0.127 # Phosphate reported as P
    Si        19.5
    Al        0.01562
    Br        -
    B         0.0266
    Pb        0.00166
    Cu        0.00088
    Zn        0.0199
    water    1 # kg
SOLUTION 36 # (Gomes, 2012) Itaboraí/RJ - P-03B  (08/09) ago/09
    temp      25.4
    pe        -0.422 # Calculated with eh-to-pe.xls file
    pH        8.6
    redox     pe
    units     mg/l
    density   1
    Ba        0.19
    Cd        0.00088
    Na        90.2
    K         1.1
    Ca        4.1
    Mg        0.88
    Fe        0.02 # Dissolved Iron
    Mn        0.59
    Alkalinity 196.72 as Ca.5(CO3).5 # Total Alkalinity calculated as mgCaCO3/L
    S(6)      5.2
    Cl        7.8
    F         1.82
    N(-3)     0.007 # NH3 reported as N
    N(+3)     0.006 # Nitrite reported as N
    N(+5)     0.061 # Nitrate reported as N
    P         0.095 # Phosphate reported as P
    Si        18.9
    Al        0.04564
    Br        -
    B         0.0141
    Pb        0.00167
    Cu        0.00211
    Zn        0.012
    water    1 # kg
SOLUTION 37 # (Gomes, 2012) Itaboraí/RJ - P-04A  (08/09) ago/09
    temp      25.56
```

```
    pe        -2.682 # Calculated with eh-to-pe.xls file
    pH        7.7
    redox     pe
    units     mg/l
    density   1
    Ba        0.26
    Cd        0.00069
    Na        33.6
    K         8
    Ca        16.1
    Mg        6.65
    Fe        1.52 # Dissolved Iron
    Mn        1.35
    Alkalinity 40.98 as Ca.5(CO3).5 # Total Alkalinity calculated as mgCaCO3/L
    S(6)      22.5
    Cl        122
    F         6.14
    N(-3)     0.049 # NH3 reported as N
    N(+3)     0.007 # Nitrite reported as N
    N(+5)     0.018 # Nitrate reported as N
    P         0.004 # Phosphate reported as P
    Si        37.5
    Al        0.00115
    Br        -
    B         0.0122
    Pb        0.00317
    Cu        0.00336
    Zn        0.0098
    water    1 # kg
SOLUTION 38 # (Gomes, 2012) Itaboraí/RJ - P-04B  (08/09) ago/09
    temp      25.6
    pe        -1.839 # Calculated with eh-to-pe.xls file
    pH        6.8
    redox     pe
    units     mg/l
    density   1
    Ba        0.22
    Cd        0.00068
    Na        97
    K         6
    Ca        19
    Mg        8
    Fe        0.02 # Dissolved Iron
    Mn        0.48
    Alkalinity 55.74 as Ca.5(CO3).5 # Total Alkalinity calculated as mgCaCO3/L
    S(6)      15
    Cl        158
    F         0.37
    N(-3)     0.009 # NH3 reported as N
    N(+3)     0.004 # Nitrite reported as N
    N(+5)     0.023 # Nitrate reported as N
    P         0.03 # Phosphate reported as P
    Si        22.5
    Al        0.0021
    Br        -
    B         0.0317
    Pb        0.00337
    Cu        0.00317
    Zn        0.0058
    water    1 # kg
SOLUTION 39 # (Gomes, 2012) Itaboraí/RJ - P-05  (08/09) ago/09
    units     mg/l
    density   1
    Ba        0.07
    Cd        0.00067
    Fe        0.35 # Dissolved Iron
    Mn        0.36
    F         0.65
```

```
    N(-3)     0.161 # NH3 reported as N
    N(+3)     0.014 # Nitrite reported as N
    N(+5)     0.014 # Nitrate reported as N
    P         0.048 # Phosphate reported as P
    Si        14.5
    Al        0.00803
    Br        -
    B         0.7341
    Pb        0.00233
    Cu        0.00474
    Zn        0.0119
    water    1 # kg
SOLUTION 40 # (Marcolan, 2009) Urânia/SP - PM-1  (PM1-BX-1) set/07
    temp      26.2
    pe        7.037 # Calculated with eh-to-pe.xls file
    pH        7.47
    redox     pe
    units     mg/l
    density   1
    O(0)      0.8
    Ba        0.419
    Na        8.4
    K         6.4
    Ca        44
    Mg        21
    Fe        0 # Dissolved Iron
    Mn        0
    Alkalinity 165.05 as Ca.5(CO3).5 # Total Alkalinity reported as mgCaCO3/L
    S(6)      0.27
    Cl        8.2
    F         0.28
    N(-3)     0 # NH3 reported as N
    N(+3)     0 # Nitrite reported as N
    N(+5)     40 # Nitrate reported as N
    P         0 # Phosphate reported as P
    Si        65.6
    Al        0
    Br        0
    Cu        0
    Sr        0.55
    Zn        0.01
    water    1 # kg
SOLUTION 41 # (Marcolan, 2009) Urânia/SP - PM-2  (PM-2-24h) set/07
    temp      26.9
    pe        6.483 # Calculated with eh-to-pe.xls file
    pH        9.17
    redox     pe
    units     mg/l
    density   1
    O(0)      3.3
    Ba        0.017
    Na        45
    K         3.6
    Ca        1.9
    Mg        0.2
    Fe        0.003 # Dissolved Iron
    Mn        0
    Alkalinity 97.91 as Ca.5(CO3).5 # Total Alkalinity reported as mgCaCO3/L
    S(6)      1.7
    Cl        1.2
    F         0.32
    N(-3)     0 # NH3 reported as N
    N(+3)     0 # Nitrite reported as N
    N(+5)     0.23 # Nitrate reported as N
    P         0.24 # Phosphate reported as P
    Si        17.5
    Al        0.05
    Br        0
```

```
    Cu        0
    Sr        0.09
    Zn        0.01
    water    1 # kg
SOLUTION 42 # (Marcolan, 2009) Urânia/SP - PM-3A  (PM3A-BX-2) set/07
    temp      30.5
    pe        8.149 # Calculated with eh-to-pe.xls file
    pH        6.33
    redox     pe
    units     mg/l
    density   1
    O(0)      4.2
    Ba        0.217
    Na        9.2
    K         4.3
    Ca        15
    Mg        5.7
    Fe        0 # Dissolved Iron
    Mn        0.02
    Alkalinity 65.19 as Ca.5(CO3).5 # Total Alkalinity reported as mgCaCO3/L
    S(6)      0.28
    Cl        3
    F         0.14
    N(-3)     0 # NH3 reported as N
    N(+3)     0 # Nitrite reported as N
    N(+5)     11 # Nitrate reported as N
    P         0.1 # Phosphate reported as P
    Si        26.3
    Al        0
    Br        0
    Cu        0
    Sr        0.12
    Zn        0.04
    water    1 # kg
SOLUTION 43 # (Marcolan, 2009) Urânia/SP - PM-3B  (PM3B-BX-2) set/07
    temp      30.4
    pe        7.653 # Calculated with eh-to-pe.xls file
    pH        7.77
    redox     pe
    units     mg/l
    density   1
    O(0)      2.4
    Ba        0.116
    Na        8.4
    K         4.3
    Ca        23
    Mg        13
    Fe        0 # Dissolved Iron
    Mn        0.01
    Alkalinity 121.69 as Ca.5(CO3).5 # Total Alkalinity reported as mgCaCO3/L
    S(6)      0.11
    Cl        0.25
    F         0.17
    N(-3)     0 # NH3 reported as N
    N(+3)     0 # Nitrite reported as N
    N(+5)     0.06 # Nitrate reported as N
    P         0.012 # Phosphate reported as P
    Si        62.6
    Al        0.01
    Br        0
    Cu        0
    Sr        0.83
    Zn        0.01
    water    1 # kg
SOLUTION 44 # (Marcolan, 2009) Urânia/SP - PM-3C  (PM3C-BX) set/07
    temp      28.1
    pe        4.349 # Calculated with eh-to-pe.xls file
    pH        11.13
```

```
          redox     pe
          units     mg/l
          density   1
          O(0)      1
          Ba        0.055
          Na        23
          K         10.7
          Ca        39
          Mg        0
          Fe        0 # Dissolved Iron
          Mn        0
          Alkalinity 139.88 as Ca.5(CO3).5 # Total Alkalinity reported as mgCaCO3/L (18.16
as HCO3-)
          C         74.84
          S(6)      14
          Cl        3.3
          F         0.44
          N(-3)     0 # NH3 reported as N
          N(+3)     0.23 # Nitrite reported as N
          N(+5)     0.25 # Nitrate reported as N
          P         0.05 # Phosphate reported as P
          Si        10.1
          Al        2.01
          Br        0
          Cu        0
          Sr        0.9
          Zn        0
          water    1 # kg
      PRINT
       alkalinity true
      SELECTED_OUTPUT
       file Monografia_PAP_phreeqc_PAP_lnll.txt
       reset true
       ph
       pe
       alkalinity
       charge_balance
       percent_error
       totals Ba Cd S(6) Cl
       molalities Ba+2 BaCO3 BaSO4 BaHCO3+ BaOH+ BaCl+ BaNO3+ Cd+2 CdHCO3+ CdCO3 CdCl+
CdSO4
       saturation_indices Barite Witherite BaCl2 BaCl2:2H2O BaCl2:H2O BaS Greenockite Cd
(OH)2 Otavite CdSO4
-------------------------------------------
Beginning of initial solution calculations.
-------------------------------------------

Initial solution 1.

-----------------------------Solution composition------------------------------

      Elements           Molality       Moles

      Alkalinity        3.601e-03   3.601e-03
      Ba                2.039e-06   2.039e-06
      Ca                1.575e-03   1.575e-03
      Cl                1.292e-04   1.292e-04
      F                 3.686e-06   3.686e-06
      K                 5.884e-05   5.884e-05
      Mg                6.649e-04   6.649e-04
      Mn                5.462e-07   5.462e-07
      N(3)              1.428e-06   1.428e-06
      N(5)              1.152e-03   1.152e-03
      Na                1.175e-04   1.175e-04
      P                 1.615e-06   1.615e-06
      S(6)              4.613e-05   4.613e-05
      Si                2.392e-04   2.392e-04
      Sr                6.051e-06   6.051e-06
```

----------Description of solution----------

pH	= 7.040
pe	= 4.883
Specific Conductance (µS/cm, 24°C)	= 449
Density (g/cm³)	= 0.99766
Volume (L)	= 1.00278
Activity of water	= 1.000
Ionic strength (mol/kgw)	= 6.946e-03
Mass of water (kg)	= 1.000e+00
Total carbon (mol/kg)	= 4.266e-03
Total CO2 (mol/kg)	= 4.266e-03
Temperature (°C)	= 23.80
Electrical balance (eq)	= -3.088e-04
Percent error, 100*(Cat-|An|)/(Cat+|An|)	= -3.26
Iterations	= 8
Total H	= 1.110170e+02
Total O	= 5.552295e+01

----------Redox couples----------

Redox couple	pe	Eh (volts)
N(3)/N(5)	8.7631	0.5163

----------Distribution of species----------

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma	mole V cm³/mol
OH-	1.106e-07	1.012e-07	-6.956	-6.995	-0.039	-4.10
H+	9.864e-08	9.120e-08	-7.006	-7.040	-0.034	0.00
H2O	5.551e+01	9.999e-01	1.744	-0.000	0.000	18.06
Ba	2.039e-06					
Ba+2	1.973e-06	1.391e-06	-5.705	-5.857	-0.152	-12.65
BaHCO3+	4.533e-08	4.152e-08	-7.344	-7.382	-0.038	(0)
BaSO4	1.880e-08	1.883e-08	-7.726	-7.725	0.001	(0)
BaCO3	1.136e-09	1.138e-09	-8.944	-8.944	0.001	-10.71
BaCl+	5.544e-10	5.079e-10	-9.256	-9.294	-0.038	(0)
BaNO3+	2.012e-10	1.843e-10	-9.696	-9.734	-0.038	(0)
BaOH+	5.631e-13	5.167e-13	-12.249	-12.287	-0.037	(0)
C(4)	4.266e-03					
HCO3-	3.521e-03	3.234e-03	-2.453	-2.490	-0.037	24.66
CO2	6.723e-04	6.734e-04	-3.172	-3.172	0.001	34.37
CaHCO3+	4.755e-05	4.373e-05	-4.323	-4.359	-0.036	9.67
MgHCO3+	1.886e-05	1.727e-05	-4.724	-4.763	-0.038	5.48
CaCO3	2.870e-06	2.875e-06	-5.542	-5.541	0.001	-14.60
CO3-2	2.280e-06	1.623e-06	-5.642	-5.790	-0.148	-5.17
MgCO3	6.962e-07	6.974e-07	-6.157	-6.157	0.001	-17.09
SrHCO3+	2.139e-07	1.964e-07	-6.670	-6.707	-0.037	(0)
NaHCO3	1.965e-07	1.968e-07	-6.707	-6.706	0.001	1.80
MnHCO3+	9.288e-08	8.523e-08	-7.032	-7.069	-0.037	(0)
BaHCO3+	4.533e-08	4.152e-08	-7.344	-7.382	-0.038	(0)
MnCO3	3.805e-08	3.811e-08	-7.420	-7.419	0.001	(0)
(CO2)2	7.984e-09	7.997e-09	-8.098	-8.097	0.001	68.75
SrCO3	4.130e-09	4.137e-09	-8.384	-8.383	0.001	-14.13
NaCO3-	3.336e-09	3.056e-09	-8.477	-8.515	-0.038	-1.06
BaCO3	1.136e-09	1.138e-09	-8.944	-8.944	0.001	-10.71
Ca	1.575e-03					
Ca+2	1.519e-03	1.080e-03	-2.819	-2.967	-0.148	-17.99
CaHCO3+	4.755e-05	4.373e-05	-4.323	-4.359	-0.036	9.67
CaSO4	5.133e-06	5.141e-06	-5.290	-5.289	0.001	7.45
CaCO3	2.870e-06	2.875e-06	-5.542	-5.541	0.001	-14.60
CaHPO4	2.320e-07	2.324e-07	-6.635	-6.634	0.001	(0)
CaH2PO4+	1.745e-08	1.603e-08	-7.758	-7.795	-0.037	(0)
CaPO4-	6.416e-09	5.893e-09	-8.193	-8.230	-0.037	(0)
CaOH+	2.145e-09	1.965e-09	-8.669	-8.707	-0.038	(0)

CaHSO4+	3.308e-12	3.030e-12	-11.480	-11.519	-0.038	(0)
Cl	1.292e-04					
Cl-	1.291e-04	1.182e-04	-3.889	-3.927	-0.038	18.09
NaCl	7.525e-08	7.537e-08	-7.123	-7.123	0.001	(0)
BaCl+	5.544e-10	5.079e-10	-9.256	-9.294	-0.038	(0)
MnCl+	1.552e-10	1.424e-10	-9.809	-9.846	-0.037	-3.35
MnCl2	7.336e-15	7.348e-15	-14.135	-14.134	0.001	87.38
MnCl3-	2.607e-19	2.392e-19	-18.584	-18.621	-0.037	43.46
F	3.686e-06					
F-	3.579e-06	3.274e-06	-5.446	-5.485	-0.039	-1.28
MgF+	1.059e-07	9.709e-08	-6.975	-7.013	-0.038	-10.53
HF	4.375e-10	4.382e-10	-9.359	-9.358	0.001	12.45
NaF	2.021e-10	2.025e-10	-9.694	-9.694	0.001	7.22
MnF+	7.299e-12	6.698e-12	-11.137	-11.174	-0.037	(0)
HF2-	5.953e-15	5.453e-15	-14.225	-14.263	-0.038	22.05
SiF6-2	4.862e-35	3.448e-35	-34.313	-34.462	-0.149	42.69
H(0)	2.040e-27					
H2	1.020e-27	1.021e-27	-26.991	-26.991	0.001	28.61
K	5.884e-05					
K+	5.883e-05	5.382e-05	-4.230	-4.269	-0.039	9.01
KSO4-	1.089e-08	1.000e-08	-7.963	-8.000	-0.037	34.12
KHPO4-	4.587e-11	4.213e-11	-10.338	-10.375	-0.037	38.25
Mg	6.649e-04					
Mg+2	6.423e-04	4.588e-04	-3.192	-3.338	-0.146	-21.62
MgHCO3+	1.886e-05	1.727e-05	-4.724	-4.763	-0.038	5.48
MgSO4	2.812e-06	2.816e-06	-5.551	-5.550	0.001	5.79
MgCO3	6.962e-07	6.974e-07	-6.157	-6.157	0.001	-17.09
MgHPO4	1.333e-07	1.335e-07	-6.875	-6.875	0.001	(0)
MgF+	1.059e-07	9.709e-08	-6.975	-7.013	-0.038	-10.53
MgOH+	1.780e-08	1.638e-08	-7.750	-7.786	-0.036	(0)
MgH2PO4+	9.441e-09	8.671e-09	-8.025	-8.062	-0.037	(0)
MgPO4-	3.677e-09	3.377e-09	-8.434	-8.471	-0.037	(0)
Mn(2)	5.462e-07					
Mn+2	4.137e-07	2.957e-07	-6.383	-6.529	-0.146	-20.09
MnHCO3+	9.288e-08	8.523e-08	-7.032	-7.069	-0.037	(0)
MnCO3	3.805e-08	3.811e-08	-7.420	-7.419	0.001	(0)
MnSO4	1.386e-09	1.388e-09	-8.858	-8.858	0.001	23.08
MnCl+	1.552e-10	1.424e-10	-9.809	-9.846	-0.037	-3.35
MnOH+	8.232e-11	7.554e-11	-10.084	-10.122	-0.037	(0)
MnF+	7.299e-12	6.698e-12	-11.137	-11.174	-0.037	(0)
Mn(NO3)2	1.306e-12	1.308e-12	-11.884	-11.883	0.001	41.36
MnCl2	7.336e-15	7.348e-15	-14.135	-14.134	0.001	87.38
MnCl3-	2.607e-19	2.392e-19	-18.584	-18.621	-0.037	43.46
Mn(OH)3-	6.730e-21	6.176e-21	-20.172	-20.209	-0.037	(0)
Mn(3)	1.185e-27					
Mn+3	1.185e-27	5.854e-28	-26.926	-27.233	-0.306	(0)
N(3)	1.428e-06					
NO2-	1.428e-06	1.305e-06	-5.845	-5.884	-0.039	24.95
N(5)	1.152e-03					
NO3-	1.152e-03	1.053e-03	-2.939	-2.978	-0.039	29.42
BaNO3+	2.012e-10	1.843e-10	-9.696	-9.734	-0.038	(0)
Mn(NO3)2	1.306e-12	1.308e-12	-11.884	-11.883	0.001	41.36
Na	1.175e-04					
Na+	1.172e-04	1.075e-04	-3.931	-3.969	-0.038	-1.47
NaHCO3	1.965e-07	1.968e-07	-6.707	-6.706	0.001	1.80
NaCl	7.525e-08	7.537e-08	-7.123	-7.123	0.001	(0)
NaSO4-	1.572e-08	1.444e-08	-7.803	-7.840	-0.037	14.21
NaCO3-	3.336e-09	3.056e-09	-8.477	-8.515	-0.038	-1.06
NaF	2.021e-10	2.025e-10	-9.694	-9.694	0.001	7.22
NaHPO4-	9.159e-11	8.411e-11	-10.038	-10.075	-0.037	33.98
NaOH	1.086e-21	1.088e-21	-20.964	-20.963	0.001	(0)
O(0)	3.258e-39					
O2	1.629e-39	1.632e-39	-38.788	-38.787	0.001	30.31
P	1.615e-06					
H2PO4-	6.463e-07	5.936e-07	-6.190	-6.226	-0.037	33.29
HPO4-2	5.660e-07	4.014e-07	-6.247	-6.396	-0.149	6.94
CaHPO4	2.320e-07	2.324e-07	-6.635	-6.634	0.001	(0)
MgHPO4	1.333e-07	1.335e-07	-6.875	-6.875	0.001	(0)

CaH2PO4+	1.745e-08	1.603e-08	-7.758	-7.795	-0.037	(0)
MgH2PO4+	9.441e-09	8.671e-09	-8.025	-8.062	-0.037	(0)
CaPO4-	6.416e-09	5.893e-09	-8.193	-8.230	-0.037	(0)
MgPO4-	3.677e-09	3.377e-09	-8.434	-8.471	-0.037	(0)
NaHPO4-	9.159e-11	8.411e-11	-10.038	-10.075	-0.037	33.98
KHPO4-	4.587e-11	4.213e-11	-10.338	-10.375	-0.037	38.25
H3PO4	7.845e-12	7.857e-12	-11.105	-11.105	0.001	47.34
PO4-3	4.278e-12	1.937e-12	-11.369	-11.713	-0.344	-22.71
S(6)	4.613e-05					
SO4-2	3.812e-05	2.701e-05	-4.419	-4.568	-0.150	14.55
CaSO4	5.133e-06	5.141e-06	-5.290	-5.289	0.001	7.45
MgSO4	2.812e-06	2.816e-06	-5.551	-5.550	0.001	5.79
SrSO4	2.145e-08	2.149e-08	-7.669	-7.668	0.001	24.19
BaSO4	1.880e-08	1.883e-08	-7.726	-7.725	0.001	(0)
NaSO4-	1.572e-08	1.444e-08	-7.803	-7.840	-0.037	14.21
KSO4-	1.089e-08	1.000e-08	-7.963	-8.000	-0.037	34.12
MnSO4	1.386e-09	1.388e-09	-8.858	-8.858	0.001	23.08
HSO4-	2.548e-10	2.334e-10	-9.594	-9.632	-0.038	40.24
CaHSO4+	3.308e-12	3.030e-12	-11.480	-11.519	-0.038	(0)
Si	2.392e-04					
H4SiO4	2.388e-04	2.392e-04	-3.622	-3.621	0.001	52.18
H3SiO4-	4.049e-07	3.708e-07	-6.393	-6.431	-0.038	27.99
H2SiO4-2	3.593e-13	2.556e-13	-12.445	-12.592	-0.148	(0)
SiF6-2	4.862e-35	3.448e-35	-34.313	-34.462	-0.149	42.69
Sr	6.051e-06					
Sr+2	5.811e-06	4.138e-06	-5.236	-5.383	-0.147	-17.60
SrHCO3+	2.139e-07	1.964e-07	-6.670	-6.707	-0.037	(0)
SrSO4	2.145e-08	2.149e-08	-7.669	-7.668	0.001	24.19
SrCO3	4.130e-09	4.137e-09	-8.384	-8.383	0.001	-14.13
SrOH+	2.535e-12	2.327e-12	-11.596	-11.633	-0.037	(0)

----------Distribution of alkalinity----------

Total alkalinity (eq/kgw) = 3.601e-03

Species	Alkalinity	Molality	Alk/Mol
HCO3-	3.521e-03	3.521e-03	1.00
CaHCO3+	4.755e-05	4.755e-05	1.00
MgHCO3+	1.886e-05	1.886e-05	1.00
CaCO3	5.740e-06	2.870e-06	2.00
CO3-2	4.561e-06	2.280e-06	2.00
MgCO3	1.392e-06	6.962e-07	2.00
HPO4-2	5.660e-07	5.660e-07	1.00
H3SiO4-	4.049e-07	4.049e-07	1.00
CaHPO4	2.320e-07	2.320e-07	1.00
SrHCO3+	2.139e-07	2.139e-07	1.00
NaHCO3	1.965e-07	1.965e-07	1.00
MgHPO4	1.333e-07	1.333e-07	1.00
OH-	1.106e-07	1.106e-07	1.00
H+	-9.864e-08	9.864e-08	-1.00
MnHCO3+	9.288e-08	9.288e-08	1.00
MnCO3	7.611e-08	3.805e-08	2.00
BaHCO3+	4.533e-08	4.533e-08	1.00
MgOH+	1.780e-08	1.780e-08	1.00
CaPO4-	1.283e-08	6.416e-09	2.00
SrCO3	8.260e-09	4.130e-09	2.00
MgPO4-	7.354e-09	3.677e-09	2.00
NaCO3-	6.671e-09	3.336e-09	2.00
BaCO3	2.273e-09	1.136e-09	2.00
CaOH+	2.145e-09	2.145e-09	1.00
HF	-4.375e-10	4.375e-10	-1.00
HSO4-	-2.548e-10	2.548e-10	-1.00
NaHPO4-	9.159e-11	9.159e-11	1.00
MnOH+	8.232e-11	8.232e-11	1.00
KHPO4-	4.587e-11	4.587e-11	1.00
PO4-3	8.556e-12	4.278e-12	2.00
H3PO4	-7.845e-12	7.845e-12	-1.00

CaHSO4+	-3.308e-12	3.308e-12	-1.00
SrOH+	2.535e-12	2.535e-12	1.00
H2SiO4-2	7.186e-13	3.593e-13	2.00
BaOH+	5.631e-13	5.631e-13	1.00
HF2-	-5.953e-15	5.953e-15	-1.00
Mn(OH)3-	2.019e-20	6.730e-21	3.00
NaOH	1.086e-21	1.086e-21	1.00
SiF6-2	-1.945e-34	4.862e-35	-4.00

----------Saturation indices----------

Phase	SI**	log IAP	log K(296 K, 1 atm)	
Anhydrite	-3.27	-7.54	-4.26	CaSO4
Aragonite	-0.43	-8.76	-8.33	CaCO3
BaCl2	-15.95	-13.71	2.24	BaCl2
BaCl2:2H2O	-13.91	-13.71	0.20	BaCl2:2H2O
BaCl2:H2O	-14.53	-13.71	0.82	BaCl2:H2O
Barite	-0.57	-10.43	-9.86	BaSO4
Calcite	-0.28	-8.76	-8.47	CaCO3
Celestite	-3.30	-9.95	-6.65	SrSO4
Chalcedony	-0.06	-3.62	-3.57	SiO2
Chrysotile	-7.37	24.98	32.35	Mg3Si2O5(OH)4
CO2(g)	-1.72	-3.17	-1.45	CO2
Dolomite	-0.82	-17.88	-17.06	CaMg(CO3)2
Fluorite	-3.32	-13.94	-10.61	CaF2
Gypsum	-2.95	-7.54	-4.58	CaSO4:2H2O
H2(g)	-23.89	-26.99	-3.10	H2
H2O(g)	-1.53	-0.00	1.53	H2O
Halite	-9.47	-7.90	1.57	NaCl
Hausmannite	-14.83	46.50	61.33	Mn3O4
Hydroxyapatite	-2.55	-5.86	-3.31	Ca5(PO4)3OH
Manganite	-5.87	19.47	25.34	MnOOH
O2(g)	-35.90	-38.79	-2.88	O2
Pyrochroite	-7.65	7.55	15.20	Mn(OH)2
Pyrolusite	-10.18	31.40	41.57	MnO2:H2O
Quartz	0.38	-3.62	-4.00	SiO2
Rhodochrosite	-1.19	-12.32	-11.13	MnCO3
Sepiolite	-5.17	10.62	15.79	Mg2Si3O7.5OH:3H2O
Sepiolite(d)	-8.04	10.62	18.66	Mg2Si3O7.5OH:3H2O
SiO2(a)	-0.90	-3.62	-2.72	SiO2
Strontianite	-1.90	-11.17	-9.27	SrCO3
Sylvite	-9.09	-8.20	0.89	KCl
Talc	-3.80	17.74	21.54	Mg3Si4O10(OH)2
Witherite	-3.08	-11.65	-8.56	BaCO3

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
For ideal gases, phi = 1.

Initial solution 2.

----------Solution composition----------

Elements	Molality	Moles
Alkalinity	2.631e-03	2.631e-03
Ba	1.122e-05	1.122e-05
Ca	5.261e-04	5.261e-04
Cl	8.040e-05	8.040e-05
F	4.212e-06	4.212e-06
K	1.458e-04	1.458e-04
Mg	7.603e-04	7.603e-04
Mn	5.462e-07	5.462e-07
N(3)	6.427e-07	6.427e-07
N(5)	8.926e-05	8.926e-05
Na	2.045e-04	2.045e-04
P	1.292e-06	1.292e-06
S(6)	1.343e-05	1.343e-05

Si	1.928e-04	1.928e-04
Sr	6.621e-06	6.621e-06

----------Description of solution----------

pH	= 8.860
pe	= 4.473
Specific Conductance (µS/cm, 27°C)	= 269
Density (g/cm³)	= 0.99669
Volume (L)	= 1.00355
Activity of water	= 1.000
Ionic strength (mol/kgw)	= 3.990e-03
Mass of water (kg)	= 1.000e+00
Total carbon (mol/kg)	= 2.422e-03
Total CO2 (mol/kg)	= 2.422e-03
Temperature (°C)	= 27.00
Electrical balance (eq)	= 1.257e-04
Percent error, 100*(Cat-|An|)/(Cat+|An|)	= 2.33
Iterations	= 7 (15 overall)
Total H	= 1.110154e+02
Total O	= 5.551459e+01

----------Redox couples----------

Redox couple	pe	Eh (volts)
N(3)/N(5)	6.3895	0.3805

----------Distribution of species----------

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma	mole V cm³/mol
OH-	9.140e-06	8.527e-06	-5.039	-5.069	-0.030	-4.00
H+	1.470e-09	1.380e-09	-8.833	-8.860	-0.027	0.00
H2O	5.551e+01	9.999e-01	1.744	-0.000	0.000	18.08
Ba	1.122e-05					
Ba+2	1.067e-05	8.120e-06	-4.972	-5.090	-0.119	-12.54
BaCO3	3.186e-07	3.189e-07	-6.497	-6.496	0.000	-10.68
BaHCO3+	1.835e-07	1.713e-07	-6.736	-6.766	-0.030	(0)
BaSO4	3.605e-08	3.608e-08	-7.443	-7.443	0.000	(0)
BaCl+	2.113e-09	1.973e-09	-8.675	-8.705	-0.030	(0)
BaOH+	2.132e-10	1.993e-10	-9.671	-9.700	-0.029	(0)
BaNO3+	9.112e-11	8.507e-11	-10.040	-10.070	-0.030	(0)
C(4)	2.422e-03					
HCO3-	2.210e-03	2.067e-03	-2.656	-2.685	-0.029	24.86
CO3-2	9.545e-05	7.303e-05	-4.020	-4.137	-0.116	-5.02
CaCO3	4.582e-05	4.586e-05	-4.339	-4.339	0.000	-14.59
MgCO3	3.875e-05	3.878e-05	-4.412	-4.411	0.000	-17.09
MgHCO3+	1.411e-05	1.317e-05	-4.850	-4.880	-0.030	5.55
CaHCO3+	1.040e-05	9.737e-06	-4.983	-5.012	-0.029	9.77
CO2	6.260e-06	6.266e-06	-5.203	-5.203	0.000	34.53
MnCO3	4.324e-07	4.328e-07	-6.364	-6.364	0.000	(0)
BaCO3	3.186e-07	3.189e-07	-6.497	-6.496	0.000	-10.68
NaCO3-	3.067e-07	2.863e-07	-6.513	-6.543	-0.030	-0.82
SrCO3	2.347e-07	2.349e-07	-6.630	-6.629	0.000	-14.12
NaHCO3	2.187e-07	2.189e-07	-6.660	-6.660	0.000	1.80
BaHCO3+	1.835e-07	1.713e-07	-6.736	-6.766	-0.030	(0)
SrHCO3+	1.719e-07	1.608e-07	-6.765	-6.794	-0.029	(0)
MnHCO3+	1.470e-08	1.374e-08	-7.833	-7.862	-0.029	(0)
(CO2)2	7.685e-13	7.692e-13	-12.114	-12.114	0.000	69.06
Ca	5.261e-04					
Ca+2	4.690e-04	3.586e-04	-3.329	-3.445	-0.116	-18.02
CaCO3	4.582e-05	4.586e-05	-4.339	-4.339	0.000	-14.59
CaHCO3+	1.040e-05	9.737e-06	-4.983	-5.012	-0.029	9.77
CaSO4	5.734e-07	5.739e-07	-6.242	-6.241	0.000	7.57
CaPO4-	1.602e-07	1.498e-07	-6.795	-6.824	-0.029	(0)
CaHPO4	8.413e-08	8.421e-08	-7.075	-7.075	0.000	(0)

CaOH+	4.618e-08	4.311e-08	-7.336	-7.365	-0.030	(0)
CaH2PO4+	9.248e-11	8.650e-11	-10.034	-10.063	-0.029	(0)
CaHSO4+	5.742e-15	5.361e-15	-14.241	-14.271	-0.030	(0)
Cl	8.040e-05					
Cl-	8.032e-05	7.496e-05	-4.095	-4.125	-0.030	18.16
NaCl	8.656e-08	8.664e-08	-7.063	-7.062	0.000	(0)
BaCl+	2.113e-09	1.973e-09	-8.675	-8.705	-0.030	(0)
MnCl+	2.437e-11	2.278e-11	-10.613	-10.642	-0.029	-2.60
MnCl2	7.447e-16	7.454e-16	-15.128	-15.128	0.000	83.51
MnCl3-	1.646e-20	1.539e-20	-19.784	-19.813	-0.029	43.31
F	4.212e-06					
F-	4.061e-06	3.789e-06	-5.391	-5.421	-0.030	-1.27
MgF+	1.499e-07	1.401e-07	-6.824	-6.854	-0.030	-10.55
NaF	4.149e-10	4.153e-10	-9.382	-9.382	0.000	7.33
HF	8.125e-12	8.133e-12	-11.090	-11.090	0.000	12.59
MnF+	2.092e-12	1.956e-12	-11.679	-11.709	-0.029	(0)
HF2-	1.286e-16	1.200e-16	-15.891	-15.921	-0.030	22.18
SiF6-2	0.000e+00	0.000e+00	-41.516	-41.633	-0.117	42.80
H(0)	2.993e-30					
H2	1.496e-30	1.498e-30	-29.825	-29.825	0.000	28.60
K	1.458e-04					
K+	1.458e-04	1.360e-04	-3.836	-3.866	-0.030	9.10
KSO4-	9.381e-09	8.773e-09	-8.028	-8.057	-0.029	34.18
KHPO4-	1.170e-10	1.095e-10	-9.932	-9.961	-0.029	38.01
Mg	7.603e-04					
Mg+2	7.038e-04	5.397e-04	-3.153	-3.268	-0.115	-21.79
MgCO3	3.875e-05	3.878e-05	-4.412	-4.411	0.000	-17.09
MgHCO3+	1.411e-05	1.317e-05	-4.850	-4.880	-0.030	5.55
MgOH+	1.814e-06	1.698e-06	-5.741	-5.770	-0.028	(0)
MgSO4	1.180e-06	1.181e-06	-5.928	-5.928	0.000	5.91
MgPO4-	3.252e-07	3.042e-07	-6.488	-6.517	-0.029	(0)
MgHPO4	1.712e-07	1.713e-07	-6.767	-6.766	0.000	(0)
MgF+	1.499e-07	1.401e-07	-6.824	-6.854	-0.030	-10.55
MgH2PO4+	1.772e-10	1.658e-10	-9.751	-9.780	-0.029	(0)
Mn(2)	5.462e-07					
MnCO3	4.324e-07	4.328e-07	-6.364	-6.364	0.000	(0)
Mn+2	9.722e-08	7.460e-08	-7.012	-7.127	-0.115	-20.34
MnHCO3+	1.470e-08	1.374e-08	-7.833	-7.862	-0.029	(0)
MnOH+	1.747e-09	1.633e-09	-8.758	-8.787	-0.029	(0)
MnSO4	1.221e-10	1.222e-10	-9.913	-9.913	0.000	21.68
MnCl+	2.437e-11	2.278e-11	-10.613	-10.642	-0.029	-2.60
MnF+	2.092e-12	1.956e-12	-11.679	-11.709	-0.029	(0)
Mn(NO3)2	2.046e-15	2.048e-15	-14.689	-14.689	0.000	40.52
MnCl2	7.447e-16	7.454e-16	-15.128	-15.128	0.000	83.51
Mn(OH)3-	4.808e-16	4.494e-16	-15.318	-15.347	-0.029	(0)
MnCl3-	1.646e-20	1.539e-20	-19.784	-19.813	-0.029	43.31
Mn(3)	1.610e-28					
Mn+3	1.610e-28	9.157e-29	-27.793	-28.038	-0.245	(0)
N(3)	6.427e-07					
NO2-	6.427e-07	5.992e-07	-6.192	-6.222	-0.030	25.09
N(5)	8.926e-05					
NO3-	8.926e-05	8.322e-05	-4.049	-4.080	-0.030	29.70
BaNO3+	9.112e-11	8.507e-11	-10.040	-10.070	-0.030	(0)
Mn(NO3)2	2.046e-15	2.048e-15	-14.689	-14.689	0.000	40.52
Na	2.045e-04					
Na+	2.039e-04	1.905e-04	-3.691	-3.720	-0.029	-1.33
NaCO3-	3.067e-07	2.863e-07	-6.513	-6.543	-0.030	-0.82
NaHCO3	2.187e-07	2.189e-07	-6.660	-6.660	0.000	1.80
NaCl	8.656e-08	8.664e-08	-7.063	-7.062	0.000	(0)
NaSO4-	9.164e-09	8.571e-09	-8.038	-8.067	-0.029	13.94
NaF	4.149e-10	4.153e-10	-9.382	-9.382	0.000	7.33
NaHPO4-	1.639e-10	1.533e-10	-9.786	-9.815	-0.029	33.68
NaOH	1.623e-19	1.624e-19	-18.790	-18.789	0.000	(0)
O(0)	1.625e-32					
O2	8.126e-33	8.133e-33	-32.090	-32.090	0.000	30.55
P	1.292e-06					
HPO4-2	5.404e-07	4.126e-07	-6.267	-6.384	-0.117	6.76
MgPO4-	3.252e-07	3.042e-07	-6.488	-6.517	-0.029	(0)

MgHPO4	1.712e-07	1.713e-07	-6.767	-6.766	0.000	(0)
CaPO4-	1.602e-07	1.498e-07	-6.795	-6.824	-0.029	(0)
CaHPO4	8.413e-08	8.421e-08	-7.075	-7.075	0.000	(0)
H2PO4-	9.701e-09	9.073e-09	-8.013	-8.042	-0.029	33.19
PO4-3	2.603e-10	1.402e-10	-9.585	-9.853	-0.269	-23.15
MgH2PO4+	1.772e-10	1.658e-10	-9.751	-9.780	-0.029	(0)
NaHPO4-	1.639e-10	1.533e-10	-9.786	-9.815	-0.029	33.68
KHPO4-	1.170e-10	1.095e-10	-9.932	-9.961	-0.029	38.01
CaH2PO4+	9.248e-11	8.650e-11	-10.034	-10.063	-0.029	(0)
H3PO4	1.886e-15	1.888e-15	-14.724	-14.724	0.000	47.51
S(6)	1.343e-05					
SO4-2	1.162e-05	8.866e-06	-4.935	-5.052	-0.117	14.87
MgSO4	1.180e-06	1.181e-06	-5.928	-5.928	0.000	5.91
CaSO4	5.734e-07	5.739e-07	-6.242	-6.241	0.000	7.57
BaSO4	3.605e-08	3.608e-08	-7.443	-7.443	0.000	(0)
KSO4-	9.381e-09	8.773e-09	-8.028	-8.057	-0.029	34.18
NaSO4-	9.164e-09	8.571e-09	-8.038	-8.067	-0.029	13.94
SrSO4	8.398e-09	8.405e-09	-8.076	-8.075	0.000	24.31
MnSO4	1.221e-10	1.222e-10	-9.913	-9.913	0.000	21.68
HSO4-	1.332e-12	1.243e-12	-11.876	-11.905	-0.030	40.43
CaHSO4+	5.742e-15	5.361e-15	-14.241	-14.271	-0.030	(0)
Si	1.928e-04					
H4SiO4	1.717e-04	1.719e-04	-3.765	-3.765	0.000	51.91
H3SiO4-	2.106e-05	1.966e-05	-4.677	-4.706	-0.030	28.05
H2SiO4-2	1.440e-09	1.102e-09	-8.842	-8.958	-0.116	(0)
SiF6-2	0.000e+00	0.000e+00	-41.516	-41.633	-0.117	42.80
Sr	6.621e-06					
Sr+2	6.206e-06	4.750e-06	-5.207	-5.323	-0.116	-17.73
SrCO3	2.347e-07	2.349e-07	-6.630	-6.629	0.000	-14.12
SrHCO3+	1.719e-07	1.608e-07	-6.765	-6.794	-0.029	(0)
SrSO4	8.398e-09	8.405e-09	-8.076	-8.075	0.000	24.31
SrOH+	1.888e-10	1.765e-10	-9.724	-9.753	-0.029	(0)

----------Distribution of alkalinity----------

Total alkalinity (eq/kgw) = 2.631e-03

Species	Alkalinity	Molality	Alk/Mol
HCO3-	2.210e-03	2.210e-03	1.00
CO3-2	1.909e-04	9.545e-05	2.00
CaCO3	9.164e-05	4.582e-05	2.00
MgCO3	7.750e-05	3.875e-05	2.00
H3SiO4-	2.106e-05	2.106e-05	1.00
MgHCO3+	1.411e-05	1.411e-05	1.00
CaHCO3+	1.040e-05	1.040e-05	1.00
OH-	9.140e-06	9.140e-06	1.00
MgOH+	1.814e-06	1.814e-06	1.00
MnCO3	8.647e-07	4.324e-07	2.00
MgPO4-	6.505e-07	3.252e-07	2.00
BaCO3	6.372e-07	3.186e-07	2.00
NaCO3-	6.133e-07	3.067e-07	2.00
HPO4-2	5.404e-07	5.404e-07	1.00
SrCO3	4.694e-07	2.347e-07	2.00
CaPO4-	3.204e-07	1.602e-07	2.00
NaHCO3	2.187e-07	2.187e-07	1.00
BaHCO3+	1.835e-07	1.835e-07	1.00
SrHCO3+	1.719e-07	1.719e-07	1.00
MgHPO4	1.712e-07	1.712e-07	1.00
CaHPO4	8.413e-08	8.413e-08	1.00
CaOH+	4.618e-08	4.618e-08	1.00
MnHCO3+	1.470e-08	1.470e-08	1.00
H2SiO4-2	2.881e-09	1.440e-09	2.00
MnOH+	1.747e-09	1.747e-09	1.00
H+	-1.470e-09	1.470e-09	-1.00
PO4-3	5.206e-10	2.603e-10	2.00
BaOH+	2.132e-10	2.132e-10	1.00
SrOH+	1.888e-10	1.888e-10	1.00

NaHPO4-	1.639e-10	1.639e-10	1.00
KHPO4-	1.170e-10	1.170e-10	1.00
HF	-8.125e-12	8.125e-12	-1.00
HSO4-	-1.332e-12	1.332e-12	-1.00
CaHSO4+	-5.742e-15	5.742e-15	-1.00
H3PO4	-1.886e-15	1.886e-15	-1.00
Mn(OH)3-	1.442e-15	4.808e-16	3.00
HF2-	-1.286e-16	1.286e-16	-1.00
NaOH	1.623e-19	1.623e-19	1.00
SiF6-2	-0.000e+00	0.000e+00	-4.00

----------Saturation indices----------

Phase	SI**	log IAP	log K(300 K, 1 atm)	
Anhydrite	-4.20	-8.50	-4.30	CaSO4
Aragonite	0.77	-7.58	-8.35	CaCO3
BaCl2	-15.55	-13.34	2.21	BaCl2
BaCl2:2H2O	-13.57	-13.34	0.23	BaCl2:2H2O
BaCl2:H2O	-14.17	-13.34	0.83	BaCl2:H2O
Barite	-0.32	-10.14	-9.83	BaSO4
Calcite	0.91	-7.58	-8.49	CaCO3
Celestite	-3.71	-10.38	-6.67	SrSO4
Chalcedony	-0.24	-3.76	-3.53	SiO2
Chrysotile	3.87	35.83	31.95	Mg3Si2O5(OH)4
CO2(g)	-3.71	-5.20	-1.49	CO2
Dolomite	2.15	-14.99	-17.14	CaMg(CO3)2
Fluorite	-3.71	-14.29	-10.58	CaF2
Gypsum	-3.92	-8.50	-4.58	CaSO4:2H2O
H2(g)	-26.72	-29.82	-3.11	H2
H2O(g)	-1.45	-0.00	1.45	H2O
Halite	-9.42	-7.85	1.57	NaCl
Hausmannite	-2.09	58.44	60.54	Mn3O4
Hydroxyapatite	2.66	-0.94	-3.60	Ca5(PO4)3OH
Manganite	-1.41	23.93	25.34	MnOOH
O2(g)	-29.18	-32.09	-2.91	O2
Pyrochroite	-4.61	10.59	15.20	Mn(OH)2
Pyrolusite	-3.80	37.26	41.06	MnO2:H2O
Quartz	0.19	-3.76	-3.95	SiO2
Rhodochrosite	-0.13	-11.26	-11.14	MnCO3
Sepiolite	1.90	17.61	15.71	Mg2Si3O7.5OH:3H2O
Sepiolite(d)	-1.05	17.61	18.66	Mg2Si3O7.5OH:3H2O
SiO2(a)	-1.07	-3.76	-2.70	SiO2
Strontianite	-0.19	-9.46	-9.27	SrCO3
Sylvite	-8.90	-7.99	0.91	KCl
Talc	7.12	28.30	21.17	Mg3Si4O10(OH)2
Witherite	-0.67	-9.23	-8.56	BaCO3

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
For ideal gases, phi = 1.

Initial solution 3.

----------Solution composition----------

Elements	Molality	Moles
Alkalinity	1.729e-03	1.729e-03
Ba	2.476e-06	2.476e-06
Ca	1.852e-04	1.852e-04
Cl	3.794e-04	3.794e-04
F	6.317e-06	6.317e-06
K	4.297e-04	4.297e-04
Mg	2.999e-04	2.999e-04
Mn	5.462e-07	5.462e-07
N(3)	1.428e-06	1.428e-06
N(5)	5.691e-04	5.691e-04
Na	9.397e-04	9.397e-04

P	1.937e-06	1.937e-06
S(6)	8.100e-05	8.100e-05
Si	8.773e-05	8.773e-05
Sr	1.667e-05	1.667e-05

----------Description of solution----------

pH	= 9.370
pe	= 6.553
Specific Conductance (µS/cm, 24°C)	= 270
Density (g/cm³)	= 0.99743
Volume (L)	= 1.00279
Activity of water	= 1.000
Ionic strength (mol/kgw)	= 3.165e-03
Mass of water (kg)	= 1.000e+00
Total carbon (mol/kg)	= 1.464e-03
Total CO2 (mol/kg)	= 1.464e-03
Temperature (°C)	= 24.10
Electrical balance (eq)	= -4.704e-04
Percent error, 100*(Cat-|An|)/(Cat+|An|)	= -9.46
Iterations	= 7 (22 overall)
Total H	= 1.110140e+02
Total O	= 5.551303e+01

----------Redox couples----------

Redox couple	pe	Eh (volts)
N(3)/N(5)	6.2638	0.3694

----------Distribution of species----------

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma	mole V cm³/mol
OH-	2.356e-05	2.214e-05	-4.628	-4.655	-0.027	-4.12
H+	4.514e-10	4.266e-10	-9.345	-9.370	-0.025	0.00
H2O	5.551e+01	9.999e-01	1.744	-0.000	0.000	18.07
Ba	2.476e-06					
Ba+2	2.285e-06	1.789e-06	-5.641	-5.747	-0.106	-12.72
BaCO3	1.146e-07	1.147e-07	-6.941	-6.941	0.000	-10.71
BaSO4	5.359e-08	5.363e-08	-7.271	-7.271	0.000	(0)
BaHCO3+	2.074e-08	1.951e-08	-7.683	-7.710	-0.027	(0)
BaCl+	2.095e-09	1.971e-09	-8.679	-8.705	-0.027	(0)
BaOH+	1.509e-10	1.421e-10	-9.821	-9.847	-0.026	(0)
BaNO3+	1.280e-10	1.204e-10	-9.893	-9.919	-0.027	(0)
C(4)	1.464e-03					
HCO3-	1.243e-03	1.170e-03	-2.906	-2.932	-0.026	24.65
CO3-2	1.606e-04	1.263e-04	-3.794	-3.899	-0.104	-5.25
CaCO3	2.556e-05	2.558e-05	-4.592	-4.592	0.000	-14.60
MgCO3	2.495e-05	2.497e-05	-4.603	-4.603	0.000	-17.09
MgHCO3+	3.046e-06	2.865e-06	-5.516	-5.543	-0.027	5.47
NaCO3-	2.102e-06	1.977e-06	-5.677	-5.704	-0.027	-1.08
CaHCO3+	1.917e-06	1.806e-06	-5.717	-5.743	-0.026	9.66
CO2	1.134e-06	1.135e-06	-5.945	-5.945	0.000	34.39
SrCO3	9.481e-07	9.488e-07	-6.023	-6.023	0.000	-14.13
NaHCO3	5.815e-07	5.820e-07	-6.235	-6.235	0.000	1.80
MnCO3	4.771e-07	4.775e-07	-6.321	-6.321	0.000	(0)
SrHCO3+	2.227e-07	2.097e-07	-6.652	-6.678	-0.026	(0)
BaCO3	1.146e-07	1.147e-07	-6.941	-6.941	0.000	-10.71
BaHCO3+	2.074e-08	1.951e-08	-7.683	-7.710	-0.027	(0)
MnHCO3+	5.273e-09	4.964e-09	-8.278	-8.304	-0.026	(0)
(CO2)2	2.295e-14	2.296e-14	-13.639	-13.639	0.000	68.78
Ca	1.852e-04					
Ca+2	1.560e-04	1.227e-04	-3.807	-3.911	-0.104	-18.07
CaCO3	2.556e-05	2.558e-05	-4.592	-4.592	0.000	-14.60
CaHCO3+	1.917e-06	1.806e-06	-5.717	-5.743	-0.026	9.66
CaSO4	1.295e-06	1.296e-06	-5.888	-5.887	0.000	7.47

CaPO4-	2.677e-07	2.521e-07	-6.572	-6.598	-0.026	(0)
CaOH+	5.075e-08	4.773e-08	-7.295	-7.321	-0.027	(0)
CaHPO4	4.621e-08	4.624e-08	-7.335	-7.335	0.000	(0)
CaH2PO4+	1.581e-11	1.489e-11	-10.801	-10.827	-0.026	(0)
CaHSO4+	3.816e-15	3.588e-15	-14.418	-14.445	-0.027	(0)
Cl	3.794e-04					
Cl-	3.776e-04	3.550e-04	-3.423	-3.450	-0.027	18.07
NaCl	1.856e-06	1.857e-06	-5.731	-5.731	0.000	(0)
BaCl+	2.095e-09	1.971e-09	-8.679	-8.705	-0.027	(0)
MnCl+	7.310e-11	6.882e-11	-10.136	-10.162	-0.026	-3.29
MnCl2	1.066e-14	1.066e-14	-13.972	-13.972	0.000	87.00
MnCl3-	1.108e-18	1.043e-18	-17.956	-17.982	-0.026	43.41
F	6.317e-06					
F-	6.230e-06	5.855e-06	-5.206	-5.232	-0.027	-1.30
MgF+	8.495e-08	7.993e-08	-7.071	-7.097	-0.026	-10.55
NaF	2.962e-09	2.964e-09	-8.528	-8.528	0.000	7.23
HF	3.683e-12	3.686e-12	-11.434	-11.433	0.000	12.46
MnF+	2.048e-12	1.928e-12	-11.689	-11.715	-0.026	(0)
HF2-	8.742e-17	8.222e-17	-16.058	-16.085	-0.027	22.04
SiF6-2	0.000e+00	0.000e+00	-42.743	-42.847	-0.105	42.61
H(0)	2.035e-35					
H2	1.018e-35	1.018e-35	-34.992	-34.992	0.000	28.61
K	4.297e-04					
K+	4.295e-04	4.038e-04	-3.367	-3.394	-0.027	9.00
KSO4-	1.774e-07	1.671e-07	-6.751	-6.777	-0.026	34.11
KHPO4-	5.844e-10	5.504e-10	-9.233	-9.259	-0.026	38.20
Mg	2.999e-04					
Mg+2	2.665e-04	2.100e-04	-3.574	-3.678	-0.103	-21.71
MgCO3	2.495e-05	2.497e-05	-4.603	-4.603	0.000	-17.09
MgHCO3+	3.046e-06	2.865e-06	-5.516	-5.543	-0.027	5.47
MgSO4	2.875e-06	2.877e-06	-5.541	-5.541	0.000	5.80
MgOH+	1.747e-06	1.648e-06	-5.758	-5.783	-0.026	(0)
MgPO4-	6.182e-07	5.822e-07	-6.209	-6.235	-0.026	(0)
MgHPO4	1.069e-07	1.070e-07	-6.971	-6.971	0.000	(0)
MgF+	8.495e-08	7.993e-08	-7.071	-7.097	-0.026	-10.55
MgH2PO4+	3.447e-11	3.247e-11	-10.463	-10.489	-0.026	(0)
Mn(2)	5.462e-07					
MnCO3	4.771e-07	4.775e-07	-6.321	-6.321	0.000	(0)
Mn+2	6.035e-08	4.759e-08	-7.219	-7.323	-0.103	-20.51
MnHCO3+	5.273e-09	4.964e-09	-8.278	-8.304	-0.026	(0)
MnOH+	2.830e-09	2.664e-09	-8.548	-8.574	-0.026	(0)
MnSO4	4.972e-10	4.976e-10	-9.303	-9.303	0.000	22.94
MnCl+	7.310e-11	6.882e-11	-10.136	-10.162	-0.026	-3.29
MnF+	2.048e-12	1.928e-12	-11.689	-11.715	-0.026	(0)
Mn(NO3)2	5.422e-14	5.426e-14	-13.266	-13.266	0.000	41.28
MnCl2	1.066e-14	1.066e-14	-13.972	-13.972	0.000	87.00
Mn(OH)3-	1.032e-14	9.714e-15	-13.986	-14.013	-0.026	(0)
MnCl3-	1.108e-18	1.043e-18	-17.956	-17.982	-0.026	43.41
Mn(3)	7.662e-27					
Mn+3	7.662e-27	4.605e-27	-26.116	-26.337	-0.221	(0)
N(3)	1.428e-06					
NO2-	1.428e-06	1.342e-06	-5.845	-5.872	-0.027	24.94
N(5)	5.691e-04					
NO3-	5.691e-04	5.346e-04	-3.245	-3.272	-0.027	29.43
BaNO3+	1.280e-10	1.204e-10	-9.893	-9.919	-0.027	(0)
Mn(NO3)2	5.422e-14	5.426e-14	-13.266	-13.266	0.000	41.28
Na	9.397e-04					
Na+	9.349e-04	8.798e-04	-3.029	-3.056	-0.026	-1.49
NaCO3-	2.102e-06	1.977e-06	-5.677	-5.704	-0.027	-1.08
NaCl	1.856e-06	1.857e-06	-5.731	-5.731	0.000	(0)
NaHCO3	5.815e-07	5.820e-07	-6.235	-6.235	0.000	1.80
NaSO4-	2.785e-07	2.622e-07	-6.555	-6.581	-0.026	13.97
NaF	2.962e-09	2.964e-09	-8.528	-8.528	0.000	7.23
NaHPO4-	1.273e-09	1.199e-09	-8.895	-8.921	-0.026	33.69
NaOH	1.947e-18	1.948e-18	-17.711	-17.710	0.000	(0)
O(0)	4.107e-23					
O2	2.053e-23	2.055e-23	-22.688	-22.687	0.000	30.33
P	1.937e-06					

HPO4-2	8.901e-07	6.991e-07	-6.051	-6.155	-0.105	6.83
MgPO4-	6.182e-07	5.822e-07	-6.209	-6.235	-0.026	(0)
CaPO4-	2.677e-07	2.521e-07	-6.572	-6.598	-0.026	(0)
MgHPO4	1.069e-07	1.070e-07	-6.971	-6.971	0.000	(0)
CaHPO4	4.621e-08	4.624e-08	-7.335	-7.335	0.000	(0)
H2PO4-	5.126e-09	4.828e-09	-8.290	-8.316	-0.026	33.25
NaHPO4-	1.273e-09	1.199e-09	-8.895	-8.921	-0.026	33.69
PO4-3	1.261e-09	7.256e-10	-8.899	-9.139	-0.240	-22.96
KHPO4-	5.844e-10	5.504e-10	-9.233	-9.259	-0.026	38.20
MgH2PO4+	3.447e-11	3.247e-11	-10.463	-10.489	-0.026	(0)
CaH2PO4+	1.581e-11	1.489e-11	-10.801	-10.827	-0.026	(0)
H3PO4	2.997e-16	3.000e-16	-15.523	-15.523	0.000	47.36
S(6)	8.100e-05					
SO4-2	7.618e-05	5.982e-05	-4.118	-4.223	-0.105	14.49
MgSO4	2.875e-06	2.877e-06	-5.541	-5.541	0.000	5.80
CaSO4	1.295e-06	1.296e-06	-5.888	-5.887	0.000	7.47
NaSO4-	2.785e-07	2.622e-07	-6.555	-6.581	-0.026	13.97
KSO4-	1.774e-07	1.671e-07	-6.751	-6.777	-0.026	34.11
SrSO4	1.393e-07	1.394e-07	-6.856	-6.856	0.000	24.20
BaSO4	5.359e-08	5.363e-08	-7.271	-7.271	0.000	(0)
MnSO4	4.972e-10	4.976e-10	-9.303	-9.303	0.000	22.94
HSO4-	2.587e-12	2.433e-12	-11.587	-11.614	-0.027	40.24
CaHSO4+	3.816e-15	3.588e-15	-14.418	-14.445	-0.027	(0)
Si	8.773e-05					
H4SiO4	6.467e-05	6.472e-05	-4.189	-4.189	0.000	52.15
H3SiO4-	2.305e-05	2.168e-05	-4.637	-4.664	-0.027	27.98
H2SiO4-2	4.143e-09	3.259e-09	-8.383	-8.487	-0.104	(0)
SiF6-2	0.000e+00	0.000e+00	-42.743	-42.847	-0.105	42.61
Sr	1.667e-05					
Sr+2	1.535e-05	1.208e-05	-4.814	-4.918	-0.104	-17.69
SrCO3	9.481e-07	9.488e-07	-6.023	-6.023	0.000	-14.13
SrHCO3+	2.227e-07	2.097e-07	-6.652	-6.678	-0.026	(0)
SrSO4	1.393e-07	1.394e-07	-6.856	-6.856	0.000	24.20
SrOH+	1.543e-09	1.453e-09	-8.812	-8.838	-0.026	(0)

----------Distribution of alkalinity----------

Total alkalinity (eq/kgw) = 1.729e-03

Species	Alkalinity	Molality	Alk/Mol
HCO3-	1.243e-03	1.243e-03	1.00
CO3-2	3.211e-04	1.606e-04	2.00
CaCO3	5.112e-05	2.556e-05	2.00
MgCO3	4.990e-05	2.495e-05	2.00
OH-	2.356e-05	2.356e-05	1.00
H3SiO4-	2.305e-05	2.305e-05	1.00
NaCO3-	4.205e-06	2.102e-06	2.00
MgHCO3+	3.046e-06	3.046e-06	1.00
CaHCO3+	1.917e-06	1.917e-06	1.00
SrCO3	1.896e-06	9.481e-07	2.00
MgOH+	1.747e-06	1.747e-06	1.00
MgPO4-	1.236e-06	6.182e-07	2.00
MnCO3	9.543e-07	4.771e-07	2.00
HPO4-2	8.901e-07	8.901e-07	1.00
NaHCO3	5.815e-07	5.815e-07	1.00
CaPO4-	5.354e-07	2.677e-07	2.00
BaCO3	2.291e-07	1.146e-07	2.00
SrHCO3+	2.227e-07	2.227e-07	1.00
MgHPO4	1.069e-07	1.069e-07	1.00
CaOH+	5.075e-08	5.075e-08	1.00
CaHPO4	4.621e-08	4.621e-08	1.00
BaHCO3+	2.074e-08	2.074e-08	1.00
H2SiO4-2	8.285e-09	4.143e-09	2.00
MnHCO3+	5.273e-09	5.273e-09	1.00
MnOH+	2.830e-09	2.830e-09	1.00
PO4-3	2.522e-09	1.261e-09	2.00
SrOH+	1.543e-09	1.543e-09	1.00

NaHPO4-	1.273e-09	1.273e-09	1.00
KHPO4-	5.844e-10	5.844e-10	1.00
H+	-4.514e-10	4.514e-10	-1.00
BaOH+	1.509e-10	1.509e-10	1.00
HF	-3.683e-12	3.683e-12	-1.00
HSO4-	-2.587e-12	2.587e-12	-1.00
Mn(OH)3-	3.096e-14	1.032e-14	3.00
CaHSO4+	-3.816e-15	3.816e-15	-1.00
H3PO4	-2.997e-16	2.997e-16	-1.00
HF2-	-8.742e-17	8.742e-17	-1.00
NaOH	1.947e-18	1.947e-18	1.00
SiF6-2	-0.000e+00	0.000e+00	-4.00

----------Saturation indices----------

Phase	SI**	log IAP	log K(297 K, 1 atm)	
Anhydrite	-3.87	-8.13	-4.27	CaSO4
Aragonite	0.52	-7.81	-8.33	CaCO3
BaCl2	-14.88	-12.65	2.24	BaCl2
BaCl2:2H2O	-12.85	-12.65	0.20	BaCl2:2H2O
BaCl2:H2O	-13.47	-12.65	0.82	BaCl2:H2O
Barite	-0.12	-9.97	-9.85	BaSO4
Calcite	0.67	-7.81	-8.47	CaCO3
Celestite	-2.49	-9.14	-6.65	SrSO4
Chalcedony	-0.63	-4.19	-3.56	SiO2
Chrysotile	4.50	36.81	32.31	Mg3Si2O5(OH)4
CO2(g)	-4.49	-5.94	-1.46	CO2
Dolomite	1.68	-15.39	-17.07	CaMg(CO3)2
Fluorite	-3.77	-14.38	-10.61	CaF2
Gypsum	-3.55	-8.13	-4.58	CaSO4:2H2O
H2(g)	-31.89	-34.99	-3.10	H2
H2O(g)	-1.53	-0.00	1.53	H2O
Halite	-8.07	-6.51	1.57	NaCl
Hausmannite	4.85	66.10	61.25	Mn3O4
Hydroxyapatite	2.80	-0.54	-3.34	Ca5(PO4)3OH
Manganite	2.00	27.34	25.34	MnOOH
O2(g)	-19.80	-22.69	-2.89	O2
Pyrochroite	-3.78	11.42	15.20	Mn(OH)2
Pyrolusite	1.74	43.26	41.52	MnO2:H2O
Quartz	-0.20	-4.19	-3.99	SiO2
Rhodochrosite	-0.09	-11.22	-11.13	MnCO3
Sepiolite	1.77	17.56	15.78	Mg2Si3O7.5OH:3H2O
Sepiolite(d)	-1.10	17.56	18.66	Mg2Si3O7.5OH:3H2O
SiO2(a)	-1.47	-4.19	-2.72	SiO2
Strontianite	0.45	-8.82	-9.27	SrCO3
Sylvite	-7.74	-6.84	0.90	KCl
Talc	6.93	28.43	21.50	Mg3Si4O10(OH)2
Witherite	-1.08	-9.65	-8.56	BaCO3

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
For ideal gases, phi = 1.

Initial solution 4.

----------Solution composition----------

Elements	Molality	Moles
Al	7.413e-07	7.413e-07
Alkalinity	3.001e-04	3.001e-04
Ba	5.097e-07	5.097e-07
Ca	1.397e-05	1.397e-05
Cl	6.488e-06	6.488e-06
F	2.105e-06	2.105e-06
Fe	1.612e-06	1.612e-06
K	5.115e-06	5.115e-06
Mg	2.057e-06	2.057e-06

Mn	1.820e-07	1.820e-07
N(5)	1.642e-05	1.642e-05
Na	2.175e-05	2.175e-05
O(0)	2.950e-04	2.950e-04
P	9.686e-07	9.686e-07
S(6)	8.328e-07	8.328e-07
Si	5.825e-06	5.825e-06
Sr	1.712e-06	1.712e-06

----------Description of solution----------

pH	= 5.580
pe	= 5.386
Specific Conductance (µS/cm, 23°C)	= 18
Density (g/cm³)	= 0.99769
Volume (L)	= 1.00243
Activity of water	= 1.000
Ionic strength (mol/kgw)	= 2.211e-04
Mass of water (kg)	= 1.000e+00
Total carbon (mol/kg)	= 2.118e-03
Total CO2 (mol/kg)	= 2.118e-03
Temperature (°C)	= 22.50
Electrical balance (eq)	= -2.586e-04
Percent error, 100*(Cat-|An|)/(Cat+|An|)	= -64.68
Iterations	= 13 (35 overall)
Total H	= 1.110128e+02
Total O	= 5.551113e+01

----------Redox couples----------

Redox couple	pe	Eh (volts)
O(-2)/O(0)	15.1911	0.8911

----------Distribution of species----------

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma	mole V cm³/mol
H+	2.674e-06	2.630e-06	-5.573	-5.580	-0.007	0.00
OH-	3.227e-09	3.172e-09	-8.491	-8.499	-0.007	-4.23
H2O	5.551e+01	1.000e+00	1.744	-0.000	0.000	18.06
Al	7.413e-07					
AlF+2	2.906e-07	2.716e-07	-6.537	-6.566	-0.029	(0)
AlF2+	1.905e-07	1.873e-07	-6.720	-6.727	-0.007	(0)
Al(OH)2+	1.540e-07	1.514e-07	-6.813	-6.820	-0.007	(0)
AlOH+2	6.785e-08	6.340e-08	-7.168	-7.198	-0.029	-27.72
Al+3	2.297e-08	1.977e-08	-7.639	-7.704	-0.065	-42.24
Al(OH)3	7.034e-09	7.034e-09	-8.153	-8.153	0.000	(0)
Al(OH)4-	4.964e-09	4.880e-09	-8.304	-8.312	-0.007	(0)
AlF3	3.280e-09	3.280e-09	-8.484	-8.484	0.000	(0)
AlSO4+	4.772e-11	4.691e-11	-10.321	-10.329	-0.007	(0)
AlF4-	1.851e-12	1.820e-12	-11.733	-11.740	-0.007	(0)
Al(SO4)2-	1.156e-15	1.137e-15	-14.937	-14.944	-0.007	(0)
AlHSO4+2	1.147e-17	1.071e-17	-16.941	-16.970	-0.030	(0)
Ba	5.097e-07					
Ba+2	5.082e-07	4.747e-07	-6.294	-6.324	-0.030	-12.95
BaHCO3+	1.271e-09	1.250e-09	-8.896	-8.903	-0.007	(0)
BaSO4	1.844e-10	1.845e-10	-9.734	-9.734	0.000	(0)
BaCl+	9.326e-12	9.168e-12	-11.030	-11.038	-0.007	(0)
BaCO3	1.173e-12	1.173e-12	-11.931	-11.931	0.000	-10.72
BaNO3+	9.814e-13	9.648e-13	-12.008	-12.016	-0.007	(0)
BaOH+	6.220e-15	6.116e-15	-14.206	-14.214	-0.007	(0)
C(4)	2.118e-03					
CO2	1.816e-03	1.816e-03	-2.741	-2.741	0.000	34.31
HCO3-	3.022e-04	2.972e-04	-3.520	-3.527	-0.007	24.47
(CO2)2	5.565e-08	5.566e-08	-7.255	-7.254	0.000	68.62
CaHCO3+	4.819e-08	4.738e-08	-7.317	-7.324	-0.007	9.56

FeHCO3+	4.403e-08	4.329e-08	-7.356	-7.364	-0.007	(0)
SrHCO3+	6.762e-09	6.648e-09	-8.170	-8.177	-0.007	(0)
MgHCO3+	6.704e-09	6.590e-09	-8.174	-8.181	-0.007	5.39
CO3-2	5.382e-09	5.030e-09	-8.269	-8.298	-0.029	-5.54
MnHCO3+	4.468e-09	4.393e-09	-8.350	-8.357	-0.007	(0)
NaHCO3	3.624e-09	3.624e-09	-8.441	-8.441	0.000	1.80
BaHCO3+	1.271e-09	1.250e-09	-8.896	-8.903	-0.007	(0)
FeCO3	1.757e-10	1.758e-10	-9.755	-9.755	0.000	(0)
CaCO3	1.048e-10	1.048e-10	-9.980	-9.980	0.000	-14.61
MnCO3	6.626e-11	6.627e-11	-10.179	-10.179	0.000	(0)
MgCO3	8.846e-12	8.846e-12	-11.053	-11.053	0.000	-17.09
SrCO3	4.751e-12	4.751e-12	-11.323	-11.323	0.000	-14.14
NaCO3-	1.793e-12	1.763e-12	-11.746	-11.754	-0.007	-1.29
BaCO3	1.173e-12	1.173e-12	-11.931	-11.931	0.000	-10.72
Ca	1.397e-05					
Ca+2	1.392e-05	1.301e-05	-4.856	-4.886	-0.029	-18.23
CaHCO3+	4.819e-08	4.738e-08	-7.317	-7.324	-0.007	9.56
CaSO4	1.760e-09	1.760e-09	-8.755	-8.755	0.000	7.40
CaH2PO4+	2.993e-10	2.942e-10	-9.524	-9.531	-0.007	(0)
CaHPO4	1.469e-10	1.469e-10	-9.833	-9.833	0.000	(0)
CaCO3	1.048e-10	1.048e-10	-9.980	-9.980	0.000	-14.61
CaOH+	8.349e-13	8.208e-13	-12.078	-12.086	-0.007	(0)
CaPO4-	1.282e-13	1.260e-13	-12.892	-12.899	-0.007	(0)
CaHSO4+	2.988e-14	2.938e-14	-13.525	-13.532	-0.007	(0)
Cl	6.488e-06					
Cl-	6.487e-06	6.377e-06	-5.188	-5.195	-0.007	17.98
NaCl	8.014e-10	8.014e-10	-9.096	-9.096	0.000	(0)
FeCl+	1.304e-11	1.282e-11	-10.885	-10.892	-0.007	(0)
BaCl+	9.326e-12	9.168e-12	-11.030	-11.038	-0.007	(0)
MnCl+	4.383e-12	4.309e-12	-11.358	-11.366	-0.007	-3.75
MnCl2	1.199e-17	1.199e-17	-16.921	-16.921	0.000	89.06
FeCl+2	5.607e-18	5.239e-18	-17.251	-17.281	-0.029	(0)
FeCl2+	1.644e-22	1.617e-22	-21.784	-21.791	-0.007	(0)
MnCl3-	2.143e-23	2.107e-23	-22.669	-22.676	-0.007	43.43
FeCl3	1.031e-28	1.031e-28	-27.987	-27.987	0.000	(0)
F	2.105e-06					
F-	1.419e-06	1.394e-06	-5.848	-5.856	-0.007	-1.36
AlF+2	2.906e-07	2.716e-07	-6.537	-6.566	-0.029	(0)
AlF2+	1.905e-07	1.873e-07	-6.720	-6.727	-0.007	(0)
HF	5.260e-09	5.260e-09	-8.279	-8.279	0.000	12.38
AlF3	3.280e-09	3.280e-09	-8.484	-8.484	0.000	(0)
MgF+	1.715e-10	1.686e-10	-9.766	-9.773	-0.007	-10.58
FeF+	2.066e-11	2.031e-11	-10.685	-10.692	-0.007	(0)
NaF	1.715e-11	1.715e-11	-10.766	-10.766	0.000	7.16
AlF4-	1.851e-12	1.820e-12	-11.733	-11.740	-0.007	(0)
MnF+	1.628e-12	1.600e-12	-11.788	-11.796	-0.007	(0)
FeF+2	6.707e-14	6.267e-14	-13.173	-13.203	-0.029	(0)
HF2-	2.806e-14	2.758e-14	-13.552	-13.559	-0.007	21.93
FeF2+	3.434e-15	3.376e-15	-14.464	-14.472	-0.007	(0)
FeF3	7.398e-18	7.398e-18	-17.131	-17.131	0.000	(0)
SiF6-2	4.189e-33	3.914e-33	-32.378	-32.407	-0.029	42.35
Fe(2)	1.604e-06					
Fe+2	1.559e-06	1.457e-06	-5.807	-5.837	-0.029	-22.35
FeHCO3+	4.403e-08	4.329e-08	-7.356	-7.364	-0.007	(0)
FeH2PO4+	6.890e-10	6.775e-10	-9.162	-9.169	-0.007	(0)
FeSO4	1.918e-10	1.918e-10	-9.717	-9.717	0.000	21.68
FeCO3	1.757e-10	1.758e-10	-9.755	-9.755	0.000	(0)
FeOH+	1.475e-10	1.451e-10	-9.831	-9.838	-0.007	(0)
FeHPO4	1.252e-10	1.252e-10	-9.902	-9.902	0.000	(0)
FeF+	2.066e-11	2.031e-11	-10.685	-10.692	-0.007	(0)
FeCl+	1.304e-11	1.282e-11	-10.885	-10.892	-0.007	(0)
FeHSO4+	3.346e-15	3.290e-15	-14.475	-14.483	-0.007	(0)
Fe(OH)2	3.769e-16	3.770e-16	-15.424	-15.424	0.000	(0)
Fe(OH)3-	5.283e-21	5.194e-21	-20.277	-20.284	-0.007	(0)
Fe(3)	7.636e-09					
Fe(OH)2+	7.256e-09	7.134e-09	-8.139	-8.147	-0.007	(0)
Fe(OH)3	3.130e-10	3.130e-10	-9.504	-9.504	0.000	(0)
FeOH+2	6.674e-11	6.236e-11	-10.176	-10.205	-0.029	(0)

Fe(OH)4-	9.976e-14	9.808e-14	-13.001	-13.008	-0.007	(0)
FeF+2	6.707e-14	6.267e-14	-13.173	-13.203	-0.029	(0)
Fe+3	3.424e-14	2.947e-14	-13.466	-13.531	-0.065	(0)
FeH2PO4+2	7.876e-15	7.360e-15	-14.104	-14.133	-0.029	(0)
FeF2+	3.434e-15	3.376e-15	-14.464	-14.472	-0.007	(0)
FeSO4+	2.410e-16	2.369e-16	-15.618	-15.625	-0.007	(0)
FeHPO4+	1.605e-16	1.578e-16	-15.795	-15.802	-0.007	(0)
FeF3	7.398e-18	7.398e-18	-17.131	-17.131	0.000	(0)
FeCl+2	5.607e-18	5.239e-18	-17.251	-17.281	-0.029	(0)
Fe2(OH)2+4	1.526e-19	1.162e-19	-18.816	-18.935	-0.119	(0)
Fe(SO4)2-	4.047e-21	3.979e-21	-20.393	-20.400	-0.007	(0)
FeHSO4+2	1.790e-21	1.672e-21	-20.747	-20.777	-0.030	(0)
FeCl2+	1.644e-22	1.617e-22	-21.784	-21.791	-0.007	(0)
Fe3(OH)4+5	3.347e-25	2.185e-25	-24.475	-24.661	-0.185	(0)
FeCl3	1.031e-28	1.031e-28	-27.987	-27.987	0.000	(0)
H(0)	1.698e-25					
H2	8.489e-26	8.490e-26	-25.071	-25.071	0.000	28.61
K	5.115e-06					
K+	5.115e-06	5.028e-06	-5.291	-5.299	-0.007	8.91
KSO4-	2.666e-11	2.621e-11	-10.574	-10.582	-0.007	34.02
KHPO4-	2.154e-13	2.117e-13	-12.667	-12.674	-0.007	38.28
Mg	2.057e-06					
Mg+2	2.049e-06	1.915e-06	-5.688	-5.718	-0.029	-21.79
MgHCO3+	6.704e-09	6.590e-09	-8.174	-8.181	-0.007	5.39
MgSO4	3.262e-10	3.262e-10	-9.487	-9.487	0.000	5.74
MgF+	1.715e-10	1.686e-10	-9.766	-9.773	-0.007	-10.58
MgH2PO4+	5.611e-11	5.517e-11	-10.251	-10.258	-0.007	(0)
MgHPO4	2.925e-11	2.925e-11	-10.534	-10.534	0.000	(0)
MgCO3	8.846e-12	8.846e-12	-11.053	-11.053	0.000	-17.09
MgOH+	2.141e-12	2.105e-12	-11.669	-11.677	-0.007	(0)
MgPO4-	2.546e-14	2.503e-14	-13.594	-13.601	-0.007	(0)
Mn(2)	1.820e-07					
Mn+2	1.775e-07	1.659e-07	-6.751	-6.780	-0.029	-21.63
MnHCO3+	4.468e-09	4.393e-09	-8.350	-8.357	-0.007	(0)
MnCO3	6.626e-11	6.627e-11	-10.179	-10.179	0.000	(0)
MnSO4	2.179e-11	2.179e-11	-10.662	-10.662	0.000	23.69
MnCl+	4.383e-12	4.309e-12	-11.358	-11.366	-0.007	-3.75
MnF+	1.628e-12	1.600e-12	-11.788	-11.796	-0.007	(0)
MnOH+	1.342e-12	1.320e-12	-11.872	-11.880	-0.007	(0)
Mn(NO3)2	1.730e-16	1.730e-16	-15.762	-15.762	0.000	41.72
MnCl2	1.199e-17	1.199e-17	-16.921	-16.921	0.000	89.06
MnCl3-	2.143e-23	2.107e-23	-22.669	-22.676	-0.007	43.43
Mn(OH)3-	1.469e-25	1.444e-25	-24.833	-24.840	-0.007	(0)
Mn(3)	1.002e-27					
Mn+3	1.002e-27	8.627e-28	-26.999	-27.064	-0.065	(0)
N(5)	1.642e-05					
NO3-	1.642e-05	1.614e-05	-4.785	-4.792	-0.007	29.23
BaNO3+	9.814e-13	9.648e-13	-12.008	-12.016	-0.007	(0)
Mn(NO3)2	1.730e-16	1.730e-16	-15.762	-15.762	0.000	41.72
Na	2.175e-05					
Na+	2.174e-05	2.138e-05	-4.663	-4.670	-0.007	-1.64
NaHCO3	3.624e-09	3.624e-09	-8.441	-8.441	0.000	1.80
NaCl	8.014e-10	8.014e-10	-9.096	-9.096	0.000	(0)
NaSO4-	8.314e-11	8.175e-11	-10.080	-10.088	-0.007	13.67
NaF	1.715e-11	1.715e-11	-10.766	-10.766	0.000	7.16
NaCO3-	1.793e-12	1.763e-12	-11.746	-11.754	-0.007	-1.29
NaHPO4-	9.156e-13	9.002e-13	-12.038	-12.046	-0.007	33.49
NaOH	6.782e-24	6.782e-24	-23.169	-23.169	0.000	(0)
O(0)	2.950e-04					
O2	1.475e-04	1.475e-04	-3.831	-3.831	0.000	30.20
P	9.686e-07					
H2PO4-	9.438e-07	9.279e-07	-6.025	-6.032	-0.007	33.25
HPO4-2	2.311e-08	2.160e-08	-7.636	-7.666	-0.029	6.73
FeH2PO4+	6.890e-10	6.775e-10	-9.162	-9.169	-0.007	(0)
H3PO4	3.487e-10	3.487e-10	-9.458	-9.458	0.000	47.27
CaH2PO4+	2.993e-10	2.942e-10	-9.524	-9.531	-0.007	(0)
CaHPO4	1.469e-10	1.469e-10	-9.833	-9.833	0.000	(0)
FeHPO4	1.252e-10	1.252e-10	-9.902	-9.902	0.000	(0)

MgH2PO4+	5.611e-11	5.517e-11	-10.251	-10.258	-0.007	(0)
MgHPO4	2.925e-11	2.925e-11	-10.534	-10.534	0.000	(0)
NaHPO4-	9.156e-13	9.002e-13	-12.038	-12.046	-0.007	33.49
KHPO4-	2.154e-13	2.117e-13	-12.667	-12.674	-0.007	38.28
CaPO4-	1.282e-13	1.260e-13	-12.892	-12.899	-0.007	(0)
MgPO4-	2.546e-14	2.503e-14	-13.594	-13.601	-0.007	(0)
FeH2PO4+2	7.876e-15	7.360e-15	-14.104	-14.133	-0.029	(0)
PO4-3	4.104e-15	3.520e-15	-14.387	-14.454	-0.067	-23.16
FeHPO4+	1.605e-16	1.578e-16	-15.795	-15.802	-0.007	(0)
S(6)	8.328e-07					
SO4-2	8.297e-07	7.752e-07	-6.081	-6.111	-0.029	14.12
CaSO4	1.760e-09	1.760e-09	-8.755	-8.755	0.000	7.40
MgSO4	3.262e-10	3.262e-10	-9.487	-9.487	0.000	5.74
SrSO4	2.338e-10	2.338e-10	-9.631	-9.631	0.000	24.14
FeSO4	1.918e-10	1.918e-10	-9.717	-9.717	0.000	21.68
HSO4-	1.911e-10	1.878e-10	-9.719	-9.726	-0.007	40.09
BaSO4	1.844e-10	1.845e-10	-9.734	-9.734	0.000	(0)
NaSO4-	8.314e-11	8.175e-11	-10.080	-10.088	-0.007	13.67
AlSO4+	4.772e-11	4.691e-11	-10.321	-10.329	-0.007	(0)
KSO4-	2.666e-11	2.621e-11	-10.574	-10.582	-0.007	34.02
MnSO4	2.179e-11	2.179e-11	-10.662	-10.662	0.000	23.69
CaHSO4+	2.988e-14	2.938e-14	-13.525	-13.532	-0.007	(0)
FeHSO4+	3.346e-15	3.290e-15	-14.475	-14.483	-0.007	(0)
Al(SO4)2-	1.156e-15	1.137e-15	-14.937	-14.944	-0.007	(0)
FeSO4+	2.410e-16	2.369e-16	-15.618	-15.625	-0.007	(0)
AlHSO4+2	1.147e-17	1.071e-17	-16.941	-16.970	-0.030	(0)
Fe(SO4)2-	4.047e-21	3.979e-21	-20.393	-20.400	-0.007	(0)
FeHSO4+2	1.790e-21	1.672e-21	-20.747	-20.777	-0.030	(0)
Si	5.825e-06					
H4SiO4	5.825e-06	5.825e-06	-5.235	-5.235	0.000	52.30
H3SiO4-	3.041e-10	2.989e-10	-9.517	-9.524	-0.007	27.89
H2SiO4-2	7.013e-18	6.554e-18	-17.154	-17.184	-0.029	(0)
SiF6-2	4.189e-33	3.914e-33	-32.378	-32.407	-0.029	42.35
Sr	1.712e-06					
Sr+2	1.705e-06	1.593e-06	-5.768	-5.798	-0.029	-17.79
SrHCO3+	6.762e-09	6.648e-09	-8.170	-8.177	-0.007	(0)
SrSO4	2.338e-10	2.338e-10	-9.631	-9.631	0.000	24.14
SrCO3	4.751e-12	4.751e-12	-11.323	-11.323	0.000	-14.14
SrOH+	3.160e-14	3.107e-14	-13.500	-13.508	-0.007	(0)

----------Distribution of alkalinity----------

Total alkalinity (eq/kgw) = 3.001e-04

Species	Alkalinity	Molality	Alk/Mol
HCO3-	3.022e-04	3.022e-04	1.00
H+	-2.674e-06	2.674e-06	-1.00
Al(OH)2+	3.080e-07	1.540e-07	2.00
AlOH+2	6.785e-08	6.785e-08	1.00
CaHCO3+	4.819e-08	4.819e-08	1.00
FeHCO3+	4.403e-08	4.403e-08	1.00
HPO4-2	2.311e-08	2.311e-08	1.00
Al(OH)3	2.110e-08	7.034e-09	3.00
Al(OH)4-	1.986e-08	4.964e-09	4.00
CO3-2	1.076e-08	5.382e-09	2.00
SrHCO3+	6.762e-09	6.762e-09	1.00
MgHCO3+	6.704e-09	6.704e-09	1.00
HF	-5.260e-09	5.260e-09	-1.00
MnHCO3+	4.468e-09	4.468e-09	1.00
NaHCO3	3.624e-09	3.624e-09	1.00
OH-	3.227e-09	3.227e-09	1.00
BaHCO3+	1.271e-09	1.271e-09	1.00
FeCO3	3.515e-10	1.757e-10	2.00
H3PO4	-3.487e-10	3.487e-10	-1.00
Fe(OH)3	3.130e-10	3.130e-10	1.00
H3SiO4-	3.041e-10	3.041e-10	1.00
CaCO3	2.095e-10	1.048e-10	2.00

HSO4-	-1.911e-10	1.911e-10	-1.00
FeOH+	1.475e-10	1.475e-10	1.00
CaHPO4	1.469e-10	1.469e-10	1.00
MnCO3	1.325e-10	6.626e-11	2.00
FeHPO4	1.252e-10	1.252e-10	1.00
FeOH+2	-6.674e-11	6.674e-11	-1.00
MgHPO4	2.925e-11	2.925e-11	1.00
MgCO3	1.769e-11	8.846e-12	2.00
SrCO3	9.502e-12	4.751e-12	2.00
NaCO3-	3.587e-12	1.793e-12	2.00
BaCO3	2.346e-12	1.173e-12	2.00
MgOH+	2.141e-12	2.141e-12	1.00
MnOH+	1.342e-12	1.342e-12	1.00
NaHPO4-	9.156e-13	9.156e-13	1.00
CaOH+	8.349e-13	8.349e-13	1.00
CaPO4-	2.564e-13	1.282e-13	2.00
KHPO4-	2.154e-13	2.154e-13	1.00
Fe(OH)4-	1.995e-13	9.976e-14	2.00
FeF+2	-1.341e-13	6.707e-14	-2.00
Fe+3	-6.847e-14	3.424e-14	-2.00
MgPO4-	5.092e-14	2.546e-14	2.00
SrOH+	3.160e-14	3.160e-14	1.00
CaHSO4+	-2.988e-14	2.988e-14	-1.00
HF2-	-2.806e-14	2.806e-14	-1.00
FeH2PO4+2	-1.575e-14	7.876e-15	-2.00
PO4-3	8.207e-15	4.104e-15	2.00
FeF2+	-6.868e-15	3.434e-15	-2.00
BaOH+	6.220e-15	6.220e-15	1.00
FeHSO4+	-3.346e-15	3.346e-15	-1.00
Fe(OH)2	7.539e-16	3.769e-16	2.00
FeSO4+	-4.819e-16	2.410e-16	-2.00
FeHPO4+	-1.605e-16	1.605e-16	-1.00
FeF3	-1.480e-17	7.398e-18	-2.00
H2SiO4-2	1.403e-17	7.013e-18	2.00
AlHSO4+2	-1.147e-17	1.147e-17	-1.00
FeCl+2	-1.121e-17	5.607e-18	-2.00
Fe2(OH)2+4	-3.052e-19	1.526e-19	-2.00
Fe(OH)3-	1.585e-20	5.283e-21	3.00
Fe(SO4)2-	-8.094e-21	4.047e-21	-2.00
FeHSO4+2	-5.369e-21	1.790e-21	-3.00
FeCl2+	-3.289e-22	1.644e-22	-2.00
NaOH	6.782e-24	6.782e-24	1.00
Fe3(OH)4+5	-6.693e-25	3.347e-25	-2.00
Mn(OH)3-	4.408e-25	1.469e-25	3.00
FeCl3	-2.062e-28	1.031e-28	-2.00
SiF6-2	-1.676e-32	4.189e-33	-4.00

----------Saturation indices----------

Phase	SI**	log IAP	log K(295 K, 1 atm)	
Al(OH)3(a)	-1.93	9.04	10.96	Al(OH)3
Albite	-10.52	-28.69	-18.16	NaAlSi3O8
Alunite	-6.06	-7.15	-1.09	KAl3(SO4)2(OH)6
Anhydrite	-6.75	-11.00	-4.25	CaSO4
Anorthite	-12.19	-31.98	-19.79	CaAl2Si2O8
Aragonite	-4.86	-13.18	-8.32	CaCO3
BaCl2	-18.96	-16.71	2.25	BaCl2
BaCl2:2H2O	-16.90	-16.71	0.18	BaCl2:2H2O
BaCl2:H2O	-17.54	-16.71	0.82	BaCl2:H2O
Barite	-2.57	-12.43	-9.87	BaSO4
Ca-Montmorillonite	-5.15	-50.54	-45.39	Ca0.165Al2.33Si3.67O10(OH)2
Calcite	-4.72	-13.18	-8.47	CaCO3
Celestite	-5.26	-11.91	-6.64	SrSO4
Chalcedony	-1.65	-5.23	-3.58	SiO2
Chlorite(14A)	-39.74	29.58	69.32	Mg5Al2Si3O10(OH)8
Chrysotile	-26.66	5.86	32.51	Mg3Si2O5(OH)4
CO2(g)	-1.30	-2.74	-1.44	CO2

Dolomite	-10.17	-27.20	-17.03	CaMg(CO3)2
Fe(OH)3(a)	-1.68	3.21	4.89	Fe(OH)3
Fluorite	-5.97	-16.60	-10.63	CaF2
Gibbsite	0.78	9.04	8.25	Al(OH)3
Goethite	4.12	3.21	-0.91	FeOOH
Gypsum	-6.41	-11.00	-4.58	CaSO4:2H2O
H2(g)	-21.98	-25.07	-3.09	H2
H2O(g)	-1.57	-0.00	1.57	H2O
Halite	-11.43	-9.87	1.57	NaCl
Hausmannite	-26.58	35.07	61.65	Mn3O4
Hematite	10.24	6.42	-3.82	Fe2O3
Hydroxyapatite	-21.91	-25.11	-3.20	Ca5(PO4)3OH
Illite	-8.14	-48.74	-40.61	K0.6Mg0.25Al2.3Si3.5O10(OH)2
Jarosite-K	-15.62	-24.63	-9.02	KFe3(SO4)2(OH)6
K-feldspar	-8.55	-29.31	-20.76	KAlSi3O8
K-mica	-1.39	11.69	13.07	KAl3Si3O10(OH)2
Kaolinite	-0.05	7.60	7.65	Al2Si2O5(OH)4
Manganite	-9.99	15.35	25.34	MnOOH
Melanterite	-9.71	-11.95	-2.24	FeSO4:7H2O
O2(g)	-0.96	-3.83	-2.87	O2
Pyrochroite	-10.82	4.38	15.20	Mn(OH)2
Pyrolusite	-15.47	26.31	41.78	MnO2:H2O
Quartz	-1.22	-5.23	-4.02	SiO2
Rhodochrosite	-3.96	-15.08	-11.12	MnCO3
Sepiolite	-20.65	-4.82	15.83	Mg2Si3O7.5OH:3H2O
Sepiolite(d)	-23.48	-4.82	18.66	Mg2Si3O7.5OH:3H2O
Siderite	-3.26	-14.14	-10.87	FeCO3
SiO2(a)	-2.50	-5.23	-2.73	SiO2
Strontianite	-4.83	-14.10	-9.27	SrCO3
Sylvite	-11.38	-10.49	0.89	KCl
Talc	-26.30	-4.61	21.69	Mg3Si4O10(OH)2
Vivianite	-10.42	-46.42	-36.00	Fe3(PO4)2:8H2O
Witherite	-6.05	-14.62	-8.57	BaCO3

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
For ideal gases, phi = 1.

Initial solution 5.

-----------------------------Solution composition-------------------------------

Elements	Molality	Moles
Al	9.266e-07	9.266e-07
Alkalinity	2.000e-04	2.000e-04
Ba	1.602e-06	1.602e-06
Ca	2.994e-05	2.994e-05
Cl	6.945e-04	6.945e-04
F	3.158e-06	3.158e-06
Fe	3.599e-05	3.599e-05
K	5.371e-05	5.371e-05
Mg	4.360e-05	4.360e-05
Mn	9.102e-07	9.102e-07
N(3)	4.998e-06	4.998e-06
N(5)	3.570e-06	3.570e-06
Na	7.395e-04	7.395e-04
O(0)	3.938e-05	3.938e-05
P	6.457e-07	6.457e-07
S(6)	3.227e-06	3.227e-06
Si	1.012e-04	1.012e-04
Sr	2.511e-06	2.511e-06

----------------------------Description of solution----------------------------

pH = 5.320
pe = 1.592
Specific Conductance (µS/cm, 23°C) = 110
Density (g/cm³) = 0.99751

```
                              Volume (L)  =   1.00266
                       Activity of water  =   1.000
                  Ionic strength (mol/kgw)  =   1.086e-03
                        Mass of water (kg)  =   1.000e+00
                     Total carbon (mol/kg)  =   2.364e-03
                        Total CO2 (mol/kg)  =   2.364e-03
                          Temperature (°C)  =  23.40
                   Electrical balance (eq)  =   1.118e-04
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  =   5.77
                                Iterations  =  13 (48 overall)
                                   Total H  = 1.110130e+02
                                   Total O  = 5.551163e+01
```

----------Redox couples----------

Redox couple	pe	Eh (volts)
N(3)/N(5)	8.9785	0.5283
O(-2)/O(0)	15.1569	0.8918

----------Distribution of species----------

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma	mole V cm³/mol
H+	4.958e-06	4.786e-06	-5.305	-5.320	-0.015	0.00
OH-	1.941e-09	1.870e-09	-8.712	-8.728	-0.016	-4.17
H2O	5.551e+01	9.999e-01	1.744	-0.000	0.000	18.06
Al	9.266e-07					
AlF+2	4.296e-07	3.713e-07	-6.367	-6.430	-0.063	(0)
AlF2+	3.617e-07	3.487e-07	-6.442	-6.458	-0.016	(0)
Al(OH)2+	5.470e-08	5.275e-08	-7.262	-7.278	-0.016	(0)
AlOH+2	4.291e-08	3.709e-08	-7.367	-7.431	-0.063	-27.70
Al+3	2.723e-08	1.984e-08	-7.565	-7.702	-0.137	-42.17
AlF3	8.280e-09	8.282e-09	-8.082	-8.082	0.000	(0)
Al(OH)3	1.441e-09	1.442e-09	-8.841	-8.841	0.000	(0)
Al(OH)4-	5.766e-10	5.558e-10	-9.239	-9.255	-0.016	(0)
AlSO4+	1.741e-10	1.678e-10	-9.759	-9.775	-0.016	(0)
AlF4-	6.462e-12	6.228e-12	-11.190	-11.206	-0.016	(0)
Al(SO4)2-	1.492e-14	1.438e-14	-13.826	-13.842	-0.016	(0)
AlHSO4+2	8.142e-17	7.023e-17	-16.089	-16.154	-0.064	(0)
Ba	1.602e-06					
Ba+2	1.595e-06	1.376e-06	-5.797	-5.861	-0.064	-12.83
BaCl+	2.921e-09	2.815e-09	-8.534	-8.551	-0.016	(0)
BaHCO3+	2.559e-09	2.466e-09	-8.592	-8.608	-0.016	(0)
BaSO4	1.882e-09	1.883e-09	-8.725	-8.725	0.000	(0)
BaCO3	1.283e-12	1.283e-12	-11.892	-11.892	0.000	-10.71
BaNO3+	6.181e-13	5.956e-13	-12.209	-12.225	-0.016	(0)
BaOH+	1.010e-14	9.739e-15	-13.996	-14.011	-0.016	(0)
C(4)	2.364e-03					
CO2	2.159e-03	2.160e-03	-2.666	-2.666	0.000	34.35
HCO3-	2.039e-04	1.966e-04	-3.690	-3.706	-0.016	24.56
FeHCO3+	6.233e-07	6.006e-07	-6.205	-6.221	-0.016	(0)
MgHCO3+	8.917e-08	8.593e-08	-7.050	-7.066	-0.016	5.43
(CO2)2	8.117e-08	8.119e-08	-7.091	-7.090	0.000	68.71
NaHCO3	7.921e-08	7.923e-08	-7.101	-7.101	0.000	1.80
CaHCO3+	6.546e-08	6.313e-08	-7.184	-7.200	-0.016	9.61
MnHCO3+	1.405e-08	1.354e-08	-7.852	-7.868	-0.016	(0)
SrHCO3+	6.391e-09	6.162e-09	-8.194	-8.210	-0.016	(0)
BaHCO3+	2.559e-09	2.466e-09	-8.592	-8.608	-0.016	(0)
CO3-2	2.157e-09	1.864e-09	-8.666	-8.729	-0.063	-5.40
FeCO3	1.366e-09	1.366e-09	-8.865	-8.865	0.000	(0)
MnCO3	1.144e-10	1.144e-10	-9.942	-9.941	0.000	(0)
CaCO3	7.831e-11	7.833e-11	-10.106	-10.106	0.000	-14.60
MgCO3	6.526e-11	6.528e-11	-10.185	-10.185	0.000	-17.09
NaCO3-	2.358e-11	2.273e-11	-10.627	-10.643	-0.016	-1.18
SrCO3	2.456e-12	2.456e-12	-11.610	-11.610	0.000	-14.13
BaCO3	1.283e-12	1.283e-12	-11.892	-11.892	0.000	-10.71

Ca	2.994e-05					
Ca+2	2.986e-05	2.581e-05	-4.525	-4.588	-0.063	-18.15
CaHCO3+	6.546e-08	6.313e-08	-7.184	-7.200	-0.016	9.61
CaSO4	1.238e-08	1.238e-08	-7.907	-7.907	0.000	7.44
CaH2PO4+	3.997e-10	3.854e-10	-9.398	-9.414	-0.016	(0)
CaHPO4	1.062e-10	1.063e-10	-9.974	-9.974	0.000	(0)
CaCO3	7.831e-11	7.833e-11	-10.106	-10.106	0.000	-14.60
CaOH+	9.284e-13	8.947e-13	-12.032	-12.048	-0.016	(0)
CaHSO4+	3.951e-13	3.808e-13	-12.403	-12.419	-0.016	(0)
CaPO4-	5.285e-14	5.096e-14	-13.277	-13.293	-0.016	(0)
Cl	6.945e-04					
Cl-	6.917e-04	6.665e-04	-3.160	-3.176	-0.016	18.03
NaCl	2.799e-06	2.800e-06	-5.553	-5.553	0.000	(0)
FeCl+	2.916e-08	2.810e-08	-7.535	-7.551	-0.016	(0)
BaCl+	2.921e-09	2.815e-09	-8.534	-8.551	-0.016	(0)
MnCl+	2.177e-09	2.098e-09	-8.662	-8.678	-0.016	-3.49
MnCl2	6.103e-13	6.105e-13	-12.214	-12.214	0.000	87.89
MnCl3-	1.162e-16	1.121e-16	-15.935	-15.951	-0.016	43.41
FeCl+2	2.312e-18	1.997e-18	-17.636	-17.700	-0.064	(0)
FeCl2+	6.488e-21	6.255e-21	-20.188	-20.204	-0.016	(0)
FeCl3	4.168e-25	4.169e-25	-24.380	-24.380	0.000	(0)
F	3.158e-06					
F-	1.961e-06	1.890e-06	-5.707	-5.724	-0.016	-1.33
AlF+2	4.296e-07	3.713e-07	-6.367	-6.430	-0.063	(0)
AlF2+	3.617e-07	3.487e-07	-6.442	-6.458	-0.016	(0)
HF	1.318e-08	1.318e-08	-7.880	-7.880	0.000	12.43
AlF3	8.280e-09	8.282e-09	-8.082	-8.082	0.000	(0)
MgF+	4.731e-09	4.560e-09	-8.325	-8.341	-0.016	-10.57
NaF	7.719e-10	7.721e-10	-9.112	-9.112	0.000	7.20
FeF+	5.990e-10	5.772e-10	-9.223	-9.239	-0.016	(0)
MnF+	1.048e-11	1.010e-11	-10.980	-10.996	-0.016	(0)
AlF4-	6.462e-12	6.228e-12	-11.190	-11.206	-0.016	(0)
HF2-	9.791e-14	9.435e-14	-13.009	-13.025	-0.016	21.99
FeF+2	3.532e-16	3.051e-16	-15.452	-15.516	-0.064	(0)
FeF2+	2.335e-17	2.251e-17	-16.632	-16.648	-0.016	(0)
FeF3	6.704e-20	6.706e-20	-19.174	-19.174	0.000	(0)
SiF6-2	4.916e-30	4.246e-30	-29.308	-29.372	-0.064	42.48
Fe(2)	3.599e-05					
Fe+2	3.531e-05	3.055e-05	-4.452	-4.515	-0.063	-22.23
FeHCO3+	6.233e-07	6.006e-07	-6.205	-6.221	-0.016	(0)
FeCl+	2.916e-08	2.810e-08	-7.535	-7.551	-0.016	(0)
FeSO4	1.440e-08	1.440e-08	-7.842	-7.842	0.000	20.68
FeH2PO4+	9.559e-09	9.217e-09	-8.020	-8.035	-0.016	(0)
FeOH+	1.856e-09	1.789e-09	-8.731	-8.747	-0.016	(0)
FeCO3	1.366e-09	1.366e-09	-8.865	-8.865	0.000	(0)
FeHPO4	9.409e-10	9.412e-10	-9.026	-9.026	0.000	(0)
FeF+	5.990e-10	5.772e-10	-9.223	-9.239	-0.016	(0)
FeHSO4+	4.677e-13	4.507e-13	-12.330	-12.346	-0.016	(0)
Fe(OH)2	2.766e-15	2.766e-15	-14.558	-14.558	0.000	(0)
Fe(OH)3-	2.193e-20	2.114e-20	-19.659	-19.675	-0.016	(0)
Fe(3)	9.004e-12					
Fe(OH)2+	8.646e-12	8.337e-12	-11.063	-11.079	-0.016	(0)
Fe(OH)3	2.091e-13	2.092e-13	-12.680	-12.679	0.000	(0)
FeOH+2	1.483e-13	1.281e-13	-12.829	-12.892	-0.064	(0)
FeF+2	3.532e-16	3.051e-16	-15.452	-15.516	-0.064	(0)
Fe+3	1.433e-16	1.044e-16	-15.844	-15.981	-0.137	(0)
Fe(OH)4-	3.875e-17	3.736e-17	-16.412	-16.428	-0.016	(0)
FeF2+	2.335e-17	2.251e-17	-16.632	-16.648	-0.016	(0)
FeH2PO4+2	1.957e-17	1.692e-17	-16.708	-16.772	-0.063	(0)
FeSO4+	3.129e-18	3.016e-18	-17.505	-17.521	-0.016	(0)
FeCl+2	2.312e-18	1.997e-18	-17.636	-17.700	-0.064	(0)
FeHPO4+	2.140e-19	2.064e-19	-18.669	-18.685	-0.016	(0)
FeF3	6.704e-20	6.706e-20	-19.174	-19.174	0.000	(0)
FeCl2+	6.488e-21	6.255e-21	-20.188	-20.204	-0.016	(0)
Fe(SO4)2-	1.858e-22	1.790e-22	-21.731	-21.747	-0.016	(0)
FeHSO4+2	4.486e-23	3.869e-23	-22.348	-22.412	-0.064	(0)
Fe2(OH)2+4	8.529e-25	4.720e-25	-24.069	-24.326	-0.257	(0)
FeCl3	4.168e-25	4.169e-25	-24.380	-24.380	0.000	(0)

Fe3(OH)4+5	2.404e-33	9.536e-34	-32.619	-33.021	-0.402	(0)
H(0)	2.157e-17					
H2	1.079e-17	1.079e-17	-16.967	-16.967	0.000	28.61
K	5.371e-05					
K+	5.371e-05	5.175e-05	-4.270	-4.286	-0.016	8.96
KSO4-	1.001e-09	9.654e-10	-8.999	-9.015	-0.016	34.06
KHPO4-	8.099e-13	7.809e-13	-12.092	-12.107	-0.016	38.23
Mg	4.360e-05					
Mg+2	4.348e-05	3.761e-05	-4.362	-4.425	-0.063	-21.76
MgHCO3+	8.917e-08	8.593e-08	-7.050	-7.066	-0.016	5.43
MgSO4	2.309e-08	2.309e-08	-7.637	-7.636	0.000	5.77
MgF+	4.731e-09	4.560e-09	-8.325	-8.341	-0.016	-10.57
MgH2PO4+	7.418e-10	7.152e-10	-9.130	-9.146	-0.016	(0)
MgHPO4	2.093e-10	2.094e-10	-9.679	-9.679	0.000	(0)
MgCO3	6.526e-11	6.528e-11	-10.185	-10.185	0.000	-17.09
MgOH+	2.557e-11	2.467e-11	-10.592	-10.608	-0.016	(0)
MgPO4-	1.039e-13	1.002e-13	-12.983	-12.999	-0.016	(0)
Mn(2)	9.102e-07					
Mn+2	8.935e-07	7.729e-07	-6.049	-6.112	-0.063	-21.02
MnHCO3+	1.405e-08	1.354e-08	-7.852	-7.868	-0.016	(0)
MnCl+	2.177e-09	2.098e-09	-8.662	-8.678	-0.016	-3.49
MnSO4	3.638e-10	3.639e-10	-9.439	-9.439	0.000	23.26
MnCO3	1.144e-10	1.144e-10	-9.942	-9.941	0.000	(0)
MnF+	1.048e-11	1.010e-11	-10.980	-10.996	-0.016	(0)
MnOH+	3.776e-12	3.640e-12	-11.423	-11.439	-0.016	(0)
MnCl2	6.103e-13	6.105e-13	-12.214	-12.214	0.000	87.89
MnCl3-	1.162e-16	1.121e-16	-15.935	-15.951	-0.016	43.41
Mn(NO3)2	3.651e-17	3.652e-17	-16.438	-16.437	0.000	41.47
Mn(OH)3-	1.159e-25	1.117e-25	-24.936	-24.952	-0.016	(0)
Mn(3)	1.013e-30					
Mn+3	1.013e-30	7.380e-31	-29.994	-30.132	-0.137	(0)
N(3)	4.998e-06					
NO2-	4.998e-06	4.815e-06	-5.301	-5.317	-0.016	24.88
N(5)	3.570e-06					
NO3-	3.570e-06	3.439e-06	-5.447	-5.464	-0.016	29.34
BaNO3+	6.181e-13	5.956e-13	-12.209	-12.225	-0.016	(0)
Mn(NO3)2	3.651e-17	3.652e-17	-16.438	-16.437	0.000	41.47
Na	7.395e-04					
Na+	7.366e-04	7.100e-04	-3.133	-3.149	-0.016	-1.56
NaCl	2.799e-06	2.800e-06	-5.553	-5.553	0.000	(0)
NaHCO3	7.921e-08	7.923e-08	-7.101	-7.101	0.000	1.80
NaSO4-	9.975e-09	9.618e-09	-8.001	-8.017	-0.016	13.80
NaF	7.719e-10	7.721e-10	-9.112	-9.112	0.000	7.20
NaCO3-	2.358e-11	2.273e-11	-10.627	-10.643	-0.016	-1.18
NaHPO4-	1.111e-11	1.071e-11	-10.954	-10.970	-0.016	33.54
NaOH	1.327e-22	1.328e-22	-21.877	-21.877	0.000	(0)
O(0)	3.938e-05					
O2	1.969e-05	1.969e-05	-4.706	-4.706	0.000	30.27
P	6.457e-07					
H2PO4-	6.244e-07	6.020e-07	-6.205	-6.220	-0.016	33.25
FeH2PO4+	9.559e-09	9.217e-09	-8.020	-8.035	-0.016	(0)
HPO4-2	8.960e-09	7.739e-09	-8.048	-8.111	-0.064	6.77
FeHPO4	9.409e-10	9.412e-10	-9.026	-9.026	0.000	(0)
MgH2PO4+	7.418e-10	7.152e-10	-9.130	-9.146	-0.016	(0)
H3PO4	4.161e-10	4.162e-10	-9.381	-9.381	0.000	47.32
CaH2PO4+	3.997e-10	3.854e-10	-9.398	-9.414	-0.016	(0)
MgHPO4	2.093e-10	2.094e-10	-9.679	-9.679	0.000	(0)
CaHPO4	1.062e-10	1.063e-10	-9.974	-9.974	0.000	(0)
NaHPO4-	1.111e-11	1.071e-11	-10.954	-10.970	-0.016	33.54
KHPO4-	8.099e-13	7.809e-13	-12.092	-12.107	-0.016	38.23
MgPO4-	1.039e-13	1.002e-13	-12.983	-12.999	-0.016	(0)
CaPO4-	5.285e-14	5.096e-14	-13.277	-13.293	-0.016	(0)
PO4-3	9.849e-16	7.059e-16	-15.007	-15.151	-0.145	-23.09
FeH2PO4+2	1.957e-17	1.692e-17	-16.708	-16.772	-0.063	(0)
FeHPO4+	2.140e-19	2.064e-19	-18.669	-18.685	-0.016	(0)
S(6)	3.227e-06					
SO4-2	3.162e-06	2.730e-06	-5.500	-5.564	-0.064	14.31
MgSO4	2.309e-08	2.309e-08	-7.637	-7.636	0.000	5.77

FeSO4	1.440e-08	1.440e-08	-7.842	-7.842	0.000	20.68
CaSO4	1.238e-08	1.238e-08	-7.907	-7.907	0.000	7.44
NaSO4-	9.975e-09	9.618e-09	-8.001	-8.017	-0.016	13.80
BaSO4	1.882e-09	1.883e-09	-8.725	-8.725	0.000	(0)
HSO4-	1.274e-09	1.227e-09	-8.895	-8.911	-0.016	40.17
SrSO4	1.130e-09	1.130e-09	-8.947	-8.947	0.000	24.18
KSO4-	1.001e-09	9.654e-10	-8.999	-9.015	-0.016	34.06
MnSO4	3.638e-10	3.639e-10	-9.439	-9.439	0.000	23.26
AlSO4+	1.741e-10	1.678e-10	-9.759	-9.775	-0.016	(0)
FeHSO4+	4.677e-13	4.507e-13	-12.330	-12.346	-0.016	(0)
CaHSO4+	3.951e-13	3.808e-13	-12.403	-12.419	-0.016	(0)
Al(SO4)2-	1.492e-14	1.438e-14	-13.826	-13.842	-0.016	(0)
AlHSO4+2	8.142e-17	7.023e-17	-16.089	-16.154	-0.064	(0)
FeSO4+	3.129e-18	3.016e-18	-17.505	-17.521	-0.016	(0)
Fe(SO4)2-	1.858e-22	1.790e-22	-21.731	-21.747	-0.016	(0)
FeHSO4+2	4.486e-23	3.869e-23	-22.348	-22.412	-0.064	(0)
Si	1.012e-04					
H4SiO4	1.012e-04	1.012e-04	-3.995	-3.995	0.000	52.22
H3SiO4-	3.059e-09	2.948e-09	-8.514	-8.531	-0.016	27.94
H2SiO4-2	4.363e-17	3.771e-17	-16.360	-16.424	-0.063	(0)
SiF6-2	4.916e-30	4.246e-30	-29.308	-29.372	-0.064	42.48
Sr	2.511e-06					
Sr+2	2.503e-06	2.164e-06	-5.601	-5.665	-0.063	-17.75
SrHCO3+	6.391e-09	6.162e-09	-8.194	-8.210	-0.016	(0)
SrSO4	1.130e-09	1.130e-09	-8.947	-8.947	0.000	24.18
SrCO3	2.456e-12	2.456e-12	-11.610	-11.610	0.000	-14.13
SrOH+	2.405e-14	2.318e-14	-13.619	-13.635	-0.016	(0)

----------Distribution of alkalinity----------

Total alkalinity (eq/kgw) = 2.000e-04

Species	Alkalinity	Molality	Alk/Mol
HCO3-	2.039e-04	2.039e-04	1.00
H+	-4.958e-06	4.958e-06	-1.00
FeHCO3+	6.233e-07	6.233e-07	1.00
Al(OH)2+	1.094e-07	5.470e-08	2.00
MgHCO3+	8.917e-08	8.917e-08	1.00
NaHCO3	7.921e-08	7.921e-08	1.00
CaHCO3+	6.546e-08	6.546e-08	1.00
AlOH+2	4.291e-08	4.291e-08	1.00
MnHCO3+	1.405e-08	1.405e-08	1.00
HF	-1.318e-08	1.318e-08	-1.00
HPO4-2	8.960e-09	8.960e-09	1.00
SrHCO3+	6.391e-09	6.391e-09	1.00
Al(OH)3	4.324e-09	1.441e-09	3.00
CO3-2	4.314e-09	2.157e-09	2.00
H3SiO4-	3.059e-09	3.059e-09	1.00
FeCO3	2.731e-09	1.366e-09	2.00
BaHCO3+	2.559e-09	2.559e-09	1.00
Al(OH)4-	2.306e-09	5.766e-10	4.00
OH-	1.941e-09	1.941e-09	1.00
FeOH+	1.856e-09	1.856e-09	1.00
HSO4-	-1.274e-09	1.274e-09	-1.00
FeHPO4	9.409e-10	9.409e-10	1.00
H3PO4	-4.161e-10	4.161e-10	-1.00
MnCO3	2.288e-10	1.144e-10	2.00
MgHPO4	2.093e-10	2.093e-10	1.00
CaCO3	1.566e-10	7.831e-11	2.00
MgCO3	1.305e-10	6.526e-11	2.00
CaHPO4	1.062e-10	1.062e-10	1.00
NaCO3-	4.717e-11	2.358e-11	2.00
MgOH+	2.557e-11	2.557e-11	1.00
NaHPO4-	1.111e-11	1.111e-11	1.00
SrCO3	4.911e-12	2.456e-12	2.00
MnOH+	3.776e-12	3.776e-12	1.00
BaCO3	2.566e-12	1.283e-12	2.00

CaOH+	9.284e-13	9.284e-13	1.00
KHPO4-	8.099e-13	8.099e-13	1.00
FeHSO4+	-4.677e-13	4.677e-13	-1.00
CaHSO4+	-3.951e-13	3.951e-13	-1.00
Fe(OH)3	2.091e-13	2.091e-13	1.00
MgPO4-	2.078e-13	1.039e-13	2.00
FeOH+2	-1.483e-13	1.483e-13	-1.00
CaPO4-	1.057e-13	5.285e-14	2.00
HF2-	-9.791e-14	9.791e-14	-1.00
SrOH+	2.405e-14	2.405e-14	1.00
BaOH+	1.010e-14	1.010e-14	1.00
Fe(OH)2	5.532e-15	2.766e-15	2.00
PO4-3	1.970e-15	9.849e-16	2.00
FeF+2	-7.064e-16	3.532e-16	-2.00
Fe+3	-2.865e-16	1.433e-16	-2.00
H2SiO4-2	8.727e-17	4.363e-17	2.00
AlHSO4+2	-8.142e-17	8.142e-17	-1.00
Fe(OH)4-	7.749e-17	3.875e-17	2.00
FeF2+	-4.671e-17	2.335e-17	-2.00
FeH2PO4+2	-3.915e-17	1.957e-17	-2.00
FeSO4+	-6.257e-18	3.129e-18	-2.00
FeCl+2	-4.623e-18	2.312e-18	-2.00
FeHPO4+	-2.140e-19	2.140e-19	-1.00
FeF3	-1.341e-19	6.704e-20	-2.00
Fe(OH)3-	6.578e-20	2.193e-20	3.00
FeCl2+	-1.298e-20	6.488e-21	-2.00
Fe(SO4)2-	-3.716e-22	1.858e-22	-2.00
FeHSO4+2	-1.346e-22	4.486e-23	-3.00
NaOH	1.327e-22	1.327e-22	1.00
Fe2(OH)2+4	-1.706e-24	8.529e-25	-2.00
FeCl3	-8.335e-25	4.168e-25	-2.00
Mn(OH)3-	3.476e-25	1.159e-25	3.00
SiF6-2	-1.966e-29	4.916e-30	-4.00
Fe3(OH)4+5	-4.808e-33	2.404e-33	-2.00

-------------------------------Saturation indices--------------------------------

Phase	SI**	log IAP	log K(296 K, 1 atm)	
Al(OH)3(a)	-2.65	8.26	10.90	Al(OH)3
Albite	-6.28	-24.39	-18.10	NaAlSi3O8
Alunite	-5.40	-6.60	-1.20	KAl3(SO4)2(OH)6
Anhydrite	-5.89	-10.15	-4.26	CaSO4
Anorthite	-11.33	-31.09	-19.76	CaAl2Si2O8
Aragonite	-4.99	-13.32	-8.33	CaCO3
BaCl2	-14.46	-12.21	2.24	BaCl2
BaCl2:2H2O	-12.41	-12.21	0.19	BaCl2:2H2O
BaCl2:H2O	-13.04	-12.21	0.82	BaCl2:H2O
Barite	-1.57	-11.43	-9.86	BaSO4
Ca-Montmorillonite	-2.36	-47.62	-45.26	Ca0.165Al2.33Si3.67O10(OH)2
Calcite	-4.85	-13.32	-8.47	CaCO3
Celestite	-4.58	-11.23	-6.65	SrSO4
Chalcedony	-0.42	-3.99	-3.57	SiO2
Chlorite(14A)	-33.37	35.61	68.98	Mg5Al2Si3O10(OH)8
Chrysotile	-21.74	10.66	32.40	Mg3Si2O5(OH)4
CO2(g)	-1.22	-2.67	-1.45	CO2
Dolomite	-9.42	-26.47	-17.05	CaMg(CO3)2
Fe(OH)3(a)	-4.91	-0.02	4.89	Fe(OH)3
Fluorite	-5.42	-16.04	-10.62	CaF2
Gibbsite	0.06	8.26	8.20	Al(OH)3
Goethite	0.92	-0.02	-0.94	FeOOH
Gypsum	-5.57	-10.15	-4.58	CaSO4:2H2O
H2(g)	-13.87	-16.97	-3.10	H2
H2O(g)	-1.54	-0.00	1.54	H2O
Halite	-7.89	-6.32	1.57	NaCl
Hausmannite	-34.02	27.41	61.43	Mn3O4
Hematite	3.84	-0.04	-3.89	Fe2O3
Hydroxyapatite	-22.72	-26.00	-3.28	Ca5(PO4)3OH

Illite	-4.85	-45.33	-40.48	K0.6Mg0.25Al2.3Si3.5O10(OH)2
Jarosite-K	-22.35	-31.44	-9.09	KFe3(SO4)2(OH)6
K-feldspar	-4.83	-25.53	-20.69	KAlSi3O8
K-mica	0.88	13.82	12.94	KAl3Si3O10(OH)2
Kaolinite	0.95	8.53	7.57	Al2Si2O5(OH)4
Manganite	-13.90	11.44	25.34	MnOOH
Melanterite	-7.85	-10.08	-2.23	FeSO4:7H2O
O2(g)	-1.83	-4.71	-2.88	O2
Pyrochroite	-10.67	4.53	15.20	Mn(OH)2
Pyrolusite	-23.29	18.35	41.64	MnO2:H2O
Quartz	0.01	-3.99	-4.00	SiO2
Rhodochrosite	-3.72	-14.84	-11.12	MnCO3
Sepiolite	-15.36	0.45	15.80	Mg2Si3O7.5OH:3H2O
Sepiolite(d)	-18.21	0.45	18.66	Mg2Si3O7.5OH:3H2O
Siderite	-2.36	-13.24	-10.88	FeCO3
SiO2(a)	-1.27	-3.99	-2.73	SiO2
Strontianite	-5.12	-14.39	-9.27	SrCO3
Sylvite	-8.35	-7.46	0.89	KCl
Talc	-18.92	2.67	21.58	Mg3Si4O10(OH)2
Vivianite	-7.85	-43.85	-36.00	Fe3(PO4)2:8H2O
Witherite	-6.03	-14.59	-8.56	BaCO3

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
For ideal gases, phi = 1.

Initial solution 6.

-----------------------------Solution composition------------------------------

Elements	Molality	Moles
Al	2.484e-06	2.484e-06
Alkalinity	1.501e-04	1.501e-04
Ba	5.389e-06	5.389e-06
Ca	1.233e-04	1.233e-04
Cl	2.300e-03	2.300e-03
F	4.212e-06	4.212e-06
Fe	1.970e-06	1.970e-06
K	1.432e-04	1.432e-04
Mg	2.633e-04	2.633e-04
Mn	1.019e-05	1.019e-05
N(3)	1.142e-05	1.142e-05
N(5)	2.878e-04	2.878e-04
Na	1.131e-03	1.131e-03
O(0)	3.626e-05	3.626e-05
P	1.292e-06	1.292e-06
S(6)	3.394e-05	3.394e-05
Si	1.162e-04	1.162e-04
Sr	5.707e-06	5.707e-06

----------------------------Description of solution----------------------------

pH	= 5.210
pe	= 1.724
Specific Conductance (µS/cm, 23°C)	= 291
Density (g/cm³)	= 0.99775
Volume (L)	= 1.00252
Activity of water	= 1.000
Ionic strength (mol/kgw)	= 2.889e-03
Mass of water (kg)	= 1.000e+00
Total carbon (mol/kg)	= 2.251e-03
Total CO2 (mol/kg)	= 2.251e-03
Temperature (°C)	= 22.70
Electrical balance (eq)	= -7.212e-04
Percent error, 100*(Cat-|An|)/(Cat+|An|)	= -14.73
Iterations	= 11 (59 overall)
Total H	= 1.110131e+02
Total O	= 5.551240e+01

---------------------------------Redox couples---------------------------------

Redox couple	pe	Eh (volts)
N(3)/N(5)	9.9003	0.5811
O(-2)/O(0)	15.3167	0.8991

----------------------------Distribution of species----------------------------

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma	mole V cm³/mol
H+	6.510e-06	6.166e-06	-5.186	-5.210	-0.024	0.00
OH-	1.458e-09	1.374e-09	-8.836	-8.862	-0.026	-4.18
H2O	5.551e+01	9.999e-01	1.744	-0.000	0.000	18.06
Al	2.484e-06					
AlF+2	1.335e-06	1.061e-06	-5.874	-5.974	-0.100	(0)
AlF2+	7.200e-07	6.799e-07	-6.143	-6.168	-0.025	(0)
AlOH+2	1.450e-07	1.153e-07	-6.839	-6.938	-0.100	-27.60
Al+3	1.356e-07	8.318e-08	-6.868	-7.080	-0.212	-41.98
Al(OH)2+	1.266e-07	1.195e-07	-6.898	-6.922	-0.025	(0)
AlF3	1.104e-08	1.105e-08	-7.957	-7.957	0.000	(0)
AlSO4+	6.878e-09	6.488e-09	-8.163	-8.188	-0.025	(0)
Al(OH)3	2.404e-09	2.405e-09	-8.619	-8.619	0.000	(0)
Al(OH)4-	7.564e-10	7.136e-10	-9.121	-9.147	-0.025	(0)
AlF4-	6.027e-12	5.686e-12	-11.220	-11.245	-0.025	(0)
Al(SO4)2-	5.469e-12	5.160e-12	-11.262	-11.287	-0.025	(0)
AlHSO4+2	4.398e-15	3.478e-15	-14.357	-14.459	-0.102	(0)
Ba	5.389e-06					
Ba+2	5.300e-06	4.195e-06	-5.276	-5.377	-0.102	-12.81
BaSO4	5.341e-08	5.344e-08	-7.272	-7.272	0.000	(0)
BaCl+	2.913e-08	2.747e-08	-7.536	-7.561	-0.025	(0)
BaHCO3+	5.819e-09	5.488e-09	-8.235	-8.261	-0.025	(0)
BaNO3+	1.518e-10	1.432e-10	-9.819	-9.844	-0.025	(0)
BaCO3	2.200e-12	2.201e-12	-11.658	-11.657	0.000	-10.72
BaOH+	2.442e-14	2.305e-14	-13.612	-13.637	-0.025	(0)
C(4)	2.251e-03					
CO2	2.095e-03	2.096e-03	-2.679	-2.679	0.000	34.32
HCO3-	1.554e-04	1.467e-04	-3.809	-3.834	-0.025	24.53
MgHCO3+	3.757e-07	3.543e-07	-6.425	-6.451	-0.026	5.43
CaHCO3+	1.861e-07	1.758e-07	-6.730	-6.755	-0.025	9.60
MnHCO3+	1.101e-07	1.039e-07	-6.958	-6.983	-0.025	(0)
NaHCO3	8.809e-08	8.815e-08	-7.055	-7.055	0.000	1.80
(CO2)2	7.462e-08	7.467e-08	-7.127	-7.127	0.000	68.64
FeHCO3+	2.396e-08	2.260e-08	-7.621	-7.646	-0.025	(0)
SrHCO3+	9.914e-09	9.361e-09	-8.004	-8.029	-0.025	(0)
BaHCO3+	5.819e-09	5.488e-09	-8.235	-8.261	-0.025	(0)
CO3-2	1.338e-09	1.064e-09	-8.873	-8.973	-0.100	-5.38
MnCO3	6.711e-10	6.715e-10	-9.173	-9.173	0.000	(0)
MgCO3	2.041e-10	2.042e-10	-9.690	-9.690	0.000	-17.09
CaCO3	1.665e-10	1.666e-10	-9.779	-9.778	0.000	-14.61
FeCO3	3.928e-11	3.930e-11	-10.406	-10.406	0.000	(0)
NaCO3-	1.971e-11	1.858e-11	-10.705	-10.731	-0.025	-1.22
SrCO3	2.861e-12	2.863e-12	-11.543	-11.543	0.000	-14.14
BaCO3	2.200e-12	2.201e-12	-11.658	-11.657	0.000	-10.72
Ca	1.233e-04					
Ca+2	1.226e-04	9.745e-05	-3.911	-4.011	-0.100	-18.09
CaSO4	4.326e-07	4.329e-07	-6.364	-6.364	0.000	7.41
CaHCO3+	1.861e-07	1.758e-07	-6.730	-6.755	-0.025	9.60
CaH2PO4+	3.007e-09	2.839e-09	-8.522	-8.547	-0.025	(0)
CaHPO4	6.051e-10	6.055e-10	-9.218	-9.218	0.000	(0)
CaCO3	1.665e-10	1.666e-10	-9.779	-9.778	0.000	-14.61
CaHSO4+	1.801e-11	1.699e-11	-10.744	-10.770	-0.025	(0)
CaOH+	2.781e-12	2.623e-12	-11.556	-11.581	-0.025	(0)
CaPO4-	2.355e-13	2.224e-13	-12.628	-12.653	-0.025	(0)
Cl	2.300e-03					
Cl-	2.287e-03	2.156e-03	-2.641	-2.666	-0.026	18.02

NaCl	1.337e-05	1.338e-05	-4.874	-4.874	0.000	(0)
MnCl+	7.393e-08	6.978e-08	-7.131	-7.156	-0.025	-3.66
BaCl+	2.913e-08	2.747e-08	-7.536	-7.561	-0.025	(0)
FeCl+	4.859e-09	4.582e-09	-8.313	-8.339	-0.025	(0)
MnCl2	6.562e-11	6.566e-11	-10.183	-10.183	0.000	88.80
MnCl3-	4.130e-14	3.898e-14	-13.384	-13.409	-0.025	43.46
FeCl+2	5.229e-19	4.150e-19	-18.282	-18.382	-0.100	(0)
FeCl2+	4.556e-21	4.300e-21	-20.341	-20.367	-0.025	(0)
FeCl3	9.263e-25	9.270e-25	-24.033	-24.033	0.000	(0)
F	4.212e-06					
F-	1.373e-06	1.294e-06	-5.862	-5.888	-0.026	-1.32
AlF+2	1.335e-06	1.061e-06	-5.874	-5.974	-0.100	(0)
AlF2+	7.200e-07	6.799e-07	-6.143	-6.168	-0.025	(0)
MgF+	1.810e-08	1.708e-08	-7.742	-7.768	-0.025	-10.55
HF	1.147e-08	1.148e-08	-7.940	-7.940	0.000	12.39
AlF3	1.104e-08	1.105e-08	-7.957	-7.957	0.000	(0)
NaF	7.844e-10	7.850e-10	-9.105	-9.105	0.000	7.17
MnF+	7.535e-11	7.112e-11	-10.123	-10.148	-0.025	(0)
FeF+	2.113e-11	1.992e-11	-10.675	-10.701	-0.025	(0)
AlF4-	6.027e-12	5.686e-12	-11.220	-11.245	-0.025	(0)
HF2-	5.932e-14	5.594e-14	-13.227	-13.252	-0.025	21.97
FeF+2	1.711e-17	1.358e-17	-16.767	-16.867	-0.100	(0)
FeF2+	7.207e-19	6.803e-19	-18.142	-18.167	-0.025	(0)
FeF3	1.383e-21	1.384e-21	-20.859	-20.859	0.000	(0)
SiF6-2	1.861e-30	1.477e-30	-29.730	-29.831	-0.100	42.51
Fe(2)	1.970e-06					
Fe+2	1.933e-06	1.540e-06	-5.714	-5.812	-0.099	-22.21
FeHCO3+	2.396e-08	2.260e-08	-7.621	-7.646	-0.025	(0)
FeSO4	6.668e-09	6.672e-09	-8.176	-8.176	0.000	21.46
FeCl+	4.859e-09	4.582e-09	-8.313	-8.339	-0.025	(0)
FeH2PO4+	9.733e-10	9.190e-10	-9.012	-9.037	-0.025	(0)
FeHPO4	7.251e-11	7.256e-11	-10.140	-10.139	0.000	(0)
FeOH+	7.036e-11	6.641e-11	-10.153	-10.178	-0.025	(0)
FeCO3	3.928e-11	3.930e-11	-10.406	-10.406	0.000	(0)
FeF+	2.113e-11	1.992e-11	-10.675	-10.701	-0.025	(0)
FeHSO4+	2.847e-13	2.685e-13	-12.546	-12.571	-0.025	(0)
Fe(OH)2	7.488e-17	7.493e-17	-16.126	-16.125	0.000	(0)
Fe(OH)3-	4.675e-22	4.413e-22	-21.330	-21.355	-0.025	(0)
Fe(3)	3.402e-13					
Fe(OH)2+	3.264e-13	3.082e-13	-12.486	-12.511	-0.025	(0)
FeOH+2	7.896e-15	6.267e-15	-14.103	-14.203	-0.100	(0)
Fe(OH)3	5.816e-15	5.820e-15	-14.235	-14.235	0.000	(0)
FeF+2	1.711e-17	1.358e-17	-16.767	-16.867	-0.100	(0)
Fe+3	1.118e-17	6.861e-18	-16.952	-17.164	-0.212	(0)
FeH2PO4+2	2.766e-18	2.199e-18	-17.558	-17.658	-0.100	(0)
FeSO4+	1.925e-18	1.817e-18	-17.716	-17.741	-0.025	(0)
Fe(OH)4-	8.305e-19	7.841e-19	-18.081	-18.106	-0.025	(0)
FeF2+	7.207e-19	6.803e-19	-18.142	-18.167	-0.025	(0)
FeCl+2	5.229e-19	4.150e-19	-18.282	-18.382	-0.100	(0)
FeHPO4+	2.147e-20	2.026e-20	-19.668	-19.693	-0.025	(0)
FeCl2+	4.556e-21	4.300e-21	-20.341	-20.367	-0.025	(0)
FeF3	1.383e-21	1.384e-21	-20.859	-20.859	0.000	(0)
Fe(SO4)2-	1.062e-21	1.001e-21	-20.974	-21.000	-0.025	(0)
FeHSO4+2	3.798e-23	3.004e-23	-22.420	-22.522	-0.102	(0)
FeCl3	9.263e-25	9.270e-25	-24.033	-24.033	0.000	(0)
Fe2(OH)2+4	2.973e-27	1.163e-27	-26.527	-26.934	-0.408	(0)
Fe3(OH)4+5	4.020e-37	9.277e-38	-36.396	-37.033	-0.637	(0)
H(0)	1.962e-17					
H2	9.811e-18	9.818e-18	-17.008	-17.008	0.000	28.61
K	1.432e-04					
K+	1.432e-04	1.350e-04	-3.844	-3.870	-0.026	8.95
KSO4-	2.452e-08	2.315e-08	-7.610	-7.635	-0.025	34.06
KHPO4-	3.299e-12	3.115e-12	-11.482	-11.507	-0.025	38.30
Mg	2.633e-04					
Mg+2	2.617e-04	2.084e-04	-3.582	-3.681	-0.099	-21.67
MgSO4	1.169e-06	1.170e-06	-5.932	-5.932	0.000	5.75
MgHCO3+	3.757e-07	3.543e-07	-6.425	-6.451	-0.026	5.43
MgF+	1.810e-08	1.708e-08	-7.742	-7.768	-0.025	-10.55

MgH2PO4+	8.188e-09	7.731e-09	-8.087	-8.112	-0.025	(0)
MgHPO4	1.749e-09	1.751e-09	-8.757	-8.757	0.000	(0)
MgCO3	2.041e-10	2.042e-10	-9.690	-9.690	0.000	-17.09
MgOH+	1.053e-10	9.951e-11	-9.978	-10.002	-0.024	(0)
MgPO4-	6.794e-13	6.415e-13	-12.168	-12.193	-0.025	(0)
Mn(2)	1.019e-05					
Mn+2	9.976e-06	7.946e-06	-5.001	-5.100	-0.099	-20.58
MnHCO3+	1.101e-07	1.039e-07	-6.958	-6.983	-0.025	(0)
MnCl+	7.393e-08	6.978e-08	-7.131	-7.156	-0.025	-3.66
MnSO4	3.434e-08	3.437e-08	-7.464	-7.464	0.000	23.59
MnCO3	6.711e-10	6.715e-10	-9.173	-9.173	0.000	(0)
MnF+	7.535e-11	7.112e-11	-10.123	-10.148	-0.025	(0)
MnCl2	6.562e-11	6.566e-11	-10.183	-10.183	0.000	88.80
MnOH+	2.905e-11	2.742e-11	-10.537	-10.562	-0.025	(0)
Mn(NO3)2	2.335e-12	2.337e-12	-11.632	-11.631	0.000	41.67
MnCl3-	4.130e-14	3.898e-14	-13.384	-13.409	-0.025	43.46
Mn(OH)3-	5.690e-25	5.371e-25	-24.245	-24.270	-0.025	(0)
Mn(3)	1.511e-29					
Mn+3	1.511e-29	9.272e-30	-28.821	-29.033	-0.212	(0)
N(3)	1.142e-05					
NO2-	1.142e-05	1.076e-05	-4.942	-4.968	-0.026	24.87
N(5)	2.878e-04					
NO3-	2.878e-04	2.711e-04	-3.541	-3.567	-0.026	29.28
BaNO3+	1.518e-10	1.432e-10	-9.819	-9.844	-0.025	(0)
Mn(NO3)2	2.335e-12	2.337e-12	-11.632	-11.631	0.000	41.67
Na	1.131e-03					
Na+	1.118e-03	1.054e-03	-2.952	-2.977	-0.025	-1.57
NaCl	1.337e-05	1.338e-05	-4.874	-4.874	0.000	(0)
NaSO4-	1.402e-07	1.324e-07	-6.853	-6.878	-0.025	13.99
NaHCO3	8.809e-08	8.815e-08	-7.055	-7.055	0.000	1.80
NaF	7.844e-10	7.850e-10	-9.105	-9.105	0.000	7.17
NaHPO4-	2.577e-11	2.433e-11	-10.589	-10.614	-0.025	33.70
NaCO3-	1.971e-11	1.858e-11	-10.705	-10.731	-0.025	-1.22
NaOH	1.448e-22	1.449e-22	-21.839	-21.839	0.000	(0)
O(0)	3.626e-05					
O2	1.813e-05	1.814e-05	-4.742	-4.741	0.000	30.22
P	1.292e-06					
H2PO4-	1.261e-06	1.191e-06	-5.899	-5.924	-0.025	33.28
HPO4-2	1.491e-08	1.183e-08	-7.826	-7.927	-0.100	6.86
MgH2PO4+	8.188e-09	7.731e-09	-8.087	-8.112	-0.025	(0)
CaH2PO4+	3.007e-09	2.839e-09	-8.522	-8.547	-0.025	(0)
MgHPO4	1.749e-09	1.751e-09	-8.757	-8.757	0.000	(0)
H3PO4	1.051e-09	1.051e-09	-8.978	-8.978	0.000	47.28
FeH2PO4+	9.733e-10	9.190e-10	-9.012	-9.037	-0.025	(0)
CaHPO4	6.051e-10	6.055e-10	-9.218	-9.218	0.000	(0)
FeHPO4	7.251e-11	7.256e-11	-10.140	-10.139	0.000	(0)
NaHPO4-	2.577e-11	2.433e-11	-10.589	-10.614	-0.025	33.70
KHPO4-	3.299e-12	3.115e-12	-11.482	-11.507	-0.025	38.30
MgPO4-	6.794e-13	6.415e-13	-12.168	-12.193	-0.025	(0)
CaPO4-	2.355e-13	2.224e-13	-12.628	-12.653	-0.025	(0)
PO4-3	1.401e-15	8.261e-16	-14.853	-15.083	-0.230	-22.86
FeH2PO4+2	2.766e-18	2.199e-18	-17.558	-17.658	-0.100	(0)
FeHPO4+	2.147e-20	2.026e-20	-19.668	-19.693	-0.025	(0)
S(6)	3.394e-05					
SO4-2	3.204e-05	2.542e-05	-4.494	-4.595	-0.100	14.29
MgSO4	1.169e-06	1.170e-06	-5.932	-5.932	0.000	5.75
CaSO4	4.326e-07	4.329e-07	-6.364	-6.364	0.000	7.41
NaSO4-	1.402e-07	1.324e-07	-6.853	-6.878	-0.025	13.99
BaSO4	5.341e-08	5.344e-08	-7.272	-7.272	0.000	(0)
MnSO4	3.434e-08	3.437e-08	-7.464	-7.464	0.000	23.59
KSO4-	2.452e-08	2.315e-08	-7.610	-7.635	-0.025	34.06
SrSO4	2.175e-08	2.176e-08	-7.663	-7.662	0.000	24.15
HSO4-	1.537e-08	1.450e-08	-7.813	-7.839	-0.025	40.14
AlSO4+	6.878e-09	6.488e-09	-8.163	-8.188	-0.025	(0)
FeSO4	6.668e-09	6.672e-09	-8.176	-8.176	0.000	21.46
CaHSO4+	1.801e-11	1.699e-11	-10.744	-10.770	-0.025	(0)
Al(SO4)2-	5.469e-12	5.160e-12	-11.262	-11.287	-0.025	(0)
FeHSO4+	2.847e-13	2.685e-13	-12.546	-12.571	-0.025	(0)

AlHSO4+2	4.398e-15	3.478e-15	-14.357	-14.459	-0.102	(0)
FeSO4+	1.925e-18	1.817e-18	-17.716	-17.741	-0.025	(0)
Fe(SO4)2-	1.062e-21	1.001e-21	-20.974	-21.000	-0.025	(0)
FeHSO4+2	3.798e-23	3.004e-23	-22.420	-22.522	-0.102	(0)
Si	1.162e-04					
H4SiO4	1.162e-04	1.163e-04	-3.935	-3.935	0.000	52.28
H3SiO4-	2.718e-09	2.563e-09	-8.566	-8.591	-0.026	27.94
H2SiO4-2	3.057e-17	2.430e-17	-16.515	-16.614	-0.100	(0)
SiF6-2	1.861e-30	1.477e-30	-29.730	-29.831	-0.100	42.51
Sr	5.707e-06					
Sr+2	5.676e-06	4.513e-06	-5.246	-5.346	-0.100	-17.67
SrSO4	2.175e-08	2.176e-08	-7.663	-7.662	0.000	24.15
SrHCO3+	9.914e-09	9.361e-09	-8.004	-8.029	-0.025	(0)
SrCO3	2.861e-12	2.863e-12	-11.543	-11.543	0.000	-14.14
SrOH+	3.976e-14	3.753e-14	-13.401	-13.426	-0.025	(0)

----------Distribution of alkalinity----------

Total alkalinity (eq/kgw) = 1.501e-04

Species	Alkalinity	Molality	Alk/Mol
HCO3-	1.554e-04	1.554e-04	1.00
H+	-6.510e-06	6.510e-06	-1.00
MgHCO3+	3.757e-07	3.757e-07	1.00
Al(OH)2+	2.532e-07	1.266e-07	2.00
CaHCO3+	1.861e-07	1.861e-07	1.00
AlOH+2	1.450e-07	1.450e-07	1.00
MnHCO3+	1.101e-07	1.101e-07	1.00
NaHCO3	8.809e-08	8.809e-08	1.00
FeHCO3+	2.396e-08	2.396e-08	1.00
HSO4-	-1.537e-08	1.537e-08	-1.00
HPO4-2	1.491e-08	1.491e-08	1.00
HF	-1.147e-08	1.147e-08	-1.00
SrHCO3+	9.914e-09	9.914e-09	1.00
Al(OH)3	7.212e-09	2.404e-09	3.00
BaHCO3+	5.819e-09	5.819e-09	1.00
Al(OH)4-	3.026e-09	7.564e-10	4.00
H3SiO4-	2.718e-09	2.718e-09	1.00
CO3-2	2.677e-09	1.338e-09	2.00
MgHPO4	1.749e-09	1.749e-09	1.00
OH-	1.458e-09	1.458e-09	1.00
MnCO3	1.342e-09	6.711e-10	2.00
H3PO4	-1.051e-09	1.051e-09	-1.00
CaHPO4	6.051e-10	6.051e-10	1.00
MgCO3	4.081e-10	2.041e-10	2.00
CaCO3	3.330e-10	1.665e-10	2.00
MgOH+	1.053e-10	1.053e-10	1.00
FeCO3	7.855e-11	3.928e-11	2.00
FeHPO4	7.251e-11	7.251e-11	1.00
FeOH+	7.036e-11	7.036e-11	1.00
NaCO3-	3.941e-11	1.971e-11	2.00
MnOH+	2.905e-11	2.905e-11	1.00
NaHPO4-	2.577e-11	2.577e-11	1.00
CaHSO4+	-1.801e-11	1.801e-11	-1.00
SrCO3	5.723e-12	2.861e-12	2.00
BaCO3	4.400e-12	2.200e-12	2.00
KHPO4-	3.299e-12	3.299e-12	1.00
CaOH+	2.781e-12	2.781e-12	1.00
MgPO4-	1.359e-12	6.794e-13	2.00
CaPO4-	4.711e-13	2.355e-13	2.00
FeHSO4+	-2.847e-13	2.847e-13	-1.00
HF2-	-5.932e-14	5.932e-14	-1.00
SrOH+	3.976e-14	3.976e-14	1.00
BaOH+	2.442e-14	2.442e-14	1.00
FeOH+2	-7.896e-15	7.896e-15	-1.00
Fe(OH)3	5.816e-15	5.816e-15	1.00
AlHSO4+2	-4.398e-15	4.398e-15	-1.00

PO4-3	2.803e-15	1.401e-15	2.00
Fe(OH)2	1.498e-16	7.488e-17	2.00
H2SiO4-2	6.113e-17	3.057e-17	2.00
FeF+2	-3.422e-17	1.711e-17	-2.00
Fe+3	-2.236e-17	1.118e-17	-2.00
FeH2PO4+2	-5.532e-18	2.766e-18	-2.00
FeSO4+	-3.849e-18	1.925e-18	-2.00
Fe(OH)4-	1.661e-18	8.305e-19	2.00
FeF2+	-1.441e-18	7.207e-19	-2.00
FeCl+2	-1.046e-18	5.229e-19	-2.00
FeHPO4+	-2.147e-20	2.147e-20	-1.00
FeCl2+	-9.112e-21	4.556e-21	-2.00
FeF3	-2.766e-21	1.383e-21	-2.00
Fe(SO4)2-	-2.123e-21	1.062e-21	-2.00
Fe(OH)3-	1.403e-21	4.675e-22	3.00
NaOH	1.448e-22	1.448e-22	1.00
FeHSO4+2	-1.140e-22	3.798e-23	-3.00
FeCl3	-1.853e-24	9.263e-25	-2.00
Mn(OH)3-	1.707e-24	5.690e-25	3.00
Fe2(OH)2+4	-5.947e-27	2.973e-27	-2.00
SiF6-2	-7.443e-30	1.861e-30	-4.00
Fe3(OH)4+5	-8.040e-37	4.020e-37	-2.00

-----Saturation indices-----

Phase	SI**	log IAP	log K(295 K, 1 atm)	
Al(OH)3(a)	-2.40	8.55	10.95	Al(OH)3
Albite	-5.78	-23.93	-18.15	NaAlSi3O8
Alunite	-1.93	-3.04	-1.11	KAl3(SO4)2(OH)6
Anhydrite	-4.35	-8.61	-4.25	CaSO4
Anorthite	-10.39	-30.17	-19.78	CaAl2Si2O8
Aragonite	-4.66	-12.98	-8.32	CaCO3
BaCl2	-12.96	-10.71	2.25	BaCl2
BaCl2:2H2O	-10.90	-10.71	0.19	BaCl2:2H2O
BaCl2:H2O	-11.53	-10.71	0.82	BaCl2:H2O
Barite	-0.11	-9.97	-9.87	BaSO4
Ca-Montmorillonite	-1.47	-46.83	-45.36	Ca0.165Al2.33Si3.67O10(OH)2
Calcite	-4.52	-12.98	-8.47	CaCO3
Celestite	-3.29	-9.94	-6.65	SrSO4
Chalcedony	-0.36	-3.93	-3.58	SiO2
Chlorite(14A)	-30.25	38.99	69.24	Mg5Al2Si3O10(OH)8
Chrysotile	-20.14	12.35	32.49	Mg3Si2O5(OH)4
CO2(g)	-1.24	-2.68	-1.44	CO2
Dolomite	-8.60	-25.64	-17.04	CaMg(CO3)2
Fe(OH)3(a)	-6.42	-1.53	4.89	Fe(OH)3
Fluorite	-5.16	-15.79	-10.63	CaF2
Gibbsite	0.31	8.55	8.24	Al(OH)3
Goethite	-0.62	-1.53	-0.92	FeOOH
Gypsum	-4.02	-8.61	-4.58	CaSO4:2H2O
H2(g)	-13.91	-17.01	-3.10	H2
H2O(g)	-1.56	-0.00	1.56	H2O
Halite	-7.21	-5.64	1.57	NaCl
Hausmannite	-31.78	29.83	61.60	Mn3O4
Hematite	0.76	-3.07	-3.83	Fe2O3
Hydroxyapatite	-19.78	-23.00	-3.21	Ca5(PO4)3OH
Illite	-3.72	-44.30	-40.58	K0.6Mg0.25Al2.3Si3.5O10(OH)2
Jarosite-K	-24.26	-33.29	-9.03	KFe3(SO4)2(OH)6
K-feldspar	-4.07	-24.82	-20.75	KAlSi3O8
K-mica	2.15	15.19	13.04	KAl3Si3O10(OH)2
Kaolinite	1.59	9.23	7.64	Al2Si2O5(OH)4
Manganite	-13.09	12.25	25.34	MnOOH
Melanterite	-8.17	-10.41	-2.24	FeSO4:7H2O
O2(g)	-1.87	-4.74	-2.88	O2
Pyrochroite	-9.88	5.32	15.20	Mn(OH)2
Pyrolusite	-22.56	19.19	41.75	MnO2:H2O
Quartz	0.08	-3.93	-4.01	SiO2
Rhodochrosite	-2.95	-14.07	-11.12	MnCO3

Sepiolite	-14.15	1.67	15.82	Mg2Si3O7.5OH:3H2O
Sepiolite(d)	-16.99	1.67	18.66	Mg2Si3O7.5OH:3H2O
Siderite	-3.91	-14.79	-10.88	FeCO3
SiO2(a)	-1.20	-3.93	-2.73	SiO2
Strontianite	-5.05	-14.32	-9.27	SrCO3
Sylvite	-7.42	-6.54	0.89	KCl
Talc	-17.18	4.48	21.66	Mg3Si4O10(OH)2
Vivianite	-11.60	-47.60	-36.00	Fe3(PO4)2:8H2O
Witherite	-5.78	-14.35	-8.57	BaCO3

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
For ideal gases, phi = 1.

Initial solution 7.

-----------------------------Solution composition------------------------------

Elements	Molality	Moles
Al	4.821e-07	4.821e-07
Alkalinity	7.504e-03	7.504e-03
Ba	1.078e-05	1.078e-05
Ca	1.682e-03	1.682e-03
Cl	1.273e-04	1.273e-04
F	6.846e-06	6.846e-06
Fe	3.296e-05	3.296e-05
K	8.444e-05	8.444e-05
Mg	2.320e-03	2.320e-03
Mn	3.460e-06	3.460e-06
N(3)	7.143e-07	7.143e-07
N(5)	1.143e-05	1.143e-05
Na	4.396e-04	4.396e-04
O(0)	5.440e-05	5.440e-05
P	6.461e-07	6.461e-07
S(6)	2.500e-06	2.500e-06
Si	2.288e-04	2.288e-04
Sr	6.052e-06	6.052e-06

----------------------------Description of solution----------------------------

pH	= 7.070
pe	= -1.471
Specific Conductance (µS/cm, 21°C)	= 633
Density (g/cm³)	= 0.99847
Volume (L)	= 1.00222
Activity of water	= 1.000
Ionic strength (mol/kgw)	= 1.172e-02
Mass of water (kg)	= 1.000e+00
Total carbon (mol/kg)	= 8.794e-03
Total CO2 (mol/kg)	= 8.794e-03
Temperature (°C)	= 21.20
Electrical balance (eq)	= 9.802e-04
Percent error, 100*(Cat-|An|)/(Cat+|An|)	= 6.21
Iterations	= 10 (69 overall)
Total H	= 1.110208e+02
Total O	= 5.553231e+01

---------------------------------Redox couples---------------------------------

Redox couple	pe	Eh (volts)
N(3)/N(5)	8.0242	0.4686
O(-2)/O(0)	13.6279	0.7959

----------------------------Distribution of species----------------------------

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma	mole V cm³/mol

OH-	9.901e-08	8.848e-08	-7.004	-7.053	-0.049	-4.19
H+	9.367e-08	8.511e-08	-7.028	-7.070	-0.042	0.00
H2O	5.551e+01	9.998e-01	1.744	-0.000	0.000	18.05
Al	4.821e-07					
Al(OH)4-	4.460e-07	3.999e-07	-6.351	-6.398	-0.047	(0)
Al(OH)3	1.889e-08	1.895e-08	-7.724	-7.722	0.001	(0)
Al(OH)2+	1.621e-08	1.458e-08	-7.790	-7.836	-0.046	(0)
AlF2+	4.117e-10	3.703e-10	-9.385	-9.431	-0.046	(0)
AlOH+2	3.398e-10	2.224e-10	-9.469	-9.653	-0.184	-27.40
AlF+2	2.051e-10	1.342e-10	-9.688	-9.872	-0.184	(0)
AlF3	2.601e-11	2.608e-11	-10.585	-10.584	0.001	(0)
Al+3	5.789e-12	2.445e-12	-11.237	-11.612	-0.374	-41.58
AlF4-	6.498e-14	5.827e-14	-13.187	-13.235	-0.047	(0)
AlSO4+	1.009e-14	9.051e-15	-13.996	-14.043	-0.047	(0)
Al(SO4)2-	3.857e-19	3.459e-19	-18.414	-18.461	-0.047	(0)
AlHSO4+2	1.027e-22	6.618e-23	-21.988	-22.179	-0.191	(0)
Ba	1.078e-05					
Ba+2	1.035e-05	6.678e-06	-4.985	-5.175	-0.190	-12.73
BaHCO3+	4.130e-07	3.700e-07	-6.384	-6.432	-0.048	(0)
BaCO3	1.056e-08	1.059e-08	-7.976	-7.975	0.001	-10.74
BaSO4	4.107e-09	4.118e-09	-8.387	-8.385	0.001	(0)
BaCl+	2.514e-09	2.252e-09	-8.600	-8.647	-0.048	(0)
BaNO3+	9.567e-12	8.572e-12	-11.019	-11.067	-0.048	(0)
BaOH+	2.959e-12	2.658e-12	-11.529	-11.575	-0.047	(0)
C(4)	8.794e-03					
HCO3-	7.244e-03	6.516e-03	-2.140	-2.186	-0.046	24.48
CO2	1.309e-03	1.313e-03	-2.883	-2.882	0.001	34.25
MgHCO3+	1.212e-04	1.085e-04	-3.917	-3.965	-0.048	5.42
CaHCO3+	8.987e-05	8.098e-05	-4.046	-4.092	-0.045	9.58
FeHCO3+	1.030e-05	9.228e-06	-4.987	-5.035	-0.048	(0)
CaCO3	5.362e-06	5.377e-06	-5.271	-5.269	0.001	-14.61
CO3-2	5.062e-06	3.312e-06	-5.296	-5.480	-0.184	-5.32
MgCO3	4.297e-06	4.309e-06	-5.367	-5.366	0.001	-17.09
NaHCO3	1.467e-06	1.471e-06	-5.833	-5.832	0.001	1.80
FeCO3	1.122e-06	1.125e-06	-5.950	-5.949	0.001	(0)
MnHCO3+	9.218e-07	8.280e-07	-6.035	-6.082	-0.047	(0)
BaHCO3+	4.130e-07	3.700e-07	-6.384	-6.432	-0.048	(0)
MnCO3	3.742e-07	3.752e-07	-6.427	-6.426	0.001	(0)
SrHCO3+	3.623e-07	3.259e-07	-6.441	-6.487	-0.046	(0)
(CO2)2	2.774e-08	2.782e-08	-7.557	-7.556	0.001	68.49
NaCO3-	2.228e-08	1.996e-08	-7.652	-7.700	-0.048	-1.29
BaCO3	1.056e-08	1.059e-08	-7.976	-7.975	0.001	-10.74
SrCO3	7.019e-09	7.038e-09	-8.154	-8.153	0.001	-14.14
Ca	1.682e-03					
Ca+2	1.586e-03	1.037e-03	-2.800	-2.984	-0.184	-17.96
CaHCO3+	8.987e-05	8.098e-05	-4.046	-4.092	-0.045	9.58
CaCO3	5.362e-06	5.377e-06	-5.271	-5.269	0.001	-14.61
CaSO4	2.199e-07	2.205e-07	-6.658	-6.657	0.001	7.35
CaHPO4	7.055e-08	7.074e-08	-7.152	-7.150	0.001	(0)
CaH2PO4+	5.130e-09	4.614e-09	-8.290	-8.336	-0.046	(0)
CaOH+	2.257e-09	2.022e-09	-8.646	-8.694	-0.048	(0)
CaPO4-	2.033e-09	1.829e-09	-8.692	-8.738	-0.046	(0)
CaHSO4+	1.306e-13	1.170e-13	-12.884	-12.932	-0.048	(0)
Cl	1.273e-04					
Cl-	1.270e-04	1.136e-04	-3.896	-3.945	-0.048	18.02
NaCl	2.593e-07	2.600e-07	-6.586	-6.585	0.001	(0)
BaCl+	2.514e-09	2.252e-09	-8.600	-8.647	-0.048	(0)
FeCl+	2.479e-09	2.221e-09	-8.606	-8.653	-0.048	(0)
MnCl+	7.348e-10	6.600e-10	-9.134	-9.180	-0.047	-4.04
MnCl2	3.265e-14	3.273e-14	-13.486	-13.485	0.001	90.81
MnCl3-	1.140e-18	1.024e-18	-17.943	-17.990	-0.047	43.59
FeCl+2	1.727e-22	1.125e-22	-21.763	-21.949	-0.186	(0)
FeCl2+	7.179e-26	6.449e-26	-25.144	-25.191	-0.047	(0)
FeCl3	7.307e-31	7.327e-31	-30.136	-30.135	0.001	(0)
F	6.846e-06					
F-	6.285e-06	5.617e-06	-5.202	-5.251	-0.049	-1.29
MgF+	5.577e-07	5.001e-07	-6.254	-6.301	-0.047	-10.51

NaF	1.267e-09	1.270e-09	-8.897	-8.896	0.001	7.11
FeF+	8.879e-10	7.955e-10	-9.052	-9.099	-0.048	(0)
HF	6.681e-10	6.699e-10	-9.175	-9.174	0.001	12.32
AlF2+	4.117e-10	3.703e-10	-9.385	-9.431	-0.046	(0)
AlF+2	2.051e-10	1.342e-10	-9.688	-9.872	-0.184	(0)
MnF+	6.168e-11	5.541e-11	-10.210	-10.256	-0.047	(0)
AlF3	2.601e-11	2.608e-11	-10.585	-10.584	0.001	(0)
AlF4-	6.498e-14	5.827e-14	-13.187	-13.235	-0.047	(0)
HF2-	1.562e-14	1.399e-14	-13.806	-13.854	-0.048	21.94
FeF+2	4.774e-19	3.108e-19	-18.321	-18.507	-0.186	(0)
FeF2+	7.391e-20	6.639e-20	-19.131	-19.178	-0.047	(0)
FeF3	5.818e-22	5.833e-22	-21.235	-21.234	0.001	(0)
SiF6-2	1.251e-33	8.148e-34	-32.903	-33.089	-0.186	42.60
Fe(2)	3.296e-05					
Fe+2	2.148e-05	1.416e-05	-4.668	-4.849	-0.181	-22.16
FeHCO3+	1.030e-05	9.228e-06	-4.987	-5.035	-0.048	(0)
FeCO3	1.122e-06	1.125e-06	-5.950	-5.949	0.001	(0)
FeOH+	4.393e-08	3.946e-08	-7.357	-7.404	-0.047	(0)
FeHPO4	7.515e-09	7.536e-09	-8.124	-8.123	0.001	(0)
FeSO4	2.881e-09	2.888e-09	-8.541	-8.539	0.001	23.17
FeCl+	2.479e-09	2.221e-09	-8.606	-8.653	-0.048	(0)
FeH2PO4+	1.477e-09	1.329e-09	-8.830	-8.877	-0.046	(0)
FeF+	8.879e-10	7.955e-10	-9.052	-9.099	-0.048	(0)
Fe(OH)2	2.815e-12	2.823e-12	-11.551	-11.549	0.001	(0)
FeHSO4+	1.783e-15	1.598e-15	-14.749	-14.796	-0.048	(0)
Fe(OH)3-	1.321e-15	1.186e-15	-14.879	-14.926	-0.047	(0)
Fe(3)	1.807e-11					
Fe(OH)3	9.603e-12	9.629e-12	-11.018	-11.016	0.001	(0)
Fe(OH)2+	8.368e-12	7.526e-12	-11.077	-11.123	-0.046	(0)
Fe(OH)4-	9.825e-14	8.837e-14	-13.008	-13.054	-0.046	(0)
FeOH+2	3.439e-15	2.239e-15	-14.464	-14.650	-0.186	(0)
FeF+2	4.774e-19	3.108e-19	-18.321	-18.507	-0.186	(0)
Fe+3	8.766e-20	3.703e-20	-19.057	-19.431	-0.374	(0)
FeF2+	7.391e-20	6.639e-20	-19.131	-19.178	-0.047	(0)
FeH2PO4+2	2.851e-21	1.866e-21	-20.545	-20.729	-0.184	(0)
FeHPO4+	1.308e-21	1.175e-21	-20.883	-20.930	-0.047	(0)
FeF3	5.818e-22	5.833e-22	-21.235	-21.234	0.001	(0)
FeSO4+	5.107e-22	4.588e-22	-21.292	-21.338	-0.047	(0)
FeCl+2	1.727e-22	1.125e-22	-21.763	-21.949	-0.186	(0)
FeCl2+	7.179e-26	6.449e-26	-25.144	-25.191	-0.047	(0)
Fe(SO4)2-	1.358e-26	1.217e-26	-25.867	-25.915	-0.048	(0)
Fe2(OH)2+4	9.179e-28	1.582e-28	-27.037	-27.801	-0.764	(0)
FeHSO4+2	1.629e-28	1.049e-28	-27.788	-27.979	-0.191	(0)
FeCl3	7.307e-31	7.327e-31	-30.136	-30.135	0.001	(0)
Fe3(OH)4+5	5.535e-36	3.548e-37	-35.257	-36.450	-1.193	(0)
H(0)	9.300e-15					
H2	4.650e-15	4.663e-15	-14.333	-14.331	0.001	28.61
K	8.444e-05					
K+	8.444e-05	7.549e-05	-4.073	-4.122	-0.049	8.94
KSO4-	6.785e-10	6.103e-10	-9.168	-9.214	-0.046	34.07
KHPO4-	2.187e-11	1.967e-11	-10.660	-10.706	-0.046	38.48
Mg	2.320e-03					
Mg+2	2.194e-03	1.445e-03	-2.659	-2.840	-0.181	-21.46
MgHCO3+	1.212e-04	1.085e-04	-3.917	-3.965	-0.048	5.42
MgCO3	4.297e-06	4.309e-06	-5.367	-5.366	0.001	-17.09
MgF+	5.577e-07	5.001e-07	-6.254	-6.301	-0.047	-10.51
MgSO4	3.765e-07	3.775e-07	-6.424	-6.423	0.001	5.68
MgHPO4	1.329e-07	1.332e-07	-6.877	-6.875	0.001	(0)
MgOH+	4.824e-08	4.354e-08	-7.317	-7.361	-0.045	(0)
MgH2PO4+	9.101e-09	8.185e-09	-8.041	-8.087	-0.046	(0)
MgPO4-	3.821e-09	3.436e-09	-8.418	-8.464	-0.046	(0)
Mn(2)	3.460e-06					
Mn+2	2.163e-06	1.426e-06	-5.665	-5.846	-0.181	-19.83
MnHCO3+	9.218e-07	8.280e-07	-6.035	-6.082	-0.047	(0)
MnCO3	3.742e-07	3.752e-07	-6.427	-6.426	0.001	(0)
MnCl+	7.348e-10	6.600e-10	-9.134	-9.180	-0.047	-4.04
MnOH+	3.502e-10	3.146e-10	-9.456	-9.502	-0.047	(0)
MnSO4	2.891e-10	2.899e-10	-9.539	-9.538	0.001	24.32

MnF+	6.168e-11	5.541e-11	-10.210	-10.256	-0.047	(0)
MnCl2	3.265e-14	3.273e-14	-13.486	-13.485	0.001	90.81
Mn(NO3)2	5.937e-16	5.953e-16	-15.226	-15.225	0.001	42.10
MnCl3-	1.140e-18	1.024e-18	-17.943	-17.990	-0.047	43.59
Mn(OH)3-	4.078e-20	3.663e-20	-19.390	-19.436	-0.047	(0)
Mn(3)	2.010e-33					
Mn+3	2.010e-33	8.491e-34	-32.697	-33.071	-0.374	(0)
N(3)	7.143e-07					
NO2-	7.143e-07	6.373e-07	-6.146	-6.196	-0.050	24.83
N(5)	1.143e-05					
NO3-	1.143e-05	1.020e-05	-4.942	-4.992	-0.050	29.18
BaNO3+	9.567e-12	8.572e-12	-11.019	-11.067	-0.048	(0)
Mn(NO3)2	5.937e-16	5.953e-16	-15.226	-15.225	0.001	42.10
Na	4.396e-04					
Na+	4.378e-04	3.929e-04	-3.359	-3.406	-0.047	-1.58
NaHCO3	1.467e-06	1.471e-06	-5.833	-5.832	0.001	1.80
NaCl	2.593e-07	2.600e-07	-6.586	-6.585	0.001	(0)
NaCO3-	2.228e-08	1.996e-08	-7.652	-7.700	-0.048	-1.29
NaSO4-	2.629e-09	2.365e-09	-8.580	-8.626	-0.046	14.50
NaF	1.267e-09	1.270e-09	-8.897	-8.896	0.001	7.11
NaHPO4-	1.138e-10	1.024e-10	-9.944	-9.990	-0.046	34.37
NaOH	3.467e-21	3.477e-21	-20.460	-20.459	0.001	(0)
O(0)	5.440e-05					
O2	2.720e-05	2.728e-05	-4.565	-4.564	0.001	30.09
P	6.461e-07					
H2PO4-	2.081e-07	1.872e-07	-6.682	-6.728	-0.046	33.37
HPO4-2	2.053e-07	1.336e-07	-6.688	-6.874	-0.186	7.10
MgHPO4	1.329e-07	1.332e-07	-6.877	-6.875	0.001	(0)
CaHPO4	7.055e-08	7.074e-08	-7.152	-7.150	0.001	(0)
MgH2PO4+	9.101e-09	8.185e-09	-8.041	-8.087	-0.046	(0)
FeHPO4	7.515e-09	7.536e-09	-8.124	-8.123	0.001	(0)
CaH2PO4+	5.130e-09	4.614e-09	-8.290	-8.336	-0.046	(0)
MgPO4-	3.821e-09	3.436e-09	-8.418	-8.464	-0.046	(0)
CaPO4-	2.033e-09	1.829e-09	-8.692	-8.738	-0.046	(0)
FeH2PO4+	1.477e-09	1.329e-09	-8.830	-8.877	-0.046	(0)
NaHPO4-	1.138e-10	1.024e-10	-9.944	-9.990	-0.046	34.37
KHPO4-	2.187e-11	1.967e-11	-10.660	-10.706	-0.046	38.48
H3PO4	2.235e-12	2.241e-12	-11.651	-11.650	0.001	47.19
PO4-3	1.774e-12	6.555e-13	-11.751	-12.183	-0.432	-22.29
FeH2PO4+2	2.851e-21	1.866e-21	-20.545	-20.729	-0.184	(0)
FeHPO4+	1.308e-21	1.175e-21	-20.883	-20.930	-0.047	(0)
S(6)	2.500e-06					
SO4-2	1.892e-06	1.230e-06	-5.723	-5.910	-0.187	14.26
MgSO4	3.765e-07	3.775e-07	-6.424	-6.423	0.001	5.68
CaSO4	2.199e-07	2.205e-07	-6.658	-6.657	0.001	7.35
BaSO4	4.107e-09	4.118e-09	-8.387	-8.385	0.001	(0)
FeSO4	2.881e-09	2.888e-09	-8.541	-8.539	0.001	23.17
NaSO4-	2.629e-09	2.365e-09	-8.580	-8.626	-0.046	14.50
SrSO4	8.515e-10	8.538e-10	-9.070	-9.069	0.001	24.09
KSO4-	6.785e-10	6.103e-10	-9.168	-9.214	-0.046	34.07
MnSO4	2.891e-10	2.899e-10	-9.539	-9.538	0.001	24.32
HSO4-	1.047e-11	9.384e-12	-10.980	-11.028	-0.048	40.07
CaHSO4+	1.306e-13	1.170e-13	-12.884	-12.932	-0.048	(0)
AlSO4+	1.009e-14	9.051e-15	-13.996	-14.043	-0.047	(0)
FeHSO4+	1.783e-15	1.598e-15	-14.749	-14.796	-0.048	(0)
Al(SO4)2-	3.857e-19	3.459e-19	-18.414	-18.461	-0.047	(0)
FeSO4+	5.107e-22	4.588e-22	-21.292	-21.338	-0.047	(0)
AlHSO4+2	1.027e-22	6.618e-23	-21.988	-22.179	-0.191	(0)
Fe(SO4)2-	1.358e-26	1.217e-26	-25.867	-25.915	-0.048	(0)
FeHSO4+2	1.629e-28	1.049e-28	-27.788	-27.979	-0.191	(0)
Si	2.288e-04					
H4SiO4	2.284e-04	2.290e-04	-3.641	-3.640	0.001	52.41
H3SiO4-	3.870e-07	3.465e-07	-6.412	-6.460	-0.048	27.94
H2SiO4-2	3.285e-13	2.150e-13	-12.483	-12.668	-0.184	(0)
SiF6-2	1.251e-33	8.148e-34	-32.903	-33.089	-0.186	42.60
Sr	6.052e-06					
Sr+2	5.682e-06	3.724e-06	-5.246	-5.429	-0.184	-17.48
SrHCO3+	3.623e-07	3.259e-07	-6.441	-6.487	-0.046	(0)

SrCO3	7.019e-09	7.038e-09	-8.154	-8.153	0.001	-14.14
SrSO4	8.515e-10	8.538e-10	-9.070	-9.069	0.001	24.09
SrOH+	2.497e-12	2.243e-12	-11.603	-11.649	-0.047	(0)

----------Distribution of alkalinity----------

Total alkalinity (eq/kgw) = 7.504e-03

Species	Alkalinity	Molality	Alk/Mol
HCO3-	7.244e-03	7.244e-03	1.00
MgHCO3+	1.212e-04	1.212e-04	1.00
CaHCO3+	8.987e-05	8.987e-05	1.00
CaCO3	1.072e-05	5.362e-06	2.00
FeHCO3+	1.030e-05	1.030e-05	1.00
CO3-2	1.012e-05	5.062e-06	2.00
MgCO3	8.594e-06	4.297e-06	2.00
FeCO3	2.245e-06	1.122e-06	2.00
Al(OH)4-	1.784e-06	4.460e-07	4.00
NaHCO3	1.467e-06	1.467e-06	1.00
MnHCO3+	9.218e-07	9.218e-07	1.00
MnCO3	7.483e-07	3.742e-07	2.00
BaHCO3+	4.130e-07	4.130e-07	1.00
H3SiO4-	3.870e-07	3.870e-07	1.00
SrHCO3+	3.623e-07	3.623e-07	1.00
HPO4-2	2.053e-07	2.053e-07	1.00
MgHPO4	1.329e-07	1.329e-07	1.00
OH-	9.901e-08	9.901e-08	1.00
H+	-9.367e-08	9.367e-08	-1.00
CaHPO4	7.055e-08	7.055e-08	1.00
Al(OH)3	5.668e-08	1.889e-08	3.00
MgOH+	4.824e-08	4.824e-08	1.00
NaCO3-	4.456e-08	2.228e-08	2.00
FeOH+	4.393e-08	4.393e-08	1.00
Al(OH)2+	3.243e-08	1.621e-08	2.00
BaCO3	2.112e-08	1.056e-08	2.00
SrCO3	1.404e-08	7.019e-09	2.00
MgPO4-	7.642e-09	3.821e-09	2.00
FeHPO4	7.515e-09	7.515e-09	1.00
CaPO4-	4.066e-09	2.033e-09	2.00
CaOH+	2.257e-09	2.257e-09	1.00
HF	-6.681e-10	6.681e-10	-1.00
MnOH+	3.502e-10	3.502e-10	1.00
AlOH+2	3.398e-10	3.398e-10	1.00
NaHPO4-	1.138e-10	1.138e-10	1.00
KHPO4-	2.187e-11	2.187e-11	1.00
HSO4-	-1.047e-11	1.047e-11	-1.00
Fe(OH)3	9.603e-12	9.603e-12	1.00
Fe(OH)2	5.630e-12	2.815e-12	2.00
PO4-3	3.548e-12	1.774e-12	2.00
BaOH+	2.959e-12	2.959e-12	1.00
SrOH+	2.497e-12	2.497e-12	1.00
H3PO4	-2.235e-12	2.235e-12	-1.00
H2SiO4-2	6.571e-13	3.285e-13	2.00
Fe(OH)4-	1.965e-13	9.825e-14	2.00
CaHSO4+	-1.306e-13	1.306e-13	-1.00
HF2-	-1.562e-14	1.562e-14	-1.00
Fe(OH)3-	3.962e-15	1.321e-15	3.00
FeOH+2	-3.439e-15	3.439e-15	-1.00
FeHSO4+	-1.783e-15	1.783e-15	-1.00
FeF+2	-9.548e-19	4.774e-19	-2.00
Fe+3	-1.753e-19	8.766e-20	-2.00
FeF2+	-1.478e-19	7.391e-20	-2.00
Mn(OH)3-	1.223e-19	4.078e-20	3.00
FeH2PO4+2	-5.703e-21	2.851e-21	-2.00
NaOH	3.467e-21	3.467e-21	1.00
FeHPO4+	-1.308e-21	1.308e-21	-1.00
FeF3	-1.164e-21	5.818e-22	-2.00

FeSO4+	-1.021e-21	5.107e-22	-2.00
FeCl+2	-3.455e-22	1.727e-22	-2.00
AlHSO4+2	-1.027e-22	1.027e-22	-1.00
FeCl2+	-1.436e-25	7.179e-26	-2.00
Fe(SO4)2-	-2.716e-26	1.358e-26	-2.00
Fe2(OH)2+4	-1.836e-27	9.179e-28	-2.00
FeHSO4+2	-4.886e-28	1.629e-28	-3.00
FeCl3	-1.461e-30	7.307e-31	-2.00
SiF6-2	-5.006e-33	1.251e-33	-4.00
Fe3(OH)4+5	-1.107e-35	5.535e-36	-2.00

----------Saturation indices----------

Phase	SI**	log IAP	log K(294 K, 1 atm)	
Al(OH)3(a)	-1.45	9.60	11.05	Al(OH)3
Albite	-2.48	-20.72	-18.25	NaAlSi3O8
Alunite	-7.43	-8.36	-0.92	KAl3(SO4)2(OH)6
Anhydrite	-4.66	-8.89	-4.24	CaSO4
Anorthite	-3.24	-23.06	-19.82	CaAl2Si2O8
Aragonite	-0.15	-8.46	-8.31	CaCO3
BaCl2	-15.32	-13.06	2.26	BaCl2
BaCl2:2H2O	-13.24	-13.06	0.17	BaCl2:2H2O
BaCl2:H2O	-13.88	-13.06	0.82	BaCl2:H2O
Barite	-1.20	-11.09	-9.88	BaSO4
Ca-Montmorillonite	2.68	-42.90	-45.58	Ca0.165Al2.33Si3.67O10(OH)2
Calcite	-0.00	-8.46	-8.46	CaCO3
Celestite	-4.70	-11.34	-6.64	SrSO4
Chalcedony	-0.04	-3.64	-3.60	SiO2
Chlorite(14A)	-5.04	64.78	69.81	Mg5Al2Si3O10(OH)8
Chrysotile	-6.06	26.62	32.68	Mg3Si2O5(OH)4
CO2(g)	-1.46	-2.88	-1.42	CO2
Dolomite	0.22	-16.78	-17.00	CaMg(CO3)2
Fe(OH)3(a)	-3.11	1.78	4.89	Fe(OH)3
Fluorite	-2.84	-13.49	-10.65	CaF2
Gibbsite	1.27	9.60	8.33	Al(OH)3
Goethite	2.64	1.78	-0.86	FeOOH
Gypsum	-4.31	-8.89	-4.58	CaSO4:2H2O
H2(g)	-11.24	-14.33	-3.09	H2
H2O(g)	-1.60	-0.00	1.60	H2O
Halite	-8.92	-7.35	1.57	NaCl
Hausmannite	-25.90	36.08	61.98	Mn3O4
Hematite	7.27	3.56	-3.72	Fe2O3
Hydroxyapatite	-4.18	-7.26	-3.08	Ca5(PO4)3OH
Illite	1.66	-39.12	-40.78	K0.6Mg0.25Al2.3Si3.5O10(OH)2
Jarosite-K	-22.90	-31.82	-8.91	KFe3(SO4)2(OH)6
K-feldspar	-0.57	-21.44	-20.86	KAlSi3O8
K-mica	7.56	20.82	13.26	KAl3Si3O10(OH)2
Kaolinite	4.15	11.92	7.77	Al2Si2O5(OH)4
Manganite	-11.45	13.89	25.34	MnOOH
Melanterite	-8.50	-10.76	-2.26	FeSO4:7H2O
O2(g)	-1.70	-4.56	-2.86	O2
Pyrochroite	-6.91	8.29	15.20	Mn(OH)2
Pyrolusite	-22.50	19.49	42.00	MnO2:H2O
Quartz	0.40	-3.64	-4.04	SiO2
Rhodochrosite	-0.21	-11.33	-11.12	MnCO3
Sepiolite	-4.18	11.68	15.86	Mg2Si3O7.5OH:3H2O
Sepiolite(d)	-6.98	11.68	18.66	Mg2Si3O7.5OH:3H2O
Siderite	0.54	-10.33	-10.87	FeCO3
SiO2(a)	-0.90	-3.64	-2.74	SiO2
Strontianite	-1.64	-10.91	-9.27	SrCO3
Sylvite	-8.95	-8.07	0.88	KCl
Talc	-2.50	19.34	21.84	Mg3Si4O10(OH)2
Vivianite	-2.91	-38.91	-36.00	Fe3(PO4)2:8H2O
Witherite	-2.08	-10.66	-8.57	BaCO3

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
For ideal gases, phi = 1.

Initial solution 8.

-----------------------------Solution composition-----------------------------

Elements	Molality	Moles
Al	5.195e-07	5.195e-07
Alkalinity	8.009e-04	8.009e-04
Ba	1.385e-05	1.385e-05
Ca	2.026e-03	2.026e-03
Cl	2.213e-02	2.213e-02
F	6.851e-06	6.851e-06
Fe	8.964e-07	8.964e-07
K	1.511e-04	1.511e-04
Mg	6.624e-03	6.624e-03
Mn	2.078e-05	2.078e-05
N(3)	6.434e-06	6.434e-06
N(5)	2.706e-03	2.706e-03
Na	5.575e-03	5.575e-03
O(0)	7.259e-05	7.259e-05
P	4.849e-06	4.849e-06
S(6)	1.624e-04	1.624e-04
Si	1.433e-04	1.433e-04
Sr	1.383e-05	1.383e-05

----------------------------Description of solution----------------------------

pH	= 5.650
pe	= 3.135
Specific Conductance (µS/cm, 25°C)	= 2660
Density (g/cm³)	= 0.99816
Volume (L)	= 1.00340
Activity of water	= 0.999
Ionic strength (mol/kgw)	= 3.263e-02
Mass of water (kg)	= 1.000e+00
Total carbon (mol/kg)	= 4.033e-03
Total CO2 (mol/kg)	= 4.033e-03
Temperature (°C)	= 25.00
Electrical balance (eq)	= -2.851e-03
Percent error, 100*(Cat-|An|)/(Cat+|An|)	= -5.96
Iterations	= 13 (82 overall)
Total H	= 1.110138e+02
Total O	= 5.552453e+01

---------------------------------Redox couples---------------------------------

Redox couple	pe	Eh (volts)
N(3)/N(5)	9.9471	0.5884
O(-2)/O(0)	14.7609	0.8732

----------------------------Distribution of species----------------------------

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma	mole V cm³/mol
H+	2.571e-06	2.239e-06	-5.590	-5.650	-0.060	0.00
OH-	5.385e-09	4.518e-09	-8.269	-8.345	-0.076	-3.93
H2O	5.551e+01	9.993e-01	1.744	-0.000	0.000	18.07
Al	5.195e-07					
AlF2+	2.435e-07	2.073e-07	-6.614	-6.683	-0.070	(0)
AlF+2	1.884e-07	9.910e-08	-6.725	-7.004	-0.279	(0)
Al(OH)2+	4.324e-08	3.682e-08	-7.364	-7.434	-0.070	(0)
AlOH+2	2.001e-08	1.053e-08	-7.699	-7.978	-0.279	-27.36
AlF3	1.081e-08	1.090e-08	-7.966	-7.963	0.003	(0)
Al+3	8.241e-09	2.374e-09	-8.084	-8.625	-0.541	-41.52
Al(OH)4-	2.409e-09	2.037e-09	-8.618	-8.691	-0.073	(0)

Al(OH)3	2.404e-09	2.422e-09	-8.619	-8.616	0.003	(0)
AlSO4+	4.861e-10	4.112e-10	-9.313	-9.386	-0.073	(0)
AlF4-	2.141e-11	1.811e-11	-10.669	-10.742	-0.073	(0)
Al(SO4)2-	8.419e-13	7.121e-13	-12.075	-12.147	-0.073	(0)
AlHSO4+2	1.599e-16	8.162e-17	-15.796	-16.088	-0.292	(0)
Ba	1.385e-05					
Ba+2	1.316e-05	6.707e-06	-4.881	-5.173	-0.293	-12.31
BaCl+	4.546e-07	3.842e-07	-6.342	-6.415	-0.073	(0)
BaSO4	1.827e-07	1.841e-07	-6.738	-6.735	0.003	(0)
BaHCO3+	4.914e-08	4.153e-08	-7.309	-7.382	-0.073	(0)
BaNO3+	2.258e-09	1.908e-09	-8.646	-8.719	-0.073	(0)
BaCO3	4.654e-11	4.689e-11	-10.332	-10.329	0.003	-10.70
BaOH+	1.195e-13	1.014e-13	-12.923	-12.994	-0.071	(0)
C(4)	4.033e-03					
CO2	3.230e-03	3.254e-03	-2.491	-2.488	0.003	34.43
HCO3-	7.586e-04	6.460e-04	-3.120	-3.190	-0.070	24.90
MgHCO3+	3.145e-05	2.649e-05	-4.502	-4.577	-0.074	5.59
CaHCO3+	1.017e-05	8.700e-06	-4.993	-5.060	-0.068	9.77
NaHCO3	1.561e-06	1.573e-06	-5.807	-5.803	0.003	1.80
MnHCO3+	6.919e-07	5.875e-07	-6.160	-6.231	-0.071	(0)
(CO2)2	1.929e-07	1.944e-07	-6.715	-6.711	0.003	68.87
SrHCO3+	8.383e-08	7.138e-08	-7.077	-7.146	-0.070	(0)
BaHCO3+	4.914e-08	4.153e-08	-7.309	-7.382	-0.073	(0)
MgCO3	4.492e-08	4.526e-08	-7.348	-7.344	0.003	-17.09
FeHCO3+	3.446e-08	2.913e-08	-7.463	-7.536	-0.073	(0)
CO3-2	2.573e-08	1.353e-08	-7.590	-7.869	-0.279	-4.69
CaCO3	2.382e-08	2.400e-08	-7.623	-7.620	0.003	-14.60
MnCO3	1.089e-08	1.097e-08	-7.963	-7.960	0.003	(0)
NaCO3-	1.291e-09	1.091e-09	-8.889	-8.962	-0.073	-0.74
FeCO3	1.453e-10	1.464e-10	-9.838	-9.835	0.003	(0)
SrCO3	6.194e-11	6.241e-11	-10.208	-10.205	0.003	-14.13
BaCO3	4.654e-11	4.689e-11	-10.332	-10.329	0.003	-10.70
Ca	2.026e-03					
Ca+2	2.006e-03	1.055e-03	-2.698	-2.977	-0.279	-17.72
CaSO4	1.020e-05	1.028e-05	-4.991	-4.988	0.003	7.50
CaHCO3+	1.017e-05	8.700e-06	-4.993	-5.060	-0.068	9.77
CaH2PO4+	1.038e-07	8.836e-08	-6.984	-7.054	-0.070	(0)
CaHPO4	5.212e-08	5.251e-08	-7.283	-7.280	0.003	(0)
CaCO3	2.382e-08	2.400e-08	-7.623	-7.620	0.003	-14.60
CaHSO4+	1.790e-10	1.513e-10	-9.747	-9.820	-0.073	(0)
CaOH+	9.251e-11	7.819e-11	-10.034	-10.107	-0.073	(0)
CaPO4-	6.517e-11	5.550e-11	-10.186	-10.256	-0.070	(0)
Cl	2.213e-02					
Cl-	2.166e-02	1.821e-02	-1.664	-1.740	-0.075	18.21
NaCl	4.683e-04	4.718e-04	-3.330	-3.326	0.003	(0)
MnCl+	8.916e-07	7.570e-07	-6.050	-6.121	-0.071	-2.99
BaCl+	4.546e-07	3.842e-07	-6.342	-6.415	-0.073	(0)
FeCl+	1.341e-08	1.133e-08	-7.873	-7.946	-0.073	(0)
MnCl2	5.973e-09	6.019e-09	-8.224	-8.221	0.003	85.89
MnCl3-	3.556e-11	3.019e-11	-10.449	-10.520	-0.071	43.57
FeCl+2	6.217e-17	3.231e-17	-16.206	-16.491	-0.284	(0)
FeCl2+	3.096e-18	2.629e-18	-17.509	-17.580	-0.071	(0)
FeCl3	4.752e-21	4.788e-21	-20.323	-20.320	0.003	(0)
F	6.851e-06					
F-	4.976e-06	4.174e-06	-5.303	-5.379	-0.076	-1.17
MgF+	1.143e-06	9.666e-07	-5.942	-6.015	-0.073	-10.47
AlF2+	2.435e-07	2.073e-07	-6.614	-6.683	-0.070	(0)
AlF+2	1.884e-07	9.910e-08	-6.725	-7.004	-0.279	(0)
HF	1.391e-08	1.402e-08	-7.857	-7.853	0.003	12.50
AlF3	1.081e-08	1.090e-08	-7.966	-7.963	0.003	(0)
NaF	1.032e-08	1.040e-08	-7.986	-7.983	0.003	7.26
MnF+	3.471e-10	2.947e-10	-9.460	-9.531	-0.071	(0)
FeF+	2.227e-11	1.882e-11	-10.652	-10.725	-0.073	(0)
AlF4-	2.141e-11	1.811e-11	-10.669	-10.742	-0.073	(0)
HF2-	2.656e-13	2.245e-13	-12.576	-12.649	-0.073	22.20
FeF+2	7.479e-16	3.887e-16	-15.126	-15.410	-0.284	(0)
FeF2+	7.608e-17	6.460e-17	-16.119	-16.190	-0.071	(0)
FeF3	4.242e-19	4.274e-19	-18.372	-18.369	0.003	(0)

SiF6-2	5.605e-29	2.913e-29	-28.251	-28.536	-0.284	43.13
Fe(2)	8.964e-07					
Fe+2	8.429e-07	4.508e-07	-6.074	-6.346	-0.272	-21.73
FeHCO3+	3.446e-08	2.913e-08	-7.463	-7.536	-0.073	(0)
FeCl+	1.341e-08	1.133e-08	-7.873	-7.946	-0.073	(0)
FeSO4	4.358e-09	4.391e-09	-8.361	-8.357	0.003	18.97
FeH2PO4+	8.682e-10	7.393e-10	-9.061	-9.131	-0.070	(0)
FeHPO4	1.617e-10	1.629e-10	-9.791	-9.788	0.003	(0)
FeCO3	1.453e-10	1.464e-10	-9.838	-9.835	0.003	(0)
FeOH+	7.495e-11	6.364e-11	-10.125	-10.196	-0.071	(0)
FeF+	2.227e-11	1.882e-11	-10.652	-10.725	-0.073	(0)
FeHSO4+	7.645e-14	6.462e-14	-13.117	-13.190	-0.073	(0)
Fe(OH)2	2.399e-16	2.418e-16	-15.620	-15.617	0.003	(0)
Fe(OH)3-	4.722e-21	4.009e-21	-20.326	-20.397	-0.071	(0)
Fe(3)	3.114e-11					
Fe(OH)2+	2.939e-11	2.503e-11	-10.532	-10.602	-0.070	(0)
Fe(OH)3	1.428e-12	1.439e-12	-11.845	-11.842	0.003	(0)
FeOH+2	3.258e-13	1.693e-13	-12.487	-12.771	-0.284	(0)
FeF+2	7.479e-16	3.887e-16	-15.126	-15.410	-0.284	(0)
Fe(OH)4-	6.879e-16	5.858e-16	-15.162	-15.232	-0.070	(0)
Fe+3	2.040e-16	5.875e-17	-15.690	-16.231	-0.541	(0)
FeH2PO4+2	9.839e-17	5.174e-17	-16.007	-16.286	-0.279	(0)
FeF2+	7.608e-17	6.460e-17	-16.119	-16.190	-0.071	(0)
FeCl+2	6.217e-17	3.231e-17	-16.206	-16.491	-0.284	(0)
FeSO4+	4.155e-17	3.528e-17	-16.381	-16.452	-0.071	(0)
FeCl2+	3.096e-18	2.629e-18	-17.509	-17.580	-0.071	(0)
FeHPO4+	1.690e-18	1.435e-18	-17.772	-17.843	-0.071	(0)
FeF3	4.242e-19	4.274e-19	-18.372	-18.369	0.003	(0)
Fe(SO4)2-	5.002e-20	4.228e-20	-19.301	-19.374	-0.073	(0)
FeCl3	4.752e-21	4.788e-21	-20.323	-20.320	0.003	(0)
FeHSO4+2	4.145e-22	2.115e-22	-21.382	-21.675	-0.292	(0)
Fe2(OH)2+4	1.138e-23	7.716e-25	-22.944	-24.113	-1.169	(0)
Fe3(OH)4+5	2.703e-31	4.034e-33	-30.568	-32.394	-1.826	(0)
H(0)	3.782e-21					
H2	1.891e-21	1.905e-21	-20.723	-20.720	0.003	28.61
K	1.511e-04					
K+	1.510e-04	1.268e-04	-3.821	-3.897	-0.076	9.13
KSO4-	5.732e-08	4.881e-08	-7.242	-7.311	-0.070	34.25
KHPO4-	2.635e-11	2.244e-11	-10.579	-10.649	-0.070	38.29
Mg	6.624e-03					
Mg+2	6.546e-03	3.505e-03	-2.184	-2.455	-0.271	-21.41
MgSO4	4.466e-05	4.500e-05	-4.350	-4.347	0.003	5.84
MgHCO3+	3.145e-05	2.649e-05	-4.502	-4.577	-0.074	5.59
MgF+	1.143e-06	9.666e-07	-5.942	-6.015	-0.073	-10.47
MgH2PO4+	4.388e-07	3.736e-07	-6.358	-6.428	-0.070	(0)
MgHPO4	2.340e-07	2.358e-07	-6.631	-6.628	0.003	(0)
MgCO3	4.492e-08	4.526e-08	-7.348	-7.344	0.003	-17.09
MgOH+	6.619e-09	5.680e-09	-8.179	-8.246	-0.066	(0)
MgPO4-	2.919e-10	2.486e-10	-9.535	-9.605	-0.070	(0)
Mn(2)	2.078e-05					
Mn+2	1.908e-05	1.020e-05	-4.719	-4.991	-0.272	-19.05
MnCl+	8.916e-07	7.570e-07	-6.050	-6.121	-0.071	-2.99
MnHCO3+	6.919e-07	5.875e-07	-6.160	-6.231	-0.071	(0)
MnSO4	9.864e-08	9.938e-08	-7.006	-7.003	0.003	22.54
MnCO3	1.089e-08	1.097e-08	-7.963	-7.960	0.003	(0)
MnCl2	5.973e-09	6.019e-09	-8.224	-8.221	0.003	85.89
MnF+	3.471e-10	2.947e-10	-9.460	-9.531	-0.071	(0)
Mn(NO3)2	2.059e-10	2.074e-10	-9.686	-9.683	0.003	41.04
MnOH+	1.379e-10	1.171e-10	-9.861	-9.932	-0.071	(0)
MnCl3-	3.556e-11	3.019e-11	-10.449	-10.520	-0.071	43.57
Mn(OH)3-	1.694e-23	1.438e-23	-22.771	-22.842	-0.071	(0)
Mn(3)	1.494e-27					
Mn+3	1.494e-27	4.303e-28	-26.826	-27.366	-0.541	(0)
N(3)	6.434e-06					
NO2-	6.434e-06	5.373e-06	-5.192	-5.270	-0.078	25.11
N(5)	2.706e-03					
NO3-	2.706e-03	2.260e-03	-2.568	-2.646	-0.078	29.63
BaNO3+	2.258e-09	1.908e-09	-8.646	-8.719	-0.073	(0)

Mn(NO3)2	2.059e-10	2.074e-10	-9.686	-9.683	0.003	41.04
Na	5.575e-03					
Na+	5.104e-03	4.329e-03	-2.292	-2.364	-0.071	-1.27
NaCl	4.683e-04	4.718e-04	-3.330	-3.326	0.003	(0)
NaHCO3	1.561e-06	1.573e-06	-5.807	-5.803	0.003	1.80
NaSO4-	1.395e-06	1.188e-06	-5.855	-5.925	-0.070	15.05
NaF	1.032e-08	1.040e-08	-7.986	-7.983	0.003	7.26
NaCO3-	1.291e-09	1.091e-09	-8.889	-8.962	-0.073	-0.74
NaHPO4-	8.994e-10	7.659e-10	-9.046	-9.116	-0.070	35.85
NaOH	1.941e-21	1.956e-21	-20.712	-20.709	0.003	(0)
O(0)	7.259e-05					
O2	3.630e-05	3.657e-05	-4.440	-4.437	0.003	30.40
P	4.849e-06					
H2PO4-	3.842e-06	3.272e-06	-5.415	-5.485	-0.070	33.38
MgH2PO4+	4.388e-07	3.736e-07	-6.358	-6.428	-0.070	(0)
MgHPO4	2.340e-07	2.358e-07	-6.631	-6.628	0.003	(0)
HPO4-2	1.746e-07	9.074e-08	-6.758	-7.042	-0.284	7.27
CaH2PO4+	1.038e-07	8.836e-08	-6.984	-7.054	-0.070	(0)
CaHPO4	5.212e-08	5.251e-08	-7.283	-7.280	0.003	(0)
H3PO4	1.070e-09	1.079e-09	-8.970	-8.967	0.003	47.41
NaHPO4-	8.994e-10	7.659e-10	-9.046	-9.116	-0.070	35.85
FeH2PO4+	8.682e-10	7.393e-10	-9.061	-9.131	-0.070	(0)
MgPO4-	2.919e-10	2.486e-10	-9.535	-9.605	-0.070	(0)
FeHPO4	1.617e-10	1.629e-10	-9.791	-9.788	0.003	(0)
CaPO4-	6.517e-11	5.550e-11	-10.186	-10.256	-0.070	(0)
KHPO4-	2.635e-11	2.244e-11	-10.579	-10.649	-0.070	38.29
PO4-3	8.549e-14	1.827e-14	-13.068	-13.738	-0.670	-22.01
FeH2PO4+2	9.839e-17	5.174e-17	-16.007	-16.286	-0.279	(0)
FeHPO4+	1.690e-18	1.435e-18	-17.772	-17.843	-0.071	(0)
S(6)	1.624e-04					
SO4-2	1.057e-04	5.477e-05	-3.976	-4.261	-0.286	15.07
MgSO4	4.466e-05	4.500e-05	-4.350	-4.347	0.003	5.84
CaSO4	1.020e-05	1.028e-05	-4.991	-4.988	0.003	7.50
NaSO4-	1.395e-06	1.188e-06	-5.855	-5.925	-0.070	15.05
BaSO4	1.827e-07	1.841e-07	-6.738	-6.735	0.003	(0)
MnSO4	9.864e-08	9.938e-08	-7.006	-7.003	0.003	22.54
SrSO4	7.657e-08	7.714e-08	-7.116	-7.113	0.003	24.24
KSO4-	5.732e-08	4.881e-08	-7.242	-7.311	-0.070	34.25
HSO4-	1.410e-08	1.192e-08	-7.851	-7.924	-0.073	40.41
FeSO4	4.358e-09	4.391e-09	-8.361	-8.357	0.003	18.97
AlSO4+	4.861e-10	4.112e-10	-9.313	-9.386	-0.073	(0)
CaHSO4+	1.790e-10	1.513e-10	-9.747	-9.820	-0.073	(0)
Al(SO4)2-	8.419e-13	7.121e-13	-12.075	-12.147	-0.073	(0)
FeHSO4+	7.645e-14	6.462e-14	-13.117	-13.190	-0.073	(0)
AlHSO4+2	1.599e-16	8.162e-17	-15.796	-16.088	-0.292	(0)
FeSO4+	4.155e-17	3.528e-17	-16.381	-16.452	-0.071	(0)
Fe(SO4)2-	5.002e-20	4.228e-20	-19.301	-19.374	-0.073	(0)
FeHSO4+2	4.145e-22	2.115e-22	-21.382	-21.675	-0.292	(0)
Si	1.433e-04					
H4SiO4	1.433e-04	1.444e-04	-3.844	-3.840	0.003	52.08
H3SiO4-	1.129e-08	9.510e-09	-7.947	-8.022	-0.074	28.11
H2SiO4-2	5.494e-16	2.889e-16	-15.260	-15.539	-0.279	(0)
SiF6-2	5.605e-29	2.913e-29	-28.251	-28.536	-0.284	43.13
Sr	1.383e-05					
Sr+2	1.367e-05	7.224e-06	-4.864	-5.141	-0.277	-17.38
SrHCO3+	8.383e-08	7.138e-08	-7.077	-7.146	-0.070	(0)
SrSO4	7.657e-08	7.714e-08	-7.116	-7.113	0.003	24.24
SrCO3	6.194e-11	6.241e-11	-10.208	-10.205	0.003	-14.13
SrOH+	1.948e-13	1.654e-13	-12.711	-12.782	-0.071	(0)

----------Distribution of alkalinity----------

Total alkalinity (eq/kgw) = 8.009e-04

Species	Alkalinity	Molality	Alk/Mol
HCO3-	7.586e-04	7.586e-04	1.00
MgHCO3+	3.145e-05	3.145e-05	1.00

CaHCO3+	1.017e-05	1.017e-05	1.00
H+	-2.571e-06	2.571e-06	-1.00
NaHCO3	1.561e-06	1.561e-06	1.00
MnHCO3+	6.919e-07	6.919e-07	1.00
MgHPO4	2.340e-07	2.340e-07	1.00
HPO4-2	1.746e-07	1.746e-07	1.00
MgCO3	8.984e-08	4.492e-08	2.00
Al(OH)2+	8.648e-08	4.324e-08	2.00
SrHCO3+	8.383e-08	8.383e-08	1.00
CaHPO4	5.212e-08	5.212e-08	1.00
CO3-2	5.147e-08	2.573e-08	2.00
BaHCO3+	4.914e-08	4.914e-08	1.00
CaCO3	4.763e-08	2.382e-08	2.00
FeHCO3+	3.446e-08	3.446e-08	1.00
MnCO3	2.177e-08	1.089e-08	2.00
AlOH+2	2.001e-08	2.001e-08	1.00
HSO4-	-1.410e-08	1.410e-08	-1.00
HF	-1.391e-08	1.391e-08	-1.00
H3SiO4-	1.129e-08	1.129e-08	1.00
Al(OH)4-	9.634e-09	2.409e-09	4.00
Al(OH)3	7.211e-09	2.404e-09	3.00
MgOH+	6.619e-09	6.619e-09	1.00
OH-	5.385e-09	5.385e-09	1.00
NaCO3-	2.581e-09	1.291e-09	2.00
H3PO4	-1.070e-09	1.070e-09	-1.00
NaHPO4-	8.994e-10	8.994e-10	1.00
MgPO4-	5.838e-10	2.919e-10	2.00
FeCO3	2.905e-10	1.453e-10	2.00
CaHSO4+	-1.790e-10	1.790e-10	-1.00
FeHPO4	1.617e-10	1.617e-10	1.00
MnOH+	1.379e-10	1.379e-10	1.00
CaPO4-	1.303e-10	6.517e-11	2.00
SrCO3	1.239e-10	6.194e-11	2.00
BaCO3	9.308e-11	4.654e-11	2.00
CaOH+	9.251e-11	9.251e-11	1.00
FeOH+	7.495e-11	7.495e-11	1.00
KHPO4-	2.635e-11	2.635e-11	1.00
Fe(OH)3	1.428e-12	1.428e-12	1.00
FeOH+2	-3.258e-13	3.258e-13	-1.00
HF2-	-2.656e-13	2.656e-13	-1.00
SrOH+	1.948e-13	1.948e-13	1.00
PO4-3	1.710e-13	8.549e-14	2.00
BaOH+	1.195e-13	1.195e-13	1.00
FeHSO4+	-7.645e-14	7.645e-14	-1.00
FeF+2	-1.496e-15	7.479e-16	-2.00
Fe(OH)4-	1.376e-15	6.879e-16	2.00
H2SiO4-2	1.099e-15	5.494e-16	2.00
Fe(OH)2	4.799e-16	2.399e-16	2.00
Fe+3	-4.079e-16	2.040e-16	-2.00
FeH2PO4+2	-1.968e-16	9.839e-17	-2.00
AlHSO4+2	-1.599e-16	1.599e-16	-1.00
FeF2+	-1.522e-16	7.608e-17	-2.00
FeCl+2	-1.243e-16	6.217e-17	-2.00
FeSO4+	-8.311e-17	4.155e-17	-2.00
FeCl2+	-6.192e-18	3.096e-18	-2.00
FeHPO4+	-1.690e-18	1.690e-18	-1.00
FeF3	-8.484e-19	4.242e-19	-2.00
Fe(SO4)2-	-1.000e-19	5.002e-20	-2.00
Fe(OH)3-	1.417e-20	4.722e-21	3.00
FeCl3	-9.504e-21	4.752e-21	-2.00
NaOH	1.941e-21	1.941e-21	1.00
FeHSO4+2	-1.243e-21	4.145e-22	-3.00
Mn(OH)3-	5.081e-23	1.694e-23	3.00
Fe2(OH)2+4	-2.276e-23	1.138e-23	-2.00
SiF6-2	-2.242e-28	5.605e-29	-4.00
Fe3(OH)4+5	-5.405e-31	2.703e-31	-2.00

Saturation indices

Phase	SI**	log IAP	log K(298 K, 1 atm)	
Al(OH)3(a)	-2.48	8.32	10.80	Al(OH)3
Albite	-4.57	-22.57	-18.00	NaAlSi3O8
Alunite	-3.00	-4.40	-1.40	KAl3(SO4)2(OH)6
Anhydrite	-2.96	-7.24	-4.28	CaSO4
Anorthite	-8.32	-28.04	-19.71	CaAl2Si2O8
Aragonite	-2.51	-10.85	-8.34	CaCO3
BaCl2	-10.88	-8.65	2.23	BaCl2
BaCl2:2H2O	-8.86	-8.65	0.21	BaCl2:2H2O
BaCl2:H2O	-9.48	-8.65	0.82	BaCl2:H2O
Barite	0.41	-9.43	-9.84	BaSO4
Ca-Montmorillonite	-1.10	-46.13	-45.03	Ca0.165Al2.33Si3.67O10(OH)2
Calcite	-2.37	-10.85	-8.48	CaCO3
Celestite	-2.74	-9.40	-6.66	SrSO4
Chalcedony	-0.29	-3.84	-3.55	SiO2
Chlorite(14A)	-19.03	49.35	68.38	Mg5Al2Si3O10(OH)8
Chrysotile	-13.35	18.85	32.20	Mg3Si2O5(OH)4
CO2(g)	-1.02	-2.49	-1.47	CO2
Dolomite	-4.08	-21.17	-17.09	CaMg(CO3)2
Fe(OH)3(a)	-4.17	0.72	4.89	Fe(OH)3
Fluorite	-3.14	-13.74	-10.60	CaF2
Gibbsite	0.21	8.32	8.11	Al(OH)3
Goethite	1.72	0.72	-1.00	FeOOH
Gypsum	-2.66	-7.24	-4.58	CaSO4:2H2O
H2(g)	-17.62	-20.72	-3.10	H2
H2O(g)	-1.50	-0.00	1.50	H2O
Halite	-5.67	-4.10	1.57	NaCl
Hausmannite	-24.54	36.49	61.03	Mn3O4
Hematite	5.45	1.44	-4.01	Fe2O3
Hydroxyapatite	-9.99	-13.41	-3.42	Ca5(PO4)3OH
Illite	-2.89	-43.16	-40.27	K0.6Mg0.25Al2.3Si3.5O10(OH)2
Jarosite-K	-18.00	-27.21	-9.21	KFe3(SO4)2(OH)6
K-feldspar	-3.53	-24.11	-20.57	KAlSi3O8
K-mica	2.51	15.21	12.70	KAl3Si3O10(OH)2
Kaolinite	1.53	8.97	7.43	Al2Si2O5(OH)4
Manganite	-10.25	15.09	25.34	MnOOH
Melanterite	-8.40	-10.61	-2.21	FeSO4:7H2O
O2(g)	-1.54	-4.44	-2.89	O2
Pyrochroite	-8.89	6.31	15.20	Mn(OH)2
Pyrolusite	-17.50	23.88	41.38	MnO2:H2O
Quartz	0.14	-3.84	-3.98	SiO2
Rhodochrosite	-1.73	-12.86	-11.13	MnCO3
Sepiolite	-9.59	6.17	15.76	Mg2Si3O7.5OH:3H2O
Sepiolite(d)	-12.49	6.17	18.66	Mg2Si3O7.5OH:3H2O
Siderite	-3.32	-14.21	-10.89	FeCO3
SiO2(a)	-1.13	-3.84	-2.71	SiO2
Strontianite	-3.74	-13.01	-9.27	SrCO3
Sylvite	-6.54	-5.64	0.90	KCl
Talc	-10.23	11.17	21.40	Mg3Si4O10(OH)2
Vivianite	-10.52	-46.52	-36.00	Fe3(PO4)2:8H2O
Witherite	-4.48	-13.04	-8.56	BaCO3

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
For ideal gases, phi = 1.

Initial solution 9.

-----Solution composition-----

Elements	Molality	Moles
Al	1.038e-06	1.038e-06
Alkalinity	5.000e-04	5.000e-04
Ba	4.442e-06	4.442e-06
Ca	3.020e-04	3.020e-04
Cl	2.605e-03	2.605e-03

F	7.370e-06	7.370e-06
Fe	1.433e-06	1.433e-06
K	7.929e-05	7.929e-05
Mg	1.160e-03	1.160e-03
Mn	2.367e-06	2.367e-06
N(3)	1.143e-05	1.143e-05
N(5)	2.242e-04	2.242e-04
Na	1.523e-04	1.523e-04
O(0)	8.064e-05	8.064e-05
P	1.937e-06	1.937e-06
S(6)	5.102e-06	5.102e-06
Si	1.343e-04	1.343e-04
Sr	3.539e-06	3.539e-06

----------Description of solution----------

pH	= 5.360
pe	= 3.315
Specific Conductance (µS/cm, 22°C)	= 352
Density (g/cm³)	= 0.99808
Volume (L)	= 1.00233
Activity of water	= 1.000
Ionic strength (mol/kgw)	= 4.734e-03
Mass of water (kg)	= 1.000e+00
Total carbon (mol/kg)	= 5.269e-03
Total CO2 (mol/kg)	= 5.269e-03
Temperature (°C)	= 21.50
Electrical balance (eq)	= -1.789e-04
Percent error, 100*(Cat-|An|)/(Cat+|An|)	= -2.74
Iterations	= 13 (95 overall)
Total H	= 1.110135e+02
Total O	= 5.551860e+01

----------Redox couples----------

Redox couple	pe	Eh (volts)
N(3)/N(5)	9.7619	0.5707
O(-2)/O(0)	15.3549	0.8977

----------Distribution of species----------

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma	mole V cm³/mol
H+	4.667e-06	4.365e-06	-5.331	-5.360	-0.029	0.00
OH-	1.903e-09	1.767e-09	-8.720	-8.753	-0.032	-4.22
H2O	5.551e+01	9.998e-01	1.744	-0.000	0.000	18.05
Al	1.038e-06					
AlF2+	6.403e-07	5.961e-07	-6.194	-6.225	-0.031	(0)
AlF+2	3.258e-07	2.446e-07	-6.487	-6.611	-0.124	(0)
AlF3	3.699e-08	3.703e-08	-7.432	-7.431	0.000	(0)
Al(OH)2+	1.289e-08	1.200e-08	-7.890	-7.921	-0.031	(0)
AlOH+2	1.215e-08	9.128e-09	-7.915	-8.040	-0.124	-27.52
Al+3	9.203e-09	5.046e-09	-8.036	-8.297	-0.261	-41.81
Al(OH)3	3.107e-10	3.110e-10	-9.508	-9.507	0.000	(0)
Al(OH)4-	1.382e-10	1.285e-10	-9.860	-9.891	-0.032	(0)
AlF4-	7.846e-11	7.294e-11	-10.105	-10.137	-0.032	(0)
AlSO4+	5.347e-11	4.971e-11	-10.272	-10.304	-0.032	(0)
Al(SO4)2-	5.424e-15	5.043e-15	-14.266	-14.297	-0.032	(0)
AlHSO4+2	2.507e-17	1.868e-17	-16.601	-16.729	-0.128	(0)
Ba	4.442e-06					
Ba+2	4.397e-06	3.280e-06	-5.357	-5.484	-0.127	-12.83
BaCl+	2.545e-08	2.365e-08	-7.594	-7.626	-0.032	(0)
BaHCO3+	1.405e-08	1.306e-08	-7.852	-7.884	-0.032	(0)
BaSO4	5.356e-09	5.362e-09	-8.271	-8.271	0.000	(0)
BaNO3+	9.244e-11	8.589e-11	-10.034	-10.066	-0.032	(0)
BaCO3	7.301e-12	7.309e-12	-11.137	-11.136	0.000	-10.73

BaOH+	2.737e-14	2.546e-14	-13.563	-13.594	-0.031	(0)
C(4)	5.269e-03					
CO2	4.764e-03	4.769e-03	-2.322	-2.322	0.000	34.26
HCO3-	4.981e-04	4.636e-04	-3.303	-3.334	-0.031	24.45
MgHCO3+	5.002e-06	4.646e-06	-5.301	-5.333	-0.032	5.40
CaHCO3+	1.352e-06	1.259e-06	-5.869	-5.900	-0.031	9.56
(CO2)2	3.706e-07	3.710e-07	-6.431	-6.431	0.000	68.52
MnHCO3+	7.601e-08	7.071e-08	-7.119	-7.151	-0.031	(0)
FeHCO3+	5.172e-08	4.805e-08	-7.286	-7.318	-0.032	(0)
NaHCO3	3.713e-08	3.717e-08	-7.430	-7.430	0.000	1.80
SrHCO3+	1.787e-08	1.664e-08	-7.748	-7.779	-0.031	(0)
BaHCO3+	1.405e-08	1.306e-08	-7.852	-7.884	-0.032	(0)
CO3-2	6.161e-09	4.627e-09	-8.210	-8.335	-0.124	-5.44
MgCO3	3.631e-09	3.635e-09	-8.440	-8.439	0.000	-17.09
CaCO3	1.639e-09	1.641e-09	-8.785	-8.785	0.000	-14.61
MnCO3	6.282e-10	6.289e-10	-9.202	-9.201	0.000	(0)
FeCO3	1.149e-10	1.150e-10	-9.940	-9.939	0.000	(0)
NaCO3-	1.084e-11	1.007e-11	-10.965	-10.997	-0.032	-1.32
BaCO3	7.301e-12	7.309e-12	-11.137	-11.136	0.000	-10.73
SrCO3	7.035e-12	7.042e-12	-11.153	-11.152	0.000	-14.14
Ca	3.020e-04					
Ca+2	3.005e-04	2.255e-04	-3.522	-3.647	-0.125	-18.06
CaHCO3+	1.352e-06	1.259e-06	-5.869	-5.900	-0.031	9.56
CaSO4	1.272e-07	1.274e-07	-6.895	-6.895	0.000	7.36
CaH2PO4+	9.855e-09	9.174e-09	-8.006	-8.037	-0.031	(0)
CaHPO4	2.744e-09	2.747e-09	-8.562	-8.561	0.000	(0)
CaCO3	1.639e-09	1.641e-09	-8.785	-8.785	0.000	-14.61
CaOH+	9.226e-12	8.572e-12	-11.035	-11.067	-0.032	(0)
CaHSO4+	3.746e-12	3.481e-12	-11.426	-11.458	-0.032	(0)
CaPO4-	1.496e-12	1.393e-12	-11.825	-11.856	-0.031	(0)
Cl	2.605e-03					
Cl-	2.603e-03	2.417e-03	-2.584	-2.617	-0.032	18.00
NaCl	1.969e-06	1.972e-06	-5.706	-5.705	0.000	(0)
BaCl+	2.545e-08	2.365e-08	-7.594	-7.626	-0.032	(0)
MnCl+	1.811e-08	1.685e-08	-7.742	-7.773	-0.031	-3.98
FeCl+	3.722e-09	3.459e-09	-8.429	-8.461	-0.032	(0)
MnCl2	1.776e-11	1.778e-11	-10.750	-10.750	0.000	90.40
MnCl3-	1.273e-14	1.184e-14	-13.895	-13.927	-0.031	43.52
FeCl+2	1.466e-17	1.099e-17	-16.834	-16.959	-0.125	(0)
FeCl2+	1.427e-19	1.327e-19	-18.846	-18.877	-0.031	(0)
FeCl3	3.205e-23	3.209e-23	-22.494	-22.494	0.000	(0)
F	7.370e-06					
F-	5.335e-06	4.952e-06	-5.273	-5.305	-0.032	-1.33
AlF2+	6.403e-07	5.961e-07	-6.194	-6.225	-0.031	(0)
AlF+2	3.258e-07	2.446e-07	-6.487	-6.611	-0.124	(0)
MgF+	2.868e-07	2.666e-07	-6.542	-6.574	-0.032	-10.54
AlF3	3.699e-08	3.703e-08	-7.432	-7.431	0.000	(0)
HF	3.042e-08	3.045e-08	-7.517	-7.516	0.000	12.33
NaF	3.977e-10	3.982e-10	-9.400	-9.400	0.000	7.12
AlF4-	7.846e-11	7.294e-11	-10.105	-10.137	-0.032	(0)
MnF+	6.302e-11	5.863e-11	-10.201	-10.232	-0.031	(0)
FeF+	5.524e-11	5.133e-11	-10.258	-10.290	-0.032	(0)
HF2-	6.052e-13	5.623e-13	-12.218	-12.250	-0.032	21.93
FeF+2	1.671e-15	1.252e-15	-14.777	-14.902	-0.125	(0)
FeF2+	2.543e-16	2.366e-16	-15.595	-15.626	-0.031	(0)
FeF3	1.833e-18	1.835e-18	-17.737	-17.736	0.000	(0)
SiF6-2	2.017e-27	1.511e-27	-26.695	-26.821	-0.125	42.48
Fe(2)	1.433e-06					
Fe+2	1.375e-06	1.036e-06	-5.862	-5.984	-0.123	-22.25
FeHCO3+	5.172e-08	4.805e-08	-7.286	-7.318	-0.032	(0)
FeCl+	3.722e-09	3.459e-09	-8.429	-8.461	-0.032	(0)
FeH2PO4+	9.498e-10	8.841e-10	-9.022	-9.053	-0.031	(0)
FeSO4	5.628e-10	5.634e-10	-9.250	-9.249	0.000	22.82
FeCO3	1.149e-10	1.150e-10	-9.940	-9.939	0.000	(0)
FeHPO4	9.782e-11	9.793e-11	-10.010	-10.009	0.000	(0)
FeOH+	6.193e-11	5.762e-11	-10.208	-10.239	-0.031	(0)
FeF+	5.524e-11	5.133e-11	-10.258	-10.290	-0.032	(0)
FeHSO4+	1.722e-14	1.600e-14	-13.764	-13.796	-0.032	(0)

Fe(OH)2	8.245e-17	8.254e-17	-16.084	-16.083	0.000	(0)
Fe(OH)3-	7.292e-22	6.784e-22	-21.137	-21.168	-0.031	(0)
Fe(3)	1.501e-11					
Fe(OH)2+	1.440e-11	1.340e-11	-10.842	-10.873	-0.031	(0)
Fe(OH)3	3.386e-13	3.389e-13	-12.470	-12.470	0.000	(0)
FeOH+2	2.698e-13	2.021e-13	-12.569	-12.694	-0.125	(0)
FeF+2	1.671e-15	1.252e-15	-14.777	-14.902	-0.125	(0)
Fe+3	3.071e-16	1.684e-16	-15.513	-15.774	-0.261	(0)
FeF2+	2.543e-16	2.366e-16	-15.595	-15.626	-0.031	(0)
FeH2PO4+2	1.027e-16	7.713e-17	-15.988	-16.113	-0.124	(0)
Fe(OH)4-	6.597e-17	6.141e-17	-16.181	-16.212	-0.031	(0)
FeCl+2	1.466e-17	1.099e-17	-16.834	-16.959	-0.125	(0)
FeSO4+	5.983e-18	5.567e-18	-17.223	-17.254	-0.031	(0)
FeF3	1.833e-18	1.835e-18	-17.737	-17.736	0.000	(0)
FeHPO4+	1.030e-18	9.582e-19	-17.987	-18.019	-0.031	(0)
FeCl2+	1.427e-19	1.327e-19	-18.846	-18.877	-0.031	(0)
Fe(SO4)2-	4.216e-22	3.917e-22	-21.375	-21.407	-0.032	(0)
FeHSO4+2	8.758e-23	6.527e-23	-22.058	-22.185	-0.128	(0)
FeCl3	3.205e-23	3.209e-23	-22.494	-22.494	0.000	(0)
Fe2(OH)2+4	4.126e-24	1.273e-24	-23.384	-23.895	-0.511	(0)
Fe3(OH)4+5	3.104e-32	4.943e-33	-31.508	-32.306	-0.798	(0)
H(0)	6.544e-21					
H2	3.272e-21	3.276e-21	-20.485	-20.485	0.000	28.61
K	7.929e-05					
K+	7.929e-05	7.362e-05	-4.101	-4.133	-0.032	8.92
KSO4-	1.704e-09	1.586e-09	-8.769	-8.800	-0.031	34.04
KHPO4-	3.660e-12	3.407e-12	-11.437	-11.468	-0.031	38.41
Mg	1.160e-03					
Mg+2	1.154e-03	8.688e-04	-2.938	-3.061	-0.123	-21.58
MgHCO3+	5.002e-06	4.646e-06	-5.301	-5.333	-0.032	5.40
MgSO4	6.057e-07	6.063e-07	-6.218	-6.217	0.000	5.70
MgF+	2.868e-07	2.666e-07	-6.542	-6.574	-0.032	-10.54
MgH2PO4+	4.835e-08	4.501e-08	-7.316	-7.347	-0.031	(0)
MgHPO4	1.429e-08	1.431e-08	-7.845	-7.844	0.000	(0)
MgCO3	3.631e-09	3.635e-09	-8.440	-8.439	0.000	-17.09
MgOH+	5.628e-10	5.248e-10	-9.250	-9.280	-0.030	(0)
MgPO4-	7.774e-12	7.237e-12	-11.109	-11.140	-0.031	(0)
Mn(2)	2.367e-06					
Mn+2	2.271e-06	1.711e-06	-5.644	-5.767	-0.123	-20.35
MnHCO3+	7.601e-08	7.071e-08	-7.119	-7.151	-0.031	(0)
MnCl+	1.811e-08	1.685e-08	-7.742	-7.773	-0.031	-3.98
MnSO4	9.266e-10	9.276e-10	-9.033	-9.033	0.000	24.17
MnCO3	6.282e-10	6.289e-10	-9.202	-9.201	0.000	(0)
MnF+	6.302e-11	5.863e-11	-10.201	-10.232	-0.031	(0)
MnCl2	1.776e-11	1.778e-11	-10.750	-10.750	0.000	90.40
MnOH+	8.113e-12	7.548e-12	-11.091	-11.122	-0.031	(0)
Mn(NO3)2	2.967e-13	2.970e-13	-12.528	-12.527	0.000	42.01
MnCl3-	1.273e-14	1.184e-14	-13.895	-13.927	-0.031	43.52
Mn(OH)3-	3.503e-25	3.259e-25	-24.456	-24.487	-0.031	(0)
Mn(3)	1.188e-28					
Mn+3	1.188e-28	6.511e-29	-27.925	-28.186	-0.261	(0)
N(3)	1.143e-05					
NO2-	1.143e-05	1.060e-05	-4.942	-4.975	-0.033	24.81
N(5)	2.242e-04					
NO3-	2.242e-04	2.080e-04	-3.649	-3.682	-0.033	29.17
BaNO3+	9.244e-11	8.589e-11	-10.034	-10.066	-0.032	(0)
Mn(NO3)2	2.967e-13	2.970e-13	-12.528	-12.527	0.000	42.01
Na	1.523e-04					
Na+	1.503e-04	1.397e-04	-3.823	-3.855	-0.032	-1.62
NaCl	1.969e-06	1.972e-06	-5.706	-5.705	0.000	(0)
NaHCO3	3.713e-08	3.717e-08	-7.430	-7.430	0.000	1.80
NaSO4-	2.399e-09	2.233e-09	-8.620	-8.651	-0.031	14.15
NaF	3.977e-10	3.982e-10	-9.400	-9.400	0.000	7.12
NaCO3-	1.084e-11	1.007e-11	-10.965	-10.997	-0.032	-1.32
NaHPO4-	6.946e-12	6.466e-12	-11.158	-11.189	-0.031	33.86
NaOH	2.466e-23	2.469e-23	-22.608	-22.608	0.000	(0)
O(0)	8.064e-05					
O2	4.032e-05	4.036e-05	-4.394	-4.394	0.000	30.12

P	1.937e-06					
H2PO4-	1.828e-06	1.702e-06	-5.738	-5.769	-0.031	33.32
MgH2PO4+	4.835e-08	4.501e-08	-7.316	-7.347	-0.031	(0)
HPO4-2	3.168e-08	2.373e-08	-7.499	-7.625	-0.125	6.95
MgHPO4	1.429e-08	1.431e-08	-7.845	-7.844	0.000	(0)
CaH2PO4+	9.855e-09	9.174e-09	-8.006	-8.037	-0.031	(0)
CaHPO4	2.744e-09	2.747e-09	-8.562	-8.561	0.000	(0)
H3PO4	1.048e-09	1.049e-09	-8.980	-8.979	0.000	47.21
FeH2PO4+	9.498e-10	8.841e-10	-9.022	-9.053	-0.031	(0)
FeHPO4	9.782e-11	9.793e-11	-10.010	-10.009	0.000	(0)
MgPO4-	7.774e-12	7.237e-12	-11.109	-11.140	-0.031	(0)
NaHPO4-	6.946e-12	6.466e-12	-11.158	-11.189	-0.031	33.86
KHPO4-	3.660e-12	3.407e-12	-11.437	-11.468	-0.031	38.41
CaPO4-	1.496e-12	1.393e-12	-11.825	-11.856	-0.031	(0)
PO4-3	4.432e-15	2.284e-15	-14.353	-14.641	-0.288	-22.63
FeH2PO4+2	1.027e-16	7.713e-17	-15.988	-16.113	-0.124	(0)
FeHPO4+	1.030e-18	9.582e-19	-17.987	-18.019	-0.031	(0)
S(6)	5.102e-06					
SO4-2	4.355e-06	3.261e-06	-5.361	-5.487	-0.126	14.17
MgSO4	6.057e-07	6.063e-07	-6.218	-6.217	0.000	5.70
CaSO4	1.272e-07	1.274e-07	-6.895	-6.895	0.000	7.36
BaSO4	5.356e-09	5.362e-09	-8.271	-8.271	0.000	(0)
NaSO4-	2.399e-09	2.233e-09	-8.620	-8.651	-0.031	14.15
KSO4-	1.704e-09	1.586e-09	-8.769	-8.800	-0.031	34.04
SrSO4	1.611e-09	1.613e-09	-8.793	-8.792	0.000	24.10
HSO4-	1.382e-09	1.284e-09	-8.860	-8.892	-0.032	40.06
MnSO4	9.266e-10	9.276e-10	-9.033	-9.033	0.000	24.17
FeSO4	5.628e-10	5.634e-10	-9.250	-9.249	0.000	22.82
AlSO4+	5.347e-11	4.971e-11	-10.272	-10.304	-0.032	(0)
CaHSO4+	3.746e-12	3.481e-12	-11.426	-11.458	-0.032	(0)
FeHSO4+	1.722e-14	1.600e-14	-13.764	-13.796	-0.032	(0)
Al(SO4)2-	5.424e-15	5.043e-15	-14.266	-14.297	-0.032	(0)
AlHSO4+2	2.507e-17	1.868e-17	-16.601	-16.729	-0.128	(0)
FeSO4+	5.983e-18	5.567e-18	-17.223	-17.254	-0.031	(0)
Fe(SO4)2-	4.216e-22	3.917e-22	-21.375	-21.407	-0.032	(0)
FeHSO4+2	8.758e-23	6.527e-23	-22.058	-22.185	-0.128	(0)
Si	1.343e-04					
H4SiO4	1.343e-04	1.345e-04	-3.872	-3.871	0.000	52.39
H3SiO4-	4.317e-09	4.011e-09	-8.365	-8.397	-0.032	27.92
H2SiO4-2	6.595e-17	4.952e-17	-16.181	-16.305	-0.124	(0)
SiF6-2	2.017e-27	1.511e-27	-26.695	-26.821	-0.125	42.48
Sr	3.539e-06					
Sr+2	3.519e-06	2.644e-06	-5.454	-5.578	-0.124	-17.60
SrHCO3+	1.787e-08	1.664e-08	-7.748	-7.779	-0.031	(0)
SrSO4	1.611e-09	1.613e-09	-8.793	-8.792	0.000	24.10
SrCO3	7.035e-12	7.042e-12	-11.153	-11.152	0.000	-14.14
SrOH+	3.338e-14	3.106e-14	-13.476	-13.508	-0.031	(0)

----------Distribution of alkalinity----------

Total alkalinity (eq/kgw) = 5.000e-04

Species	Alkalinity	Molality	Alk/Mol
HCO3-	4.981e-04	4.981e-04	1.00
MgHCO3+	5.002e-06	5.002e-06	1.00
H+	-4.667e-06	4.667e-06	-1.00
CaHCO3+	1.352e-06	1.352e-06	1.00
MnHCO3+	7.601e-08	7.601e-08	1.00
FeHCO3+	5.172e-08	5.172e-08	1.00
NaHCO3	3.713e-08	3.713e-08	1.00
HPO4-2	3.168e-08	3.168e-08	1.00
HF	-3.042e-08	3.042e-08	-1.00
Al(OH)2+	2.577e-08	1.289e-08	2.00
SrHCO3+	1.787e-08	1.787e-08	1.00
MgHPO4	1.429e-08	1.429e-08	1.00
BaHCO3+	1.405e-08	1.405e-08	1.00
CO3-2	1.232e-08	6.161e-09	2.00

AlOH+2	1.215e-08	1.215e-08	1.00
MgCO3	7.262e-09	3.631e-09	2.00
H3SiO4-	4.317e-09	4.317e-09	1.00
CaCO3	3.279e-09	1.639e-09	2.00
CaHPO4	2.744e-09	2.744e-09	1.00
OH-	1.903e-09	1.903e-09	1.00
HSO4-	-1.382e-09	1.382e-09	-1.00
MnCO3	1.256e-09	6.282e-10	2.00
H3PO4	-1.048e-09	1.048e-09	-1.00
Al(OH)3	9.320e-10	3.107e-10	3.00
MgOH+	5.628e-10	5.628e-10	1.00
Al(OH)4-	5.527e-10	1.382e-10	4.00
FeCO3	2.298e-10	1.149e-10	2.00
FeHPO4	9.782e-11	9.782e-11	1.00
FeOH+	6.193e-11	6.193e-11	1.00
NaCO3-	2.167e-11	1.084e-11	2.00
MgPO4-	1.555e-11	7.774e-12	2.00
BaCO3	1.460e-11	7.301e-12	2.00
SrCO3	1.407e-11	7.035e-12	2.00
CaOH+	9.226e-12	9.226e-12	1.00
MnOH+	8.113e-12	8.113e-12	1.00
NaHPO4-	6.946e-12	6.946e-12	1.00
CaHSO4+	-3.746e-12	3.746e-12	-1.00
KHPO4-	3.660e-12	3.660e-12	1.00
CaPO4-	2.992e-12	1.496e-12	2.00
HF2-	-6.052e-13	6.052e-13	-1.00
Fe(OH)3	3.386e-13	3.386e-13	1.00
FeOH+2	-2.698e-13	2.698e-13	-1.00
SrOH+	3.338e-14	3.338e-14	1.00
BaOH+	2.737e-14	2.737e-14	1.00
FeHSO4+	-1.722e-14	1.722e-14	-1.00
PO4-3	8.864e-15	4.432e-15	2.00
FeF+2	-3.342e-15	1.671e-15	-2.00
Fe+3	-6.141e-16	3.071e-16	-2.00
FeF2+	-5.087e-16	2.543e-16	-2.00
FeH2PO4+2	-2.054e-16	1.027e-16	-2.00
Fe(OH)2	1.649e-16	8.245e-17	2.00
Fe(OH)4-	1.319e-16	6.597e-17	2.00
H2SiO4-2	1.319e-16	6.595e-17	2.00
FeCl+2	-2.933e-17	1.466e-17	-2.00
AlHSO4+2	-2.507e-17	2.507e-17	-1.00
FeSO4+	-1.197e-17	5.983e-18	-2.00
FeF3	-3.666e-18	1.833e-18	-2.00
FeHPO4+	-1.030e-18	1.030e-18	-1.00
FeCl2+	-2.853e-19	1.427e-19	-2.00
Fe(OH)3-	2.188e-21	7.292e-22	3.00
Fe(SO4)2-	-8.432e-22	4.216e-22	-2.00
FeHSO4+2	-2.627e-22	8.758e-23	-3.00
FeCl3	-6.411e-23	3.205e-23	-2.00
NaOH	2.466e-23	2.466e-23	1.00
Fe2(OH)2+4	-8.252e-24	4.126e-24	-2.00
Mn(OH)3-	1.051e-24	3.503e-25	3.00
SiF6-2	-8.068e-27	2.017e-27	-4.00
Fe3(OH)4+5	-6.208e-32	3.104e-32	-2.00

-------------------------------Saturation indices--------------------------------

Phase	SI**	log IAP	log K(294 K, 1 atm)	
Al(OH)3(a)	-3.25	7.78	11.03	Al(OH)3
Albite	-7.13	-25.36	-18.23	NaAlSi3O8
Alunite	-6.88	-7.84	-0.96	KAl3(SO4)2(OH)6
Anhydrite	-4.89	-9.13	-4.24	CaSO4
Anorthite	-11.36	-31.17	-19.81	CaAl2Si2O8
Aragonite	-3.67	-11.98	-8.31	CaCO3
BaCl2	-12.97	-10.72	2.26	BaCl2
BaCl2:2H2O	-10.89	-10.72	0.17	BaCl2:2H2O
BaCl2:H2O	-11.54	-10.72	0.82	BaCl2:H2O

Barite	-1.09	-10.97	-9.88	BaSO4
Ca-Montmorillonite	-3.04	-48.58	-45.54	Ca0.165Al2.33Si3.67O10(OH)2
Calcite	-3.52	-11.98	-8.46	CaCO3
Celestite	-4.43	-11.06	-6.64	SrSO4
Chalcedony	-0.28	-3.87	-3.59	SiO2
Chlorite(14A)	-27.45	42.25	69.70	Mg5Al2Si3O10(OH)8
Chrysotile	-17.41	15.23	32.64	Mg3Si2O5(OH)4
CO2(g)	-0.90	-2.32	-1.43	CO2
Dolomite	-6.37	-23.38	-17.01	CaMg(CO3)2
Fe(OH)3(a)	-4.58	0.31	4.89	Fe(OH)3
Fluorite	-3.62	-14.26	-10.64	CaF2
Gibbsite	-0.53	7.78	8.31	Al(OH)3
Goethite	1.18	0.31	-0.87	FeOOH
Gypsum	-4.55	-9.13	-4.58	CaSO4:2H2O
H2(g)	-17.39	-20.48	-3.09	H2
H2O(g)	-1.59	-0.00	1.59	H2O
Halite	-8.04	-6.47	1.57	NaCl
Hausmannite	-29.70	32.21	61.91	Mn3O4
Hematite	4.35	0.61	-3.74	Fe2O3
Hydroxyapatite	-16.56	-19.67	-3.11	Ca5(PO4)3OH
Illite	-5.23	-45.98	-40.74	K0.6Mg0.25Al2.3Si3.5O10(OH)2
Jarosite-K	-21.33	-30.27	-8.94	KFe3(SO4)2(OH)6
K-feldspar	-4.80	-25.64	-20.84	KAlSi3O8
K-mica	-0.26	12.96	13.22	KAl3Si3O10(OH)2
Kaolinite	0.08	7.82	7.74	Al2Si2O5(OH)4
Manganite	-11.71	13.63	25.34	MnOOH
Melanterite	-9.22	-11.47	-2.25	FeSO4:7H2O
O2(g)	-1.53	-4.39	-2.87	O2
Pyrochroite	-10.25	4.95	15.20	Mn(OH)2
Pyrolusite	-19.64	22.30	41.95	MnO2:H2O
Quartz	0.16	-3.87	-4.03	SiO2
Rhodochrosite	-2.98	-14.10	-11.12	MnCO3
Sepiolite	-12.15	3.70	15.85	Mg2Si3O7.5OH:3H2O
Sepiolite(d)	-14.96	3.70	18.66	Mg2Si3O7.5OH:3H2O
Siderite	-3.45	-14.32	-10.87	FeCO3
SiO2(a)	-1.13	-3.87	-2.74	SiO2
Strontianite	-4.64	-13.91	-9.27	SrCO3
Sylvite	-7.63	-6.75	0.88	KCl
Talc	-14.31	7.49	21.80	Mg3Si4O10(OH)2
Vivianite	-11.24	-47.24	-36.00	Fe3(PO4)2:8H2O
Witherite	-5.25	-13.82	-8.57	BaCO3

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
For ideal gases, phi = 1.

Initial solution 10.

-----------------------------Solution composition------------------------------

Elements	Molality	Moles
Al	7.043e-07	7.043e-07
Alkalinity	7.000e-04	7.000e-04
Ba	6.554e-06	6.554e-06
Ca	2.620e-05	2.620e-05
Cl	5.743e-04	5.743e-04
F	4.211e-06	4.211e-06
Fe	1.818e-04	1.818e-04
K	2.813e-05	2.813e-05
Mg	3.990e-05	3.990e-05
Mn	6.262e-05	6.262e-05
N(3)	3.570e-06	3.570e-06
N(5)	1.071e-05	1.071e-05
Na	6.525e-04	6.525e-04
O(0)	5.501e-05	5.501e-05
P	3.229e-07	3.229e-07
S(6)	2.072e-05	2.072e-05
Si	5.659e-05	5.659e-05

Sr 1.141e-06 1.141e-06

----------Description of solution----------

pH	= 5.520
pe	= 1.241
Specific Conductance (µS/cm, 24°C)	= 137
Density (g/cm³)	= 0.99749
Volume (L)	= 1.00282
Activity of water	= 1.000
Ionic strength (mol/kgw)	= 1.635e-03
Mass of water (kg)	= 1.000e+00
Total carbon (mol/kg)	= 5.254e-03
Total CO2 (mol/kg)	= 5.254e-03
Temperature (°C)	= 23.70
Electrical balance (eq)	= -1.548e-05
Percent error, 100*(Cat-|An|)/(Cat+|An|)	= -0.59
Iterations	= 11 (106 overall)
Total H	= 1.110134e+02
Total O	= 5.551783e+01

----------Redox couples----------

Redox couple	pe	Eh (volts)
N(3)/N(5)	9.0738	0.5344
O(-2)/O(0)	14.9681	0.8816

----------Distribution of species----------

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma	mole V cm³/mol
H+	3.151e-06	3.020e-06	-5.502	-5.520	-0.018	0.00
OH-	3.173e-09	3.033e-09	-8.498	-8.518	-0.020	-4.15
H2O	5.551e+01	9.999e-01	1.744	-0.000	0.000	18.06
Al	7.043e-07					
AlF2+	3.429e-07	3.281e-07	-6.465	-6.484	-0.019	(0)
AlF+2	2.569e-07	2.153e-07	-6.590	-6.667	-0.077	(0)
Al(OH)2+	5.181e-08	4.957e-08	-7.286	-7.305	-0.019	(0)
AlOH+2	2.556e-08	2.141e-08	-7.592	-7.669	-0.077	-27.68
AlF3	1.262e-08	1.263e-08	-7.899	-7.899	0.000	(0)
Al+3	1.037e-08	7.088e-09	-7.984	-8.149	-0.165	-42.14
Al(OH)3	2.195e-09	2.196e-09	-8.659	-8.658	0.000	(0)
Al(OH)4-	1.408e-09	1.347e-09	-8.851	-8.871	-0.019	(0)
AlSO4+	3.831e-10	3.664e-10	-9.417	-9.436	-0.019	(0)
AlF4-	1.609e-11	1.539e-11	-10.793	-10.813	-0.019	(0)
Al(SO4)2-	2.002e-13	1.914e-13	-12.699	-12.718	-0.019	(0)
AlHSO4+2	1.161e-16	9.700e-17	-15.935	-16.013	-0.078	(0)
Ba	6.554e-06					
Ba+2	6.465e-06	5.403e-06	-5.189	-5.267	-0.078	-12.79
BaSO4	4.500e-08	4.502e-08	-7.347	-7.347	0.000	(0)
BaHCO3+	3.429e-08	3.278e-08	-7.465	-7.484	-0.020	(0)
BaCl+	9.532e-09	9.113e-09	-8.021	-8.040	-0.020	(0)
BaCO3	2.710e-11	2.711e-11	-10.567	-10.567	0.000	-10.71
BaNO3+	7.281e-12	6.961e-12	-11.138	-11.157	-0.020	(0)
BaOH+	6.337e-14	6.062e-14	-13.198	-13.217	-0.019	(0)
C(4)	5.254e-03					
CO2	4.550e-03	4.552e-03	-2.342	-2.342	0.000	34.37
HCO3-	6.892e-04	6.594e-04	-3.162	-3.181	-0.019	24.60
FeHCO3+	9.909e-06	9.474e-06	-5.004	-5.023	-0.020	(0)
MnHCO3+	3.055e-06	2.922e-06	-5.515	-5.534	-0.019	(0)
(CO2)2	3.641e-07	3.642e-07	-6.439	-6.439	0.000	68.74
MgHCO3+	2.659e-07	2.542e-07	-6.575	-6.595	-0.020	5.45
NaHCO3	2.322e-07	2.323e-07	-6.634	-6.634	0.000	1.80
CaHCO3+	1.872e-07	1.792e-07	-6.728	-6.747	-0.019	9.63
MnCO3	3.936e-08	3.938e-08	-7.405	-7.405	0.000	(0)
FeCO3	3.435e-08	3.436e-08	-7.464	-7.464	0.000	(0)

BaHCO3+	3.429e-08	3.278e-08	-7.465	-7.484	-0.020	(0)
CO3-2	1.190e-08	9.970e-09	-7.925	-8.001	-0.077	-5.34
SrHCO3+	9.539e-09	9.126e-09	-8.021	-8.040	-0.019	(0)
CaCO3	3.548e-10	3.549e-10	-9.450	-9.450	0.000	-14.60
MgCO3	3.089e-10	3.090e-10	-9.510	-9.510	0.000	-17.09
NaCO3-	1.131e-10	1.081e-10	-9.947	-9.966	-0.020	-1.14
BaCO3	2.710e-11	2.711e-11	-10.567	-10.567	0.000	-10.71
SrCO3	5.792e-12	5.794e-12	-11.237	-11.237	0.000	-14.13
Ca	2.620e-05					
Ca+2	2.595e-05	2.174e-05	-4.586	-4.663	-0.077	-18.13
CaHCO3+	1.872e-07	1.792e-07	-6.728	-6.747	-0.019	9.63
CaSO4	6.361e-08	6.363e-08	-7.196	-7.196	0.000	7.45
CaCO3	3.548e-10	3.549e-10	-9.450	-9.450	0.000	-14.60
CaH2PO4+	1.579e-10	1.510e-10	-9.802	-9.821	-0.019	(0)
CaHPO4	6.608e-11	6.611e-11	-10.180	-10.180	0.000	(0)
CaHSO4+	1.297e-12	1.240e-12	-11.887	-11.907	-0.020	(0)
CaOH+	1.249e-12	1.194e-12	-11.903	-11.923	-0.020	(0)
CaPO4-	5.282e-14	5.053e-14	-13.277	-13.296	-0.019	(0)
Cl	5.743e-04					
Cl-	5.721e-04	5.468e-04	-3.243	-3.262	-0.020	18.04
NaCl	2.015e-06	2.016e-06	-5.696	-5.695	0.000	(0)
MnCl+	1.158e-07	1.108e-07	-6.936	-6.956	-0.019	-3.41
FeCl+	1.134e-07	1.085e-07	-6.945	-6.965	-0.020	(0)
BaCl+	9.532e-09	9.113e-09	-8.021	-8.040	-0.020	(0)
MnCl2	2.643e-11	2.644e-11	-10.578	-10.578	0.000	87.51
MnCl3-	4.163e-15	3.982e-15	-14.381	-14.400	-0.019	43.41
FeCl+2	4.211e-18	3.525e-18	-17.376	-17.453	-0.077	(0)
FeCl2+	9.383e-21	8.975e-21	-20.028	-20.047	-0.019	(0)
FeCl3	4.906e-25	4.908e-25	-24.309	-24.309	0.000	(0)
F	4.211e-06					
F-	3.203e-06	3.062e-06	-5.494	-5.514	-0.020	-1.32
AlF2+	3.429e-07	3.281e-07	-6.465	-6.484	-0.019	(0)
AlF+2	2.569e-07	2.153e-07	-6.590	-6.667	-0.077	(0)
HF	1.354e-08	1.355e-08	-7.868	-7.868	0.000	12.44
AlF3	1.262e-08	1.263e-08	-7.899	-7.899	0.000	(0)
MgF+	6.844e-09	6.545e-09	-8.165	-8.184	-0.019	-10.56
FeF+	4.601e-09	4.399e-09	-8.337	-8.357	-0.020	(0)
MnF+	1.101e-09	1.053e-09	-8.958	-8.977	-0.019	(0)
NaF	1.095e-09	1.096e-09	-8.961	-8.960	0.000	7.21
AlF4-	1.609e-11	1.539e-11	-10.793	-10.813	-0.019	(0)
HF2-	1.647e-13	1.575e-13	-12.783	-12.803	-0.020	22.01
FeF+2	1.264e-15	1.058e-15	-14.898	-14.975	-0.077	(0)
FeF2+	1.328e-16	1.270e-16	-15.877	-15.896	-0.019	(0)
FeF3	6.133e-19	6.135e-19	-18.212	-18.212	0.000	(0)
SiF6-2	7.909e-30	6.621e-30	-29.102	-29.179	-0.077	42.52
Fe(2)	1.818e-04					
Fe+2	1.712e-04	1.437e-04	-3.766	-3.843	-0.076	-22.19
FeHCO3+	9.909e-06	9.474e-06	-5.004	-5.023	-0.020	(0)
FeSO4	4.146e-07	4.147e-07	-6.382	-6.382	0.000	20.35
FeCl+	1.134e-07	1.085e-07	-6.945	-6.965	-0.020	(0)
FeCO3	3.435e-08	3.436e-08	-7.464	-7.464	0.000	(0)
FeH2PO4+	2.096e-08	2.005e-08	-7.679	-7.698	-0.019	(0)
FeOH+	1.426e-08	1.364e-08	-7.846	-7.865	-0.019	(0)
FeF+	4.601e-09	4.399e-09	-8.337	-8.357	-0.020	(0)
FeHPO4	3.250e-09	3.251e-09	-8.488	-8.488	0.000	(0)
FeHSO4+	8.574e-12	8.197e-12	-11.067	-11.086	-0.020	(0)
Fe(OH)2	3.431e-14	3.432e-14	-13.465	-13.464	0.000	(0)
Fe(OH)3-	4.358e-19	4.168e-19	-18.361	-18.380	-0.019	(0)
Fe(3)	5.041e-11					
Fe(OH)2+	4.803e-11	4.595e-11	-10.318	-10.338	-0.019	(0)
Fe(OH)3	1.851e-12	1.852e-12	-11.733	-11.732	0.000	(0)
FeOH+2	5.261e-13	4.404e-13	-12.279	-12.356	-0.077	(0)
FeF+2	1.264e-15	1.058e-15	-14.898	-14.975	-0.077	(0)
Fe(OH)4-	5.545e-16	5.305e-16	-15.256	-15.275	-0.019	(0)
Fe+3	3.256e-16	2.225e-16	-15.487	-15.653	-0.165	(0)
FeF2+	1.328e-16	1.270e-16	-15.877	-15.896	-0.019	(0)
FeSO4+	4.119e-17	3.940e-17	-16.385	-16.404	-0.019	(0)
FeH2PO4+2	1.990e-17	1.668e-17	-16.701	-16.778	-0.077	(0)

FeCl+2	4.211e-18	3.525e-18	-17.376	-17.453	-0.077	(0)
FeF3	6.133e-19	6.135e-19	-18.212	-18.212	0.000	(0)
FeHPO4+	3.410e-19	3.262e-19	-18.467	-18.487	-0.019	(0)
Fe(SO4)2-	1.491e-20	1.426e-20	-19.826	-19.846	-0.020	(0)
FeCl2+	9.383e-21	8.975e-21	-20.028	-20.047	-0.019	(0)
FeHSO4+2	3.817e-22	3.189e-22	-21.418	-21.496	-0.078	(0)
Fe2(OH)2+4	1.131e-23	5.511e-24	-22.946	-23.259	-0.312	(0)
FeCl3	4.906e-25	4.908e-25	-24.309	-24.309	0.000	(0)
Fe3(OH)4+5	1.837e-31	5.968e-32	-30.736	-31.224	-0.488	(0)
H(0)	4.310e-17					
H2	2.155e-17	2.156e-17	-16.667	-16.666	0.000	28.61
K	2.813e-05					
K+	2.813e-05	2.689e-05	-4.551	-4.570	-0.020	8.97
KSO4-	3.209e-09	3.070e-09	-8.494	-8.513	-0.019	34.08
KHPO4-	3.115e-13	2.980e-13	-12.507	-12.526	-0.019	38.21
Mg	3.990e-05					
Mg+2	3.950e-05	3.313e-05	-4.403	-4.480	-0.076	-21.75
MgHCO3+	2.659e-07	2.542e-07	-6.575	-6.595	-0.020	5.45
MgSO4	1.248e-07	1.249e-07	-6.904	-6.904	0.000	5.79
MgF+	6.844e-09	6.545e-09	-8.165	-8.184	-0.019	-10.56
MgCO3	3.089e-10	3.090e-10	-9.510	-9.510	0.000	-17.09
MgH2PO4+	3.065e-10	2.932e-10	-9.514	-9.533	-0.019	(0)
MgHPO4	1.362e-10	1.362e-10	-9.866	-9.866	0.000	(0)
MgOH+	3.698e-11	3.540e-11	-10.432	-10.451	-0.019	(0)
MgPO4-	1.086e-13	1.039e-13	-12.964	-12.983	-0.019	(0)
Mn(2)	6.262e-05					
Mn+2	5.927e-05	4.973e-05	-4.227	-4.303	-0.076	-20.83
MnHCO3+	3.055e-06	2.922e-06	-5.515	-5.534	-0.019	(0)
MnSO4	1.433e-07	1.434e-07	-6.844	-6.843	0.000	23.13
MnCl+	1.158e-07	1.108e-07	-6.936	-6.956	-0.019	-3.41
MnCO3	3.936e-08	3.938e-08	-7.405	-7.405	0.000	(0)
MnF+	1.101e-09	1.053e-09	-8.958	-8.977	-0.019	(0)
MnOH+	3.977e-10	3.805e-10	-9.400	-9.420	-0.019	(0)
MnCl2	2.643e-11	2.644e-11	-10.578	-10.578	0.000	87.51
Mn(NO3)2	2.078e-14	2.079e-14	-13.682	-13.682	0.000	41.39
MnCl3-	4.163e-15	3.982e-15	-14.381	-14.400	-0.019	43.41
Mn(OH)3-	2.990e-23	2.860e-23	-22.524	-22.544	-0.019	(0)
Mn(3)	3.237e-29					
Mn+3	3.237e-29	2.212e-29	-28.490	-28.655	-0.165	(0)
N(3)	3.570e-06					
NO2-	3.570e-06	3.411e-06	-5.447	-5.467	-0.020	24.91
N(5)	1.071e-05					
NO3-	1.071e-05	1.023e-05	-4.970	-4.990	-0.020	29.37
BaNO3+	7.281e-12	6.961e-12	-11.138	-11.157	-0.020	(0)
Mn(NO3)2	2.078e-14	2.079e-14	-13.682	-13.682	0.000	41.39
Na	6.525e-04					
Na+	6.502e-04	6.218e-04	-3.187	-3.206	-0.019	-1.53
NaCl	2.015e-06	2.016e-06	-5.696	-5.695	0.000	(0)
NaHCO3	2.322e-07	2.323e-07	-6.634	-6.634	0.000	1.80
NaSO4-	5.371e-08	5.138e-08	-7.270	-7.289	-0.019	13.85
NaF	1.095e-09	1.096e-09	-8.961	-8.960	0.000	7.21
NaCO3-	1.131e-10	1.081e-10	-9.947	-9.966	-0.020	-1.14
NaHPO4-	7.203e-12	6.892e-12	-11.142	-11.162	-0.019	33.58
NaOH	1.885e-22	1.886e-22	-21.725	-21.724	0.000	(0)
O(0)	5.501e-05					
O2	2.750e-05	2.751e-05	-4.561	-4.560	0.000	30.30
P	3.229e-07					
H2PO4-	2.911e-07	2.785e-07	-6.536	-6.555	-0.019	33.25
FeH2PO4+	2.096e-08	2.005e-08	-7.679	-7.698	-0.019	(0)
HPO4-2	6.789e-09	5.684e-09	-8.168	-8.245	-0.077	6.78
FeHPO4	3.250e-09	3.251e-09	-8.488	-8.488	0.000	(0)
MgH2PO4+	3.065e-10	2.932e-10	-9.514	-9.533	-0.019	(0)
CaH2PO4+	1.579e-10	1.510e-10	-9.802	-9.821	-0.019	(0)
MgHPO4	1.362e-10	1.362e-10	-9.866	-9.866	0.000	(0)
H3PO4	1.219e-10	1.219e-10	-9.914	-9.914	0.000	47.34
CaHPO4	6.608e-11	6.611e-11	-10.180	-10.180	0.000	(0)
NaHPO4-	7.203e-12	6.892e-12	-11.142	-11.162	-0.019	33.58
KHPO4-	3.115e-13	2.980e-13	-12.507	-12.526	-0.019	38.21

MgPO4-	1.086e-13	1.039e-13	-12.964	-12.983	-0.019	(0)
CaPO4-	5.282e-14	5.053e-14	-13.277	-13.296	-0.019	(0)
PO4-3	1.239e-15	8.266e-16	-14.907	-15.083	-0.176	-23.05
FeH2PO4+2	1.990e-17	1.668e-17	-16.701	-16.778	-0.077	(0)
FeHPO4+	3.410e-19	3.262e-19	-18.467	-18.487	-0.019	(0)
S(6)	2.072e-05					
SO4-2	1.986e-05	1.662e-05	-4.702	-4.779	-0.077	14.38
FeSO4	4.146e-07	4.147e-07	-6.382	-6.382	0.000	20.35
MnSO4	1.433e-07	1.434e-07	-6.844	-6.843	0.000	23.13
MgSO4	1.248e-07	1.249e-07	-6.904	-6.904	0.000	5.79
CaSO4	6.361e-08	6.363e-08	-7.196	-7.196	0.000	7.45
NaSO4-	5.371e-08	5.138e-08	-7.270	-7.289	-0.019	13.85
BaSO4	4.500e-08	4.502e-08	-7.347	-7.347	0.000	(0)
HSO4-	4.964e-09	4.745e-09	-8.304	-8.324	-0.020	40.20
KSO4-	3.209e-09	3.070e-09	-8.494	-8.513	-0.019	34.08
SrSO4	3.019e-09	3.020e-09	-8.520	-8.520	0.000	24.19
AlSO4+	3.831e-10	3.664e-10	-9.417	-9.436	-0.019	(0)
FeHSO4+	8.574e-12	8.197e-12	-11.067	-11.086	-0.020	(0)
CaHSO4+	1.297e-12	1.240e-12	-11.887	-11.907	-0.020	(0)
Al(SO4)2-	2.002e-13	1.914e-13	-12.699	-12.718	-0.019	(0)
AlHSO4+2	1.161e-16	9.700e-17	-15.935	-16.013	-0.078	(0)
FeSO4+	4.119e-17	3.940e-17	-16.385	-16.404	-0.019	(0)
Fe(SO4)2-	1.491e-20	1.426e-20	-19.826	-19.846	-0.020	(0)
FeHSO4+2	3.817e-22	3.189e-22	-21.418	-21.496	-0.078	(0)
Si	5.659e-05					
H4SiO4	5.659e-05	5.661e-05	-4.247	-4.247	0.000	52.19
H3SiO4-	2.762e-09	2.641e-09	-8.559	-8.578	-0.020	27.95
H2SiO4-2	6.519e-17	5.462e-17	-16.186	-16.263	-0.077	(0)
SiF6-2	7.909e-30	6.621e-30	-29.102	-29.179	-0.077	42.52
Sr	1.141e-06					
Sr+2	1.129e-06	9.460e-07	-5.947	-6.024	-0.077	-17.73
SrHCO3+	9.539e-09	9.126e-09	-8.021	-8.040	-0.019	(0)
SrSO4	3.019e-09	3.020e-09	-8.520	-8.520	0.000	24.19
SrCO3	5.792e-12	5.794e-12	-11.237	-11.237	0.000	-14.13
SrOH+	1.679e-14	1.606e-14	-13.775	-13.794	-0.019	(0)

----------Distribution of alkalinity----------

Total alkalinity (eq/kgw) = 7.000e-04

Species	Alkalinity	Molality	Alk/Mol
HCO3-	6.892e-04	6.892e-04	1.00
FeHCO3+	9.909e-06	9.909e-06	1.00
H+	-3.151e-06	3.151e-06	-1.00
MnHCO3+	3.055e-06	3.055e-06	1.00
MgHCO3+	2.659e-07	2.659e-07	1.00
NaHCO3	2.322e-07	2.322e-07	1.00
CaHCO3+	1.872e-07	1.872e-07	1.00
Al(OH)2+	1.036e-07	5.181e-08	2.00
MnCO3	7.873e-08	3.936e-08	2.00
FeCO3	6.870e-08	3.435e-08	2.00
BaHCO3+	3.429e-08	3.429e-08	1.00
AlOH+2	2.556e-08	2.556e-08	1.00
CO3-2	2.380e-08	1.190e-08	2.00
FeOH+	1.426e-08	1.426e-08	1.00
HF	-1.354e-08	1.354e-08	-1.00
SrHCO3+	9.539e-09	9.539e-09	1.00
HPO4-2	6.789e-09	6.789e-09	1.00
Al(OH)3	6.585e-09	2.195e-09	3.00
Al(OH)4-	5.634e-09	1.408e-09	4.00
HSO4-	-4.964e-09	4.964e-09	-1.00
FeHPO4	3.250e-09	3.250e-09	1.00
OH-	3.173e-09	3.173e-09	1.00
H3SiO4-	2.762e-09	2.762e-09	1.00
CaCO3	7.095e-10	3.548e-10	2.00
MgCO3	6.177e-10	3.089e-10	2.00
MnOH+	3.977e-10	3.977e-10	1.00

NaCO3-	2.261e-10	1.131e-10	2.00
MgHPO4	1.362e-10	1.362e-10	1.00
H3PO4	-1.219e-10	1.219e-10	-1.00
CaHPO4	6.608e-11	6.608e-11	1.00
BaCO3	5.420e-11	2.710e-11	2.00
MgOH+	3.698e-11	3.698e-11	1.00
SrCO3	1.158e-11	5.792e-12	2.00
FeHSO4+	-8.574e-12	8.574e-12	-1.00
NaHPO4-	7.203e-12	7.203e-12	1.00
Fe(OH)3	1.851e-12	1.851e-12	1.00
CaHSO4+	-1.297e-12	1.297e-12	-1.00
CaOH+	1.249e-12	1.249e-12	1.00
FeOH+2	-5.261e-13	5.261e-13	-1.00
KHPO4-	3.115e-13	3.115e-13	1.00
MgPO4-	2.172e-13	1.086e-13	2.00
HF2-	-1.647e-13	1.647e-13	-1.00
CaPO4-	1.056e-13	5.282e-14	2.00
Fe(OH)2	6.862e-14	3.431e-14	2.00
BaOH+	6.337e-14	6.337e-14	1.00
SrOH+	1.679e-14	1.679e-14	1.00
FeF+2	-2.528e-15	1.264e-15	-2.00
PO4-3	2.479e-15	1.239e-15	2.00
Fe(OH)4-	1.109e-15	5.545e-16	2.00
Fe+3	-6.513e-16	3.256e-16	-2.00
FeF2+	-2.655e-16	1.328e-16	-2.00
H2SiO4-2	1.304e-16	6.519e-17	2.00
AlHSO4+2	-1.161e-16	1.161e-16	-1.00
FeSO4+	-8.238e-17	4.119e-17	-2.00
FeH2PO4+2	-3.981e-17	1.990e-17	-2.00
FeCl+2	-8.422e-18	4.211e-18	-2.00
Fe(OH)3-	1.307e-18	4.358e-19	3.00
FeF3	-1.227e-18	6.133e-19	-2.00
FeHPO4+	-3.410e-19	3.410e-19	-1.00
Fe(SO4)2-	-2.983e-20	1.491e-20	-2.00
FeCl2+	-1.877e-20	9.383e-21	-2.00
FeHSO4+2	-1.145e-21	3.817e-22	-3.00
NaOH	1.885e-22	1.885e-22	1.00
Mn(OH)3-	8.971e-23	2.990e-23	3.00
Fe2(OH)2+4	-2.263e-23	1.131e-23	-2.00
FeCl3	-9.812e-25	4.906e-25	-2.00
SiF6-2	-3.164e-29	7.909e-30	-4.00
Fe3(OH)4+5	-3.673e-31	1.837e-31	-2.00

-------------------------------Saturation indices--------------------------------

Phase	SI**	log IAP	log K(296 K, 1 atm)	
Al(OH)3(a)	-2.47	8.41	10.89	Al(OH)3
Albite	-6.73	-24.82	-18.09	NaAlSi3O8
Alunite	-4.22	-5.46	-1.24	KAl3(SO4)2(OH)6
Anhydrite	-5.18	-9.44	-4.26	CaSO4
Anorthite	-11.15	-30.90	-19.75	CaAl2Si2O8
Aragonite	-4.34	-12.66	-8.33	CaCO3
BaCl2	-14.03	-11.79	2.24	BaCl2
BaCl2:2H2O	-11.99	-11.79	0.20	BaCl2:2H2O
BaCl2:H2O	-12.61	-11.79	0.82	BaCl2:H2O
Barite	-0.19	-10.05	-9.86	BaSO4
Ca-Montmorillonite	-2.85	-48.06	-45.21	Ca0.165Al2.33Si3.67O10(OH)2
Calcite	-4.19	-12.66	-8.47	CaCO3
Celestite	-4.15	-10.80	-6.65	SrSO4
Chalcedony	-0.68	-4.25	-3.57	SiO2
Chlorite(14A)	-31.99	36.88	68.87	Mg5Al2Si3O10(OH)8
Chrysotile	-21.18	11.19	32.36	Mg3Si2O5(OH)4
CO2(g)	-0.89	-2.34	-1.45	CO2
Dolomite	-8.09	-25.15	-17.06	CaMg(CO3)2
Fe(OH)3(a)	-3.98	0.91	4.89	Fe(OH)3
Fluorite	-5.08	-15.69	-10.61	CaF2
Gibbsite	0.23	8.41	8.18	Al(OH)3

Goethite	1.86	0.91	-0.95	FeOOH
Gypsum	-4.86	-9.44	-4.58	CaSO4:2H2O
H2(g)	-13.57	-16.67	-3.10	H2
H2O(g)	-1.54	-0.00	1.54	H2O
Halite	-8.04	-6.47	1.57	NaCl
Hausmannite	-27.62	33.73	61.35	Mn3O4
Hematite	5.72	1.81	-3.91	Fe2O3
Hydroxyapatite	-22.67	-25.97	-3.30	Ca5(PO4)3OH
Illite	-5.31	-45.75	-40.44	K0.6Mg0.25Al2.3Si3.5O10(OH)2
Jarosite-K	-18.86	-27.97	-9.11	KFe3(SO4)2(OH)6
K-feldspar	-5.51	-26.18	-20.67	KAlSi3O8
K-mica	0.55	13.44	12.89	KAl3Si3O10(OH)2
Kaolinite	0.78	8.33	7.55	Al2Si2O5(OH)4
Manganite	-11.84	13.50	25.34	MnOOH
Melanterite	-6.40	-8.62	-2.23	FeSO4:7H2O
O2(g)	-1.68	-4.56	-2.88	O2
Pyrochroite	-8.46	6.74	15.20	Mn(OH)2
Pyrolusite	-21.33	20.26	41.59	MnO2:H2O
Quartz	-0.25	-4.25	-4.00	SiO2
Rhodochrosite	-1.18	-12.30	-11.13	MnCO3
Sepiolite	-15.42	0.38	15.79	Mg2Si3O7.5OH:3H2O
Sepiolite(d)	-18.28	0.38	18.66	Mg2Si3O7.5OH:3H2O
Siderite	-0.96	-11.84	-10.88	FeCO3
SiO2(a)	-1.52	-4.25	-2.72	SiO2
Strontianite	-4.76	-14.03	-9.27	SrCO3
Sylvite	-8.73	-7.83	0.89	KCl
Talc	-18.86	2.69	21.55	Mg3Si4O10(OH)2
Vivianite	-5.69	-41.69	-36.00	Fe3(PO4)2:8H2O
Witherite	-4.70	-13.27	-8.56	BaCO3

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
For ideal gases, phi = 1.

Initial solution 11.

-----------------------------Solution composition-------------------------------

Elements	Molality	Moles
Al	1.298e-06	1.298e-06
Alkalinity	5.702e-03	5.702e-03
Ba	5.908e-05	5.908e-05
Ca	1.805e-04	1.805e-04
Cl	1.631e-03	1.631e-03
F	2.791e-05	2.791e-05
Fe	2.728e-04	2.728e-04
K	3.838e-04	3.838e-04
Mg	2.140e-04	2.140e-04
Mn	1.683e-04	1.683e-04
N(3)	2.143e-06	2.143e-06
N(5)	1.071e-05	1.071e-05
Na	1.001e-03	1.001e-03
O(0)	4.690e-05	4.690e-05
P	9.690e-07	9.690e-07
S(6)	6.249e-07	6.249e-07
Si	3.646e-05	3.646e-05
Sr	2.284e-06	2.284e-06

----------------------------Description of solution----------------------------

pH	=	6.520
pe	=	-1.312
Specific Conductance (µS/cm, 23°C)	=	479
Density (g/cm³)	=	0.99784
Volume (L)	=	1.00282
Activity of water	=	1.000
Ionic strength (mol/kgw)	=	5.853e-03
Mass of water (kg)	=	1.000e+00

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                    Total carbon (mol/kg)  =   9.239e-03
                       Total CO2 (mol/kg)  =   9.239e-03
                         Temperature (°C)  =  23.30
                  Electrical balance (eq)  =  -4.194e-03
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  = -41.07
                                Iterations  =  10 (116 overall)
                                   Total H  = 1.110183e+02
                                   Total O  = 5.553062e+01
```

---------------------------------Redox couples---------------------------------

Redox couple	pe	Eh (volts)
N(3)/N(5)	8.2065	0.4827
O(-2)/O(0)	13.9844	0.8225

--------------------------Distribution of species--------------------------

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma	mole V cm³/mol
H+	3.249e-07	3.020e-07	-6.488	-6.520	-0.032	0.00
OH-	3.193e-08	2.940e-08	-7.496	-7.532	-0.036	-4.13
H2O	5.551e+01	9.998e-01	1.744	-0.000	0.000	18.06
Al	1.298e-06					
AlF2+	5.540e-07	5.120e-07	-6.256	-6.291	-0.034	(0)
Al(OH)4-	3.406e-07	3.143e-07	-6.468	-6.503	-0.035	(0)
AlF3	1.536e-07	1.538e-07	-6.814	-6.813	0.001	(0)
Al(OH)2+	1.297e-07	1.198e-07	-6.887	-6.921	-0.034	(0)
AlF+2	5.912e-08	4.312e-08	-7.228	-7.365	-0.137	(0)
Al(OH)3	5.144e-08	5.151e-08	-7.289	-7.288	0.001	(0)
AlOH+2	7.355e-09	5.365e-09	-8.133	-8.270	-0.137	-27.56
AlF4-	1.585e-09	1.463e-09	-8.800	-8.835	-0.035	(0)
Al+3	3.519e-10	1.823e-10	-9.454	-9.739	-0.286	-41.89
AlSO4+	2.548e-13	2.351e-13	-12.594	-12.629	-0.035	(0)
Al(SO4)2-	3.333e-18	3.075e-18	-17.477	-17.512	-0.035	(0)
AlHSO4+2	8.583e-21	6.203e-21	-20.066	-20.207	-0.141	(0)
Ba	5.908e-05					
Ba+2	5.678e-05	4.108e-05	-4.246	-4.386	-0.141	-12.70
BaHCO3+	2.072e-06	1.910e-06	-5.684	-5.719	-0.035	(0)
BaCl+	2.041e-07	1.882e-07	-6.690	-6.725	-0.035	(0)
BaCO3	1.572e-08	1.574e-08	-7.804	-7.803	0.001	-10.71
BaSO4	8.573e-09	8.585e-09	-8.067	-8.066	0.001	(0)
BaNO3+	5.529e-11	5.098e-11	-10.257	-10.293	-0.035	(0)
BaOH+	4.990e-12	4.608e-12	-11.302	-11.336	-0.035	(0)
C(4)	9.239e-03					
HCO3-	5.538e-03	5.118e-03	-2.257	-2.291	-0.034	24.61
CO2	3.548e-03	3.552e-03	-2.450	-2.449	0.001	34.35
FeHCO3+	7.793e-05	7.185e-05	-4.108	-4.144	-0.035	(0)
MnHCO3+	4.313e-05	3.983e-05	-4.365	-4.400	-0.035	(0)
MgHCO3+	9.627e-06	8.874e-06	-5.017	-5.052	-0.035	5.47
CaHCO3+	8.599e-06	7.955e-06	-5.066	-5.099	-0.034	9.64
MnCO3	5.315e-06	5.322e-06	-5.274	-5.274	0.001	(0)
NaHCO3	2.652e-06	2.656e-06	-5.576	-5.576	0.001	1.80
FeCO3	2.581e-06	2.585e-06	-5.588	-5.588	0.001	(0)
BaHCO3+	2.072e-06	1.910e-06	-5.684	-5.719	-0.035	(0)
CO3-2	1.052e-06	7.674e-07	-5.978	-6.115	-0.137	-5.24
(CO2)2	2.186e-07	2.189e-07	-6.660	-6.660	0.001	68.70
CaCO3	1.559e-07	1.561e-07	-6.807	-6.807	0.001	-14.60
SrHCO3+	1.258e-07	1.163e-07	-6.900	-6.935	-0.034	(0)
MgCO3	1.063e-07	1.065e-07	-6.973	-6.973	0.001	-17.09
BaCO3	1.572e-08	1.574e-08	-7.804	-7.803	0.001	-10.71
NaCO3-	1.299e-08	1.198e-08	-7.886	-7.922	-0.035	-1.12
SrCO3	7.324e-10	7.334e-10	-9.135	-9.135	0.001	-14.14
Ca	1.805e-04					
Ca+2	1.717e-04	1.252e-04	-3.765	-3.903	-0.137	-18.02
CaHCO3+	8.599e-06	7.955e-06	-5.066	-5.099	-0.034	9.64
CaCO3	1.559e-07	1.561e-07	-6.807	-6.807	0.001	-14.60

CaSO4	9.149e-09	9.161e-09	-8.039	-8.038	0.001	7.44
CaHPO4	8.203e-09	8.214e-09	-8.086	-8.085	0.001	(0)
CaH2PO4+	2.035e-09	1.881e-09	-8.691	-8.726	-0.034	(0)
CaOH+	7.458e-11	6.876e-11	-10.127	-10.163	-0.035	(0)
CaPO4-	6.743e-11	6.231e-11	-10.171	-10.205	-0.034	(0)
CaHSO4+	1.926e-14	1.775e-14	-13.715	-13.751	-0.035	(0)
Cl	1.631e-03					
Cl-	1.622e-03	1.494e-03	-2.790	-2.826	-0.036	18.07
NaCl	8.062e-06	8.073e-06	-5.094	-5.093	0.001	(0)
MnCl+	5.755e-07	5.315e-07	-6.240	-6.275	-0.035	-3.48
FeCl+	3.141e-07	2.896e-07	-6.503	-6.538	-0.035	(0)
BaCl+	2.041e-07	1.882e-07	-6.690	-6.725	-0.035	(0)
MnCl2	3.461e-10	3.466e-10	-9.461	-9.460	0.001	88.02
MnCl3-	1.545e-13	1.426e-13	-12.811	-12.846	-0.035	43.47
FeCl+2	3.498e-20	2.544e-20	-19.456	-19.594	-0.138	(0)
FeCl2+	1.941e-22	1.792e-22	-21.712	-21.747	-0.035	(0)
FeCl3	2.675e-26	2.678e-26	-25.573	-25.572	0.001	(0)
F	2.791e-05					
F-	2.595e-05	2.390e-05	-4.586	-4.622	-0.036	-1.29
AlF2+	5.540e-07	5.120e-07	-6.256	-6.291	-0.034	(0)
MgF+	2.477e-07	2.285e-07	-6.606	-6.641	-0.035	-10.53
AlF3	1.536e-07	1.538e-07	-6.814	-6.813	0.001	(0)
AlF+2	5.912e-08	4.312e-08	-7.228	-7.365	-0.137	(0)
FeF+	3.639e-08	3.356e-08	-7.439	-7.474	-0.035	(0)
MnF+	1.563e-08	1.444e-08	-7.806	-7.841	-0.035	(0)
NaF	1.255e-08	1.257e-08	-7.901	-7.901	0.001	7.20
HF	1.049e-08	1.050e-08	-7.979	-7.979	0.001	12.42
AlF4-	1.585e-09	1.463e-09	-8.800	-8.835	-0.035	(0)
HF2-	1.030e-12	9.499e-13	-11.987	-12.022	-0.035	22.02
FeF+2	3.020e-17	2.197e-17	-16.520	-16.658	-0.138	(0)
FeF2+	2.218e-17	2.048e-17	-16.654	-16.689	-0.035	(0)
FeF3	7.702e-19	7.713e-19	-18.113	-18.113	0.001	(0)
SiF6-2	1.379e-28	1.003e-28	-27.860	-27.999	-0.138	42.63
Fe(2)	2.728e-04					
Fe+2	1.917e-04	1.404e-04	-3.717	-3.853	-0.135	-22.10
FeHCO3+	7.793e-05	7.185e-05	-4.108	-4.144	-0.035	(0)
FeCO3	2.581e-06	2.585e-06	-5.588	-5.588	0.001	(0)
FeCl+	3.141e-07	2.896e-07	-6.503	-6.538	-0.035	(0)
FeOH+	1.401e-07	1.294e-07	-6.854	-6.888	-0.035	(0)
FeHPO4	6.899e-08	6.908e-08	-7.161	-7.161	0.001	(0)
FeH2PO4+	4.621e-08	4.271e-08	-7.335	-7.369	-0.034	(0)
FeF+	3.639e-08	3.356e-08	-7.439	-7.474	-0.035	(0)
FeSO4	1.008e-08	1.009e-08	-7.997	-7.996	0.001	20.79
Fe(OH)2	3.137e-12	3.141e-12	-11.503	-11.503	0.001	(0)
FeHSO4+	2.160e-14	1.992e-14	-13.666	-13.701	-0.035	(0)
Fe(OH)3-	4.114e-16	3.799e-16	-15.386	-15.420	-0.035	(0)
Fe(3)	1.749e-11					
Fe(OH)2+	1.279e-11	1.182e-11	-10.893	-10.927	-0.034	(0)
Fe(OH)3	4.673e-12	4.679e-12	-11.330	-11.330	0.001	(0)
FeOH+2	1.582e-14	1.150e-14	-13.801	-13.939	-0.138	(0)
Fe(OH)4-	1.427e-14	1.319e-14	-13.846	-13.880	-0.034	(0)
FeF+2	3.020e-17	2.197e-17	-16.520	-16.658	-0.138	(0)
FeF2+	2.218e-17	2.048e-17	-16.654	-16.689	-0.035	(0)
Fe+3	1.149e-18	5.952e-19	-17.940	-18.225	-0.286	(0)
FeF3	7.702e-19	7.713e-19	-18.113	-18.113	0.001	(0)
FeH2PO4+2	1.333e-19	9.724e-20	-18.875	-19.012	-0.137	(0)
FeCl+2	3.498e-20	2.544e-20	-19.456	-19.594	-0.138	(0)
FeHPO4+	2.028e-20	1.873e-20	-19.693	-19.728	-0.035	(0)
FeSO4+	2.837e-21	2.620e-21	-20.547	-20.582	-0.035	(0)
FeCl2+	1.941e-22	1.792e-22	-21.712	-21.747	-0.035	(0)
FeCl3	2.675e-26	2.678e-26	-25.573	-25.572	0.001	(0)
Fe(SO4)2-	2.575e-26	2.374e-26	-25.589	-25.624	-0.035	(0)
Fe2(OH)2+4	1.401e-26	3.823e-27	-25.854	-26.418	-0.564	(0)
FeHSO4+2	2.935e-27	2.121e-27	-26.532	-26.673	-0.141	(0)
Fe3(OH)4+5	8.410e-35	1.105e-35	-34.075	-34.956	-0.881	(0)
H(0)	5.519e-14					
H2	2.759e-14	2.763e-14	-13.559	-13.559	0.001	28.61
K	3.838e-04					

K+	3.838e-04	3.535e-04	-3.416	-3.452	-0.036	8.99
KSO4-	1.088e-09	1.005e-09	-8.963	-8.998	-0.034	34.10
KHPO4-	9.218e-11	8.519e-11	-10.035	-10.070	-0.034	38.28
Mg	2.140e-04					
Mg+2	2.040e-04	1.493e-04	-3.690	-3.826	-0.136	-21.62
MgHCO3+	9.627e-06	8.874e-06	-5.017	-5.052	-0.035	5.47
MgF+	2.477e-07	2.285e-07	-6.606	-6.641	-0.035	-10.53
MgCO3	1.063e-07	1.065e-07	-6.973	-6.973	0.001	-17.09
MgSO4	1.394e-08	1.396e-08	-7.856	-7.855	0.001	5.77
MgHPO4	1.323e-08	1.325e-08	-7.878	-7.878	0.001	(0)
MgH2PO4+	3.091e-09	2.857e-09	-8.510	-8.544	-0.034	(0)
MgOH+	1.661e-09	1.538e-09	-8.780	-8.813	-0.033	(0)
MgPO4-	1.085e-10	1.003e-10	-9.965	-9.999	-0.034	(0)
Mn(2)	1.683e-04					
Mn+2	1.192e-04	8.731e-05	-3.924	-4.059	-0.135	-20.19
MnHCO3+	4.313e-05	3.983e-05	-4.365	-4.400	-0.035	(0)
MnCO3	5.315e-06	5.322e-06	-5.274	-5.274	0.001	(0)
MnCl+	5.755e-07	5.315e-07	-6.240	-6.275	-0.035	-3.48
MnF+	1.563e-08	1.444e-08	-7.806	-7.841	-0.035	(0)
MnOH+	6.999e-09	6.463e-09	-8.155	-8.190	-0.035	(0)
MnSO4	6.258e-09	6.266e-09	-8.204	-8.203	0.001	23.31
MnCl2	3.461e-10	3.466e-10	-9.461	-9.460	0.001	88.02
MnCl3-	1.545e-13	1.426e-13	-12.811	-12.846	-0.035	43.47
Mn(NO3)2	3.386e-14	3.390e-14	-13.470	-13.470	0.001	41.50
Mn(OH)3-	5.437e-20	5.021e-20	-19.265	-19.299	-0.035	(0)
Mn(3)	1.978e-31					
Mn+3	1.978e-31	1.025e-31	-30.704	-30.989	-0.286	(0)
N(3)	2.143e-06					
NO2-	2.143e-06	1.971e-06	-5.669	-5.705	-0.036	24.92
N(5)	1.071e-05					
NO3-	1.071e-05	9.857e-06	-4.970	-5.006	-0.036	29.37
BaNO3+	5.529e-11	5.098e-11	-10.257	-10.293	-0.035	(0)
Mn(NO3)2	3.386e-14	3.390e-14	-13.470	-13.470	0.001	41.50
Na	1.001e-03					
Na+	9.901e-04	9.139e-04	-3.004	-3.039	-0.035	-1.50
NaCl	8.062e-06	8.073e-06	-5.094	-5.093	0.001	(0)
NaHCO3	2.652e-06	2.656e-06	-5.576	-5.576	0.001	1.80
NaCO3-	1.299e-08	1.198e-08	-7.886	-7.922	-0.035	-1.12
NaF	1.255e-08	1.257e-08	-7.901	-7.901	0.001	7.20
NaSO4-	2.044e-09	1.889e-09	-8.689	-8.724	-0.034	14.17
NaHPO4-	2.383e-10	2.202e-10	-9.623	-9.657	-0.034	33.91
NaOH	2.683e-21	2.687e-21	-20.571	-20.571	0.001	(0)
O(0)	4.690e-05					
O2	2.345e-05	2.348e-05	-4.630	-4.629	0.001	30.27
P	9.690e-07					
H2PO4-	6.568e-07	6.069e-07	-6.183	-6.217	-0.034	33.29
HPO4-2	1.699e-07	1.236e-07	-6.770	-6.908	-0.138	6.93
FeHPO4	6.899e-08	6.908e-08	-7.161	-7.161	0.001	(0)
FeH2PO4+	4.621e-08	4.271e-08	-7.335	-7.369	-0.034	(0)
MgHPO4	1.323e-08	1.325e-08	-7.878	-7.878	0.001	(0)
CaHPO4	8.203e-09	8.214e-09	-8.086	-8.085	0.001	(0)
MgH2PO4+	3.091e-09	2.857e-09	-8.510	-8.544	-0.034	(0)
CaH2PO4+	2.035e-09	1.881e-09	-8.691	-8.726	-0.034	(0)
NaHPO4-	2.383e-10	2.202e-10	-9.623	-9.657	-0.034	33.91
MgPO4-	1.085e-10	1.003e-10	-9.965	-9.999	-0.034	(0)
KHPO4-	9.218e-11	8.519e-11	-10.035	-10.070	-0.034	38.28
CaPO4-	6.743e-11	6.231e-11	-10.171	-10.205	-0.034	(0)
H3PO4	2.641e-11	2.644e-11	-10.578	-10.578	0.001	47.31
PO4-3	3.710e-13	1.783e-13	-12.431	-12.749	-0.318	-22.72
FeH2PO4+2	1.333e-19	9.724e-20	-18.875	-19.012	-0.137	(0)
FeHPO4+	2.028e-20	1.873e-20	-19.693	-19.728	-0.035	(0)
S(6)	6.249e-07					
SO4-2	5.736e-07	4.170e-07	-6.241	-6.380	-0.139	14.46
MgSO4	1.394e-08	1.396e-08	-7.856	-7.855	0.001	5.77
FeSO4	1.008e-08	1.009e-08	-7.997	-7.996	0.001	20.79
CaSO4	9.149e-09	9.161e-09	-8.039	-8.038	0.001	7.44
BaSO4	8.573e-09	8.585e-09	-8.067	-8.066	0.001	(0)
MnSO4	6.258e-09	6.266e-09	-8.204	-8.203	0.001	23.31

NaSO4-	2.044e-09	1.889e-09	-8.689	-8.724	-0.034	14.17
KSO4-	1.088e-09	1.005e-09	-8.963	-8.998	-0.034	34.10
SrSO4	1.253e-10	1.254e-10	-9.902	-9.902	0.001	24.17
HSO4-	1.280e-11	1.180e-11	-10.893	-10.928	-0.035	40.20
AlSO4+	2.548e-13	2.351e-13	-12.594	-12.629	-0.035	(0)
FeHSO4+	2.160e-14	1.992e-14	-13.666	-13.701	-0.035	(0)
CaHSO4+	1.926e-14	1.775e-14	-13.715	-13.751	-0.035	(0)
Al(SO4)2-	3.333e-18	3.075e-18	-17.477	-17.512	-0.035	(0)
AlHSO4+2	8.583e-21	6.203e-21	-20.066	-20.207	-0.141	(0)
FeSO4+	2.837e-21	2.620e-21	-20.547	-20.582	-0.035	(0)
Fe(SO4)2-	2.575e-26	2.374e-26	-25.589	-25.624	-0.035	(0)
FeHSO4+2	2.935e-27	2.121e-27	-26.532	-26.673	-0.141	(0)
Si	3.646e-05					
H4SiO4	3.645e-05	3.650e-05	-4.438	-4.438	0.001	52.22
H3SiO4-	1.821e-08	1.678e-08	-7.740	-7.775	-0.035	27.97
H2SiO4-2	4.635e-15	3.381e-15	-14.334	-14.471	-0.137	(0)
SiF6-2	1.379e-28	1.003e-28	-27.860	-27.999	-0.138	42.63
Sr	2.284e-06					
Sr+2	2.157e-06	1.574e-06	-5.666	-5.803	-0.137	-17.61
SrHCO3+	1.258e-07	1.163e-07	-6.900	-6.935	-0.034	(0)
SrCO3	7.324e-10	7.334e-10	-9.135	-9.135	0.001	-14.14
SrSO4	1.253e-10	1.254e-10	-9.902	-9.902	0.001	24.17
SrOH+	2.894e-13	2.673e-13	-12.538	-12.573	-0.035	(0)

----------Distribution of alkalinity----------

Total alkalinity (eq/kgw) = 5.702e-03

Species	Alkalinity	Molality	Alk/Mol
HCO3-	5.538e-03	5.538e-03	1.00
FeHCO3+	7.793e-05	7.793e-05	1.00
MnHCO3+	4.313e-05	4.313e-05	1.00
MnCO3	1.063e-05	5.315e-06	2.00
MgHCO3+	9.627e-06	9.627e-06	1.00
CaHCO3+	8.599e-06	8.599e-06	1.00
FeCO3	5.162e-06	2.581e-06	2.00
NaHCO3	2.652e-06	2.652e-06	1.00
CO3-2	2.104e-06	1.052e-06	2.00
BaHCO3+	2.072e-06	2.072e-06	1.00
Al(OH)4-	1.363e-06	3.406e-07	4.00
H+	-3.249e-07	3.249e-07	-1.00
CaCO3	3.118e-07	1.559e-07	2.00
Al(OH)2+	2.593e-07	1.297e-07	2.00
MgCO3	2.127e-07	1.063e-07	2.00
HPO4-2	1.699e-07	1.699e-07	1.00
Al(OH)3	1.543e-07	5.144e-08	3.00
FeOH+	1.401e-07	1.401e-07	1.00
SrHCO3+	1.258e-07	1.258e-07	1.00
FeHPO4	6.899e-08	6.899e-08	1.00
OH-	3.193e-08	3.193e-08	1.00
BaCO3	3.144e-08	1.572e-08	2.00
NaCO3-	2.598e-08	1.299e-08	2.00
H3SiO4-	1.821e-08	1.821e-08	1.00
MgHPO4	1.323e-08	1.323e-08	1.00
HF	-1.049e-08	1.049e-08	-1.00
CaHPO4	8.203e-09	8.203e-09	1.00
AlOH+2	7.355e-09	7.355e-09	1.00
MnOH+	6.999e-09	6.999e-09	1.00
MgOH+	1.661e-09	1.661e-09	1.00
SrCO3	1.465e-09	7.324e-10	2.00
NaHPO4-	2.383e-10	2.383e-10	1.00
MgPO4-	2.170e-10	1.085e-10	2.00
CaPO4-	1.349e-10	6.743e-11	2.00
KHPO4-	9.218e-11	9.218e-11	1.00
CaOH+	7.458e-11	7.458e-11	1.00
H3PO4	-2.641e-11	2.641e-11	-1.00
HSO4-	-1.280e-11	1.280e-11	-1.00

Fe(OH)2	6.274e-12	3.137e-12	2.00
BaOH+	4.990e-12	4.990e-12	1.00
Fe(OH)3	4.673e-12	4.673e-12	1.00
HF2-	-1.030e-12	1.030e-12	-1.00
PO4-3	7.420e-13	3.710e-13	2.00
SrOH+	2.894e-13	2.894e-13	1.00
Fe(OH)4-	2.854e-14	1.427e-14	2.00
FeHSO4+	-2.160e-14	2.160e-14	-1.00
CaHSO4+	-1.926e-14	1.926e-14	-1.00
FeOH+2	-1.582e-14	1.582e-14	-1.00
H2SiO4-2	9.270e-15	4.635e-15	2.00
Fe(OH)3-	1.234e-15	4.114e-16	3.00
FeF+2	-6.040e-17	3.020e-17	-2.00
FeF2+	-4.435e-17	2.218e-17	-2.00
Fe+3	-2.298e-18	1.149e-18	-2.00
FeF3	-1.540e-18	7.702e-19	-2.00
FeH2PO4+2	-2.666e-19	1.333e-19	-2.00
Mn(OH)3-	1.631e-19	5.437e-20	3.00
FeCl+2	-6.996e-20	3.498e-20	-2.00
FeHPO4+	-2.028e-20	2.028e-20	-1.00
AlHSO4+2	-8.583e-21	8.583e-21	-1.00
FeSO4+	-5.675e-21	2.837e-21	-2.00
NaOH	2.683e-21	2.683e-21	1.00
FeCl2+	-3.882e-22	1.941e-22	-2.00
FeCl3	-5.349e-26	2.675e-26	-2.00
Fe(SO4)2-	-5.150e-26	2.575e-26	-2.00
Fe2(OH)2+4	-2.802e-26	1.401e-26	-2.00
FeHSO4+2	-8.804e-27	2.935e-27	-3.00
SiF6-2	-5.518e-28	1.379e-28	-4.00
Fe3(OH)4+5	-1.682e-34	8.410e-35	-2.00

-------------------------------Saturation indices--------------------------------

Phase	SI**	log IAP	log K(296 K, 1 atm)	
Al(OH)3(a)	-1.09	9.82	10.91	Al(OH)3
Albite	-4.74	-22.85	-18.11	NaAlSi3O8
Alunite	-5.12	-6.31	-1.19	KAl3(SO4)2(OH)6
Anhydrite	-6.02	-10.28	-4.26	CaSO4
Anorthite	-6.02	-25.78	-19.76	CaAl2Si2O8
Aragonite	-1.69	-10.02	-8.33	CaCO3
BaCl2	-12.28	-10.04	2.24	BaCl2
BaCl2:2H2O	-10.23	-10.04	0.19	BaCl2:2H2O
BaCl2:H2O	-10.86	-10.04	0.82	BaCl2:H2O
Barite	-0.91	-10.77	-9.86	BaSO4
Ca-Montmorillonite	0.15	-45.12	-45.27	Ca0.165Al2.33Si3.67O10(OH)2
Calcite	-1.55	-10.02	-8.47	CaCO3
Celestite	-5.53	-12.18	-6.65	SrSO4
Chalcedony	-0.87	-4.44	-3.57	SiO2
Chlorite(14A)	-16.62	52.40	69.02	Mg5Al2Si3O10(OH)8
Chrysotile	-13.65	18.77	32.41	Mg3Si2O5(OH)4
CO2(g)	-1.00	-2.45	-1.45	CO2
Dolomite	-2.91	-19.96	-17.05	CaMg(CO3)2
Fe(OH)3(a)	-3.56	1.33	4.89	Fe(OH)3
Fluorite	-2.53	-13.15	-10.62	CaF2
Gibbsite	1.61	9.82	8.21	Al(OH)3
Goethite	2.27	1.33	-0.94	FeOOH
Gypsum	-5.70	-10.28	-4.58	CaSO4:2H2O
H2(g)	-10.46	-13.56	-3.10	H2
H2O(g)	-1.55	-0.00	1.55	H2O
Halite	-7.43	-5.86	1.57	NaCl
Hausmannite	-24.09	37.36	61.45	Mn3O4
Hematite	6.55	2.67	-3.88	Fe2O3
Hydroxyapatite	-10.89	-14.16	-3.27	Ca5(PO4)3OH
Illite	-0.84	-41.34	-40.50	K0.6Mg0.25Al2.3Si3.5O10(OH)2
Jarosite-K	-22.69	-31.77	-9.08	KFe3(SO4)2(OH)6
K-feldspar	-2.56	-23.27	-20.70	KAlSi3O8
K-mica	6.26	19.22	12.95	KAl3Si3O10(OH)2

Kaolinite	3.18	10.77	7.58	Al2Si2O5(OH)4
Manganite	-11.15	14.19	25.34	MnOOH
Melanterite	-8.00	-10.23	-2.23	FeSO4:7H2O
O2(g)	-1.75	-4.63	-2.88	O2
Pyrochroite	-6.22	8.98	15.20	Mn(OH)2
Pyrolusite	-22.26	19.40	41.65	MnO2:H2O
Quartz	-0.43	-4.44	-4.01	SiO2
Rhodochrosite	0.95	-10.17	-11.12	MnCO3
Sepiolite	-10.69	5.11	15.80	Mg2Si3O7.5OH:3H2O
Sepiolite(d)	-13.55	5.11	18.66	Mg2Si3O7.5OH:3H2O
Siderite	0.91	-9.97	-10.88	FeCO3
SiO2(a)	-1.71	-4.44	-2.73	SiO2
Strontianite	-2.65	-11.92	-9.27	SrCO3
Sylvite	-7.17	-6.28	0.89	KCl
Talc	-11.70	9.89	21.59	Mg3Si4O10(OH)2
Vivianite	-1.06	-37.06	-36.00	Fe3(PO4)2:8H2O
Witherite	-1.94	-10.50	-8.57	BaCO3

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
For ideal gases, phi = 1.

Initial solution 12.

-----------------------------Solution composition------------------------------

Elements	Molality	Moles
Alkalinity	4.915e-04	4.915e-04
Br	6.259e-06	6.259e-06
Ca	4.617e-04	4.617e-04
Cl	1.885e-03	1.885e-03
F	5.265e-07	5.265e-07
K	1.791e-04	1.791e-04
Mg	1.753e-04	1.753e-04
N(5)	2.500e-03	2.500e-03
Na	2.276e-03	2.276e-03
P	3.229e-07	3.229e-07
S(6)	7.612e-04	7.612e-04

----------------------------Description of solution----------------------------

pH	= 5.500
pe	= 0.371
Specific Conductance (µS/cm, 23°C)	= 577
Density (g/cm³)	= 0.99785
Volume (L)	= 1.00271
Activity of water	= 1.000
Ionic strength (mol/kgw)	= 6.264e-03
Mass of water (kg)	= 1.000e+00
Total carbon (mol/kg)	= 3.798e-03
Total CO2 (mol/kg)	= 3.798e-03
Temperature (°C)	= 23.06
Electrical balance (eq)	= -2.677e-03
Percent error, 100*(Cat-|An|)/(Cat+|An|)	= -27.00
Iterations	= 10 (126 overall)
Total H	= 1.110129e+02
Total O	= 5.552485e+01

---------------------------Distribution of species----------------------------

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma	mole V cm³/mol
H+	3.409e-06	3.162e-06	-5.467	-5.500	-0.033	0.00
OH-	3.000e-09	2.756e-09	-8.523	-8.560	-0.037	-4.14
H2O	5.551e+01	9.998e-01	1.744	-0.000	0.000	18.06
Br	6.259e-06					
Br-	6.259e-06	5.744e-06	-5.203	-5.241	-0.037	24.51

C(4)	3.798e-03					
CO2	3.302e-03	3.307e-03	-2.481	-2.481	0.001	34.34
HCO3-	4.919e-04	4.535e-04	-3.308	-3.343	-0.035	24.59
CaHCO3+	1.895e-06	1.749e-06	-5.722	-5.757	-0.035	9.63
MgHCO3+	6.693e-07	6.154e-07	-6.174	-6.211	-0.036	5.46
NaHCO3	5.331e-07	5.339e-07	-6.273	-6.273	0.001	1.80
(CO2)2	1.879e-07	1.882e-07	-6.726	-6.725	0.001	68.68
CO3-2	8.943e-09	6.462e-09	-8.049	-8.190	-0.141	-5.25
CaCO3	3.255e-09	3.260e-09	-8.487	-8.487	0.001	-14.60
MgCO3	6.988e-10	6.998e-10	-9.156	-9.155	0.001	-17.09
NaCO3-	2.454e-10	2.257e-10	-9.610	-9.646	-0.036	-1.14
Ca	4.617e-04					
Ca+2	4.318e-04	3.118e-04	-3.365	-3.506	-0.141	-18.01
CaSO4	2.802e-05	2.806e-05	-4.553	-4.552	0.001	7.43
CaHCO3+	1.895e-06	1.749e-06	-5.722	-5.757	-0.035	9.63
CaCO3	3.255e-09	3.260e-09	-8.487	-8.487	0.001	-14.60
CaH2PO4+	2.383e-09	2.197e-09	-8.623	-8.658	-0.035	(0)
CaHPO4	9.141e-10	9.154e-10	-9.039	-9.038	0.001	(0)
CaHSO4+	6.170e-10	5.675e-10	-9.210	-9.246	-0.036	(0)
CaOH+	1.779e-11	1.636e-11	-10.750	-10.786	-0.036	(0)
CaPO4-	7.160e-13	6.601e-13	-12.145	-12.180	-0.035	(0)
Cl	1.885e-03					
Cl-	1.864e-03	1.713e-03	-2.730	-2.766	-0.037	18.06
NaCl	2.090e-05	2.093e-05	-4.680	-4.679	0.001	(0)
F	5.265e-07					
F-	5.199e-07	4.776e-07	-6.284	-6.321	-0.037	-1.29
MgF+	3.869e-09	3.561e-09	-8.412	-8.448	-0.036	-10.53
HF	2.184e-09	2.187e-09	-8.661	-8.660	0.001	12.41
NaF	5.681e-10	5.689e-10	-9.246	-9.245	0.001	7.19
HF2-	4.291e-15	3.947e-15	-14.367	-14.404	-0.036	22.01
H(0)	2.611e-15					
H2	1.306e-15	1.308e-15	-14.884	-14.884	0.001	28.61
K	1.791e-04					
K+	1.784e-04	1.640e-04	-3.748	-3.785	-0.037	8.99
KSO4-	6.202e-07	5.718e-07	-6.207	-6.243	-0.035	34.10
KHPO4-	1.926e-12	1.775e-12	-11.715	-11.751	-0.035	38.30
Mg	1.753e-04					
Mg+2	1.612e-04	1.169e-04	-3.793	-3.932	-0.140	-21.60
MgSO4	1.337e-05	1.339e-05	-4.874	-4.873	0.001	5.76
MgHCO3+	6.693e-07	6.154e-07	-6.174	-6.211	-0.036	5.46
MgF+	3.869e-09	3.561e-09	-8.412	-8.448	-0.036	-10.53
MgH2PO4+	1.138e-09	1.049e-09	-8.944	-8.979	-0.035	(0)
MgCO3	6.988e-10	6.998e-10	-9.156	-9.155	0.001	-17.09
MgHPO4	4.634e-10	4.641e-10	-9.334	-9.333	0.001	(0)
MgOH+	1.218e-10	1.125e-10	-9.914	-9.949	-0.034	(0)
MgPO4-	3.622e-13	3.339e-13	-12.441	-12.476	-0.035	(0)
N(5)	2.500e-03					
NO3-	2.500e-03	2.294e-03	-2.602	-2.639	-0.037	29.34
Na	2.276e-03					
Na+	2.248e-03	2.070e-03	-2.648	-2.684	-0.036	-1.51
NaCl	2.090e-05	2.093e-05	-4.680	-4.679	0.001	(0)
NaSO4-	5.708e-06	5.263e-06	-5.243	-5.279	-0.035	14.20
NaHCO3	5.331e-07	5.339e-07	-6.273	-6.273	0.001	1.80
NaF	5.681e-10	5.689e-10	-9.246	-9.245	0.001	7.19
NaCO3-	2.454e-10	2.257e-10	-9.610	-9.646	-0.036	-1.14
NaHPO4-	2.431e-11	2.242e-11	-10.614	-10.649	-0.035	33.94
NaOH	5.697e-22	5.706e-22	-21.244	-21.244	0.001	(0)
O(0)	0.000e+00					
O2	0.000e+00	0.000e+00	-63.244	-63.243	0.001	30.25
P	3.229e-07					
H2PO4-	3.102e-07	2.860e-07	-6.508	-6.544	-0.035	33.30
HPO4-2	7.709e-09	5.554e-09	-8.113	-8.255	-0.142	6.95
CaH2PO4+	2.383e-09	2.197e-09	-8.623	-8.658	-0.035	(0)
MgH2PO4+	1.138e-09	1.049e-09	-8.944	-8.979	-0.035	(0)
CaHPO4	9.141e-10	9.154e-10	-9.039	-9.038	0.001	(0)
MgHPO4	4.634e-10	4.641e-10	-9.334	-9.333	0.001	(0)
H3PO4	1.299e-10	1.301e-10	-9.886	-9.886	0.001	47.30
NaHPO4-	2.431e-11	2.242e-11	-10.614	-10.649	-0.035	33.94

KHPO4-	1.926e-12	1.775e-12	-11.715	-11.751	-0.035	38.30
CaPO4-	7.160e-13	6.601e-13	-12.145	-12.180	-0.035	(0)
MgPO4-	3.622e-13	3.339e-13	-12.441	-12.476	-0.035	(0)
PO4-3	1.620e-15	7.614e-16	-14.790	-15.118	-0.328	-22.68
S(6)	7.612e-04					
SO4-2	7.133e-04	5.135e-04	-3.147	-3.289	-0.143	14.43
CaSO4	2.802e-05	2.806e-05	-4.553	-4.552	0.001	7.43
MgSO4	1.337e-05	1.339e-05	-4.874	-4.873	0.001	5.76
NaSO4-	5.708e-06	5.263e-06	-5.243	-5.279	-0.035	14.20
KSO4-	6.202e-07	5.718e-07	-6.207	-6.243	-0.035	34.10
HSO4-	1.646e-07	1.514e-07	-6.784	-6.820	-0.036	40.19
CaHSO4+	6.170e-10	5.675e-10	-9.210	-9.246	-0.036	(0)

----------Distribution of alkalinity----------

Total alkalinity (eq/kgw) = 4.915e-04

Species	Alkalinity	Molality	Alk/Mol
HCO3-	4.919e-04	4.919e-04	1.00
H+	-3.409e-06	3.409e-06	-1.00
CaHCO3+	1.895e-06	1.895e-06	1.00
MgHCO3+	6.693e-07	6.693e-07	1.00
NaHCO3	5.331e-07	5.331e-07	1.00
HSO4-	-1.646e-07	1.646e-07	-1.00
CO3-2	1.789e-08	8.943e-09	2.00
HPO4-2	7.709e-09	7.709e-09	1.00
CaCO3	6.510e-09	3.255e-09	2.00
OH-	3.000e-09	3.000e-09	1.00
HF	-2.184e-09	2.184e-09	-1.00
MgCO3	1.398e-09	6.988e-10	2.00
CaHPO4	9.141e-10	9.141e-10	1.00
CaHSO4+	-6.170e-10	6.170e-10	-1.00
NaCO3-	4.908e-10	2.454e-10	2.00
MgHPO4	4.634e-10	4.634e-10	1.00
H3PO4	-1.299e-10	1.299e-10	-1.00
MgOH+	1.218e-10	1.218e-10	1.00
NaHPO4-	2.431e-11	2.431e-11	1.00
CaOH+	1.779e-11	1.779e-11	1.00
KHPO4-	1.926e-12	1.926e-12	1.00
CaPO4-	1.432e-12	7.160e-13	2.00
MgPO4-	7.243e-13	3.622e-13	2.00
HF2-	-4.291e-15	4.291e-15	-1.00
PO4-3	3.241e-15	1.620e-15	2.00
NaOH	5.697e-22	5.697e-22	1.00

----------Saturation indices----------

Phase	SI**	log IAP	log K(296 K, 1 atm)	
Anhydrite	-2.54	-6.80	-4.26	CaSO4
Aragonite	-3.37	-11.70	-8.32	CaCO3
Calcite	-3.23	-11.70	-8.47	CaCO3
CO2(g)	-1.04	-2.48	-1.45	CO2
Dolomite	-6.77	-23.82	-17.04	CaMg(CO3)2
Fluorite	-5.53	-16.15	-10.62	CaF2
Gypsum	-2.21	-6.80	-4.58	CaSO4:2H2O
H2(g)	-11.79	-14.88	-3.10	H2
H2O(g)	-1.55	-0.00	1.55	H2O
Halite	-7.02	-5.45	1.57	NaCl
Hydroxyapatite	-17.05	-20.30	-3.25	Ca5(PO4)3OH
O2(g)	-60.37	-63.24	-2.88	O2
Sylvite	-7.44	-6.55	0.89	KCl

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
For ideal gases, phi = 1.

Initial solution 13.

----------Solution composition----------

Elements	Molality	Moles
Alkalinity	4.768e-03	4.768e-03
Ba	8.523e-06	8.523e-06
Br	7.513e-06	7.513e-06
Ca	1.772e-03	1.772e-03
Cl	2.083e-03	2.083e-03
F	3.160e-06	3.160e-06
K	1.356e-04	1.356e-04
Mg	2.226e-04	2.226e-04
N(5)	8.357e-05	8.357e-05
Na	2.833e-03	2.833e-03
P	1.938e-06	1.938e-06
S(6)	1.895e-04	1.895e-04

----------Description of solution----------

pH	= 6.500
pe	= 0.447
Specific Conductance (µS/cm, 25°C)	= 693
Density (g/cm³)	= 0.99754
Volume (L)	= 1.00314
Activity of water	= 1.000
Ionic strength (mol/kgw)	= 9.046e-03
Mass of water (kg)	= 1.000e+00
Total carbon (mol/kg)	= 7.794e-03
Total CO2 (mol/kg)	= 7.794e-03
Temperature (°C)	= 24.78
Electrical balance (eq)	= -3.507e-04
Percent error, 100*(Cat-|An|)/(Cat+|An|)	= -2.51
Iterations	= 10 (136 overall)
Total H	= 1.110172e+02
Total O	= 5.552759e+01

----------Distribution of species----------

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma	mole V cm³/mol
H+	3.450e-07	3.162e-07	-6.462	-6.500	-0.038	0.00
OH-	3.480e-08	3.147e-08	-7.458	-7.502	-0.044	-4.05
H2O	5.551e+01	9.997e-01	1.744	-0.000	0.000	18.07
Ba	8.523e-06					
Ba+2	7.953e-06	5.364e-06	-5.099	-5.271	-0.171	-12.56
BaSO4	2.944e-07	2.951e-07	-6.531	-6.530	0.001	(0)
BaHCO3+	2.398e-07	2.172e-07	-6.620	-6.663	-0.043	(0)
BaCl+	3.451e-08	3.126e-08	-7.462	-7.505	-0.043	(0)
BaCO3	1.729e-09	1.733e-09	-8.762	-8.761	0.001	-10.70
BaNO3+	5.625e-11	5.096e-11	-10.250	-10.293	-0.043	(0)
BaOH+	6.329e-13	5.746e-13	-12.199	-12.241	-0.042	(0)
Br	7.513e-06					
Br-	7.513e-06	6.784e-06	-5.124	-5.169	-0.044	24.61
C(4)	7.794e-03					
HCO3-	4.681e-03	4.255e-03	-2.330	-2.371	-0.041	24.75
CO2	3.028e-03	3.034e-03	-2.519	-2.518	0.001	34.42
CaHCO3+	6.811e-05	6.200e-05	-4.167	-4.208	-0.041	9.71
MgHCO3+	7.944e-06	7.193e-06	-5.100	-5.143	-0.043	5.52
NaHCO3	6.067e-06	6.080e-06	-5.217	-5.216	0.001	1.80
CaCO3	1.202e-06	1.204e-06	-5.920	-5.919	0.001	-14.60
CO3-2	9.206e-07	6.282e-07	-6.036	-6.202	-0.166	-5.05
BaHCO3+	2.398e-07	2.172e-07	-6.620	-6.663	-0.043	(0)
(CO2)2	1.674e-07	1.678e-07	-6.776	-6.775	0.001	68.84
MgCO3	8.622e-08	8.640e-08	-7.064	-7.063	0.001	-17.09
NaCO3-	3.241e-08	2.936e-08	-7.489	-7.532	-0.043	-0.95
BaCO3	1.729e-09	1.733e-09	-8.762	-8.761	0.001	-10.70

Ca	1.772e-03					
Ca+2	1.681e-03	1.146e-03	-2.775	-2.941	-0.166	-17.94
CaHCO3+	6.811e-05	6.200e-05	-4.167	-4.208	-0.041	9.71
CaSO4	2.228e-05	2.233e-05	-4.652	-4.651	0.001	7.49
CaCO3	1.202e-06	1.204e-06	-5.920	-5.919	0.001	-14.60
CaHPO4	1.510e-07	1.513e-07	-6.821	-6.820	0.001	(0)
CaH2PO4+	3.961e-08	3.600e-08	-7.402	-7.444	-0.041	(0)
CaPO4-	1.240e-09	1.127e-09	-8.906	-8.948	-0.041	(0)
CaOH+	6.637e-10	6.013e-10	-9.178	-9.221	-0.043	(0)
CaHSO4+	5.107e-11	4.627e-11	-10.292	-10.335	-0.043	(0)
Cl	2.083e-03					
Cl-	2.054e-03	1.859e-03	-2.687	-2.731	-0.043	18.13
NaCl	2.813e-05	2.819e-05	-4.551	-4.550	0.001	(0)
BaCl+	3.451e-08	3.126e-08	-7.462	-7.505	-0.043	(0)
F	3.160e-06					
F-	3.125e-06	2.825e-06	-5.505	-5.549	-0.044	-1.26
MgF+	2.966e-08	2.689e-08	-7.528	-7.570	-0.043	-10.52
NaF	4.118e-09	4.126e-09	-8.385	-8.384	0.001	7.25
HF	1.332e-09	1.335e-09	-8.876	-8.875	0.001	12.49
HF2-	1.594e-14	1.444e-14	-13.797	-13.840	-0.043	22.11
H(0)	1.807e-17					
H2	9.037e-18	9.056e-18	-17.044	-17.043	0.001	28.61
K	1.356e-04					
K+	1.355e-04	1.226e-04	-3.868	-3.912	-0.044	9.06
KSO4-	1.036e-07	9.416e-08	-6.985	-7.026	-0.041	34.16
KHPO4-	6.358e-11	5.779e-11	-10.197	-10.238	-0.041	38.20
Mg	2.226e-04					
Mg+2	2.108e-04	1.446e-04	-3.676	-3.840	-0.164	-21.62
MgHCO3+	7.944e-06	7.193e-06	-5.100	-5.143	-0.043	5.52
MgSO4	3.692e-06	3.700e-06	-5.433	-5.432	0.001	5.83
MgCO3	8.622e-08	8.640e-08	-7.064	-7.063	0.001	-17.09
MgF+	2.966e-08	2.689e-08	-7.528	-7.570	-0.043	-10.52
MgHPO4	2.576e-08	2.582e-08	-7.589	-7.588	0.001	(0)
MgH2PO4+	6.366e-09	5.786e-09	-8.196	-8.238	-0.041	(0)
MgOH+	1.786e-09	1.627e-09	-8.748	-8.788	-0.040	(0)
MgPO4-	2.112e-10	1.919e-10	-9.675	-9.717	-0.041	(0)
N(5)	8.357e-05					
NO3-	8.357e-05	7.546e-05	-4.078	-4.122	-0.044	29.53
BaNO3+	5.625e-11	5.096e-11	-10.250	-10.293	-0.043	(0)
Na	2.833e-03					
Na+	2.797e-03	2.538e-03	-2.553	-2.596	-0.042	-1.40
NaCl	2.813e-05	2.819e-05	-4.551	-4.550	0.001	(0)
NaHCO3	6.067e-06	6.080e-06	-5.217	-5.216	0.001	1.80
NaSO4-	1.534e-06	1.394e-06	-5.814	-5.856	-0.041	14.29
NaCO3-	3.241e-08	2.936e-08	-7.489	-7.532	-0.043	-0.95
NaF	4.118e-09	4.126e-09	-8.385	-8.384	0.001	7.25
NaHPO4-	1.316e-09	1.196e-09	-8.881	-8.922	-0.041	34.12
NaOH	7.969e-21	7.986e-21	-20.099	-20.098	0.001	(0)
O(0)	0.000e+00					
O2	0.000e+00	0.000e+00	-58.366	-58.365	0.001	30.38
P	1.938e-06					
H2PO4-	1.357e-06	1.233e-06	-5.868	-5.909	-0.041	33.28
HPO4-2	3.558e-07	2.418e-07	-6.449	-6.617	-0.168	6.96
CaHPO4	1.510e-07	1.513e-07	-6.821	-6.820	0.001	(0)
CaH2PO4+	3.961e-08	3.600e-08	-7.402	-7.444	-0.041	(0)
MgHPO4	2.576e-08	2.582e-08	-7.589	-7.588	0.001	(0)
MgH2PO4+	6.366e-09	5.786e-09	-8.196	-8.238	-0.041	(0)
NaHPO4-	1.316e-09	1.196e-09	-8.881	-8.922	-0.041	34.12
CaPO4-	1.240e-09	1.127e-09	-8.906	-8.948	-0.041	(0)
MgPO4-	2.112e-10	1.919e-10	-9.675	-9.717	-0.041	(0)
KHPO4-	6.358e-11	5.779e-11	-10.197	-10.238	-0.041	38.20
H3PO4	5.714e-11	5.726e-11	-10.243	-10.242	0.001	47.40
PO4-3	8.384e-13	3.432e-13	-12.077	-12.464	-0.388	-22.69
S(6)	1.895e-04					
SO4-2	1.616e-04	1.098e-04	-3.791	-3.960	-0.168	14.72
CaSO4	2.228e-05	2.233e-05	-4.652	-4.651	0.001	7.49
MgSO4	3.692e-06	3.700e-06	-5.433	-5.432	0.001	5.83
NaSO4-	1.534e-06	1.394e-06	-5.814	-5.856	-0.041	14.29

BaSO4	2.944e-07	2.951e-07	-6.531	-6.530	0.001	(0)
KSO4-	1.036e-07	9.416e-08	-6.985	-7.026	-0.041	34.16
HSO4-	3.707e-09	3.358e-09	-8.431	-8.474	-0.043	40.32
CaHSO4+	5.107e-11	4.627e-11	-10.292	-10.335	-0.043	(0)

----------Distribution of alkalinity----------

Total alkalinity (eq/kgw) = 4.768e-03

Species	Alkalinity	Molality	Alk/Mol
HCO3-	4.681e-03	4.681e-03	1.00
CaHCO3+	6.811e-05	6.811e-05	1.00
MgHCO3+	7.944e-06	7.944e-06	1.00
NaHCO3	6.067e-06	6.067e-06	1.00
CaCO3	2.403e-06	1.202e-06	2.00
CO3-2	1.841e-06	9.206e-07	2.00
HPO4-2	3.558e-07	3.558e-07	1.00
H+	-3.450e-07	3.450e-07	-1.00
BaHCO3+	2.398e-07	2.398e-07	1.00
MgCO3	1.724e-07	8.622e-08	2.00
CaHPO4	1.510e-07	1.510e-07	1.00
NaCO3-	6.481e-08	3.241e-08	2.00
OH-	3.480e-08	3.480e-08	1.00
MgHPO4	2.576e-08	2.576e-08	1.00
HSO4-	-3.707e-09	3.707e-09	-1.00
BaCO3	3.459e-09	1.729e-09	2.00
CaPO4-	2.481e-09	1.240e-09	2.00
MgOH+	1.786e-09	1.786e-09	1.00
HF	-1.332e-09	1.332e-09	-1.00
NaHPO4-	1.316e-09	1.316e-09	1.00
CaOH+	6.637e-10	6.637e-10	1.00
MgPO4-	4.223e-10	2.112e-10	2.00
KHPO4-	6.358e-11	6.358e-11	1.00
H3PO4	-5.714e-11	5.714e-11	-1.00
CaHSO4+	-5.107e-11	5.107e-11	-1.00
PO4-3	1.677e-12	8.384e-13	2.00
BaOH+	6.329e-13	6.329e-13	1.00
HF2-	-1.594e-14	1.594e-14	-1.00
NaOH	7.969e-21	7.969e-21	1.00

----------Saturation indices----------

Phase	SI**	log IAP	log K(297 K, 1 atm)	
Anhydrite	-2.63	-6.90	-4.28	CaSO4
Aragonite	-0.81	-9.14	-8.33	CaCO3
BaCl2	-12.96	-10.73	2.23	BaCl2
BaCl2:2H2O	-10.94	-10.73	0.21	BaCl2:2H2O
BaCl2:H2O	-11.56	-10.73	0.82	BaCl2:H2O
Barite	0.62	-9.23	-9.85	BaSO4
Calcite	-0.66	-9.14	-8.48	CaCO3
CO2(g)	-1.05	-2.52	-1.47	CO2
Dolomite	-2.10	-19.18	-17.08	CaMg(CO3)2
Fluorite	-3.44	-14.04	-10.60	CaF2
Gypsum	-2.32	-6.90	-4.58	CaSO4:2H2O
H2(g)	-13.94	-17.04	-3.10	H2
H2O(g)	-1.51	-0.00	1.51	H2O
Halite	-6.90	-5.33	1.57	NaCl
Hydroxyapatite	-5.15	-8.55	-3.40	Ca5(PO4)3OH
O2(g)	-55.47	-58.37	-2.89	O2
Sylvite	-7.54	-6.64	0.90	KCl
Witherite	-2.91	-11.47	-8.56	BaCO3

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
For ideal gases, phi = 1.

Initial solution 14.

----------Solution composition----------

Elements	Molality	Moles
Alkalinity	2.999e-03	2.999e-03
Ba	4.517e-06	4.517e-06
Br	8.891e-06	8.891e-06
Ca	1.223e-03	1.223e-03
Cl	4.911e-03	4.911e-03
F	3.687e-06	3.687e-06
K	1.100e-04	1.100e-04
Mg	2.115e-04	2.115e-04
N(3)	4.286e-06	4.286e-06
N(5)	2.329e-04	2.329e-04
Na	6.137e-03	6.137e-03
P	2.261e-06	2.261e-06
S(6)	5.427e-04	5.427e-04

----------Description of solution----------

pH	= 7.200
pe	= 0.406
Specific Conductance (µS/cm, 25°C)	= 962
Density (g/cm³)	= 0.99751
Volume (L)	= 1.00314
Activity of water	= 1.000
Ionic strength (mol/kgw)	= 1.072e-02
Mass of water (kg)	= 1.000e+00
Total carbon (mol/kg)	= 3.367e-03
Total CO2 (mol/kg)	= 3.367e-03
Temperature (°C)	= 25.08
Electrical balance (eq)	= -1.217e-04
Percent error, 100*(Cat-|An|)/(Cat+|An|)	= -0.68
Iterations	= 8 (144 overall)
Total H	= 1.110154e+02
Total O	= 5.551883e+01

----------Redox couples----------

Redox couple	pe	Eh (volts)
N(3)/N(5)	7.9483	0.4703

----------Distribution of species----------

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma	mole V cm³/mol
OH-	1.799e-07	1.614e-07	-6.745	-6.792	-0.047	-4.03
H+	6.925e-08	6.310e-08	-7.160	-7.200	-0.040	0.00
H2O	5.551e+01	9.997e-01	1.744	-0.000	0.000	18.07
Ba	4.517e-06					
Ba+2	3.988e-06	2.609e-06	-5.399	-5.584	-0.184	-12.51
BaSO4	4.128e-07	4.138e-07	-6.384	-6.383	0.001	(0)
BaHCO3+	7.409e-08	6.661e-08	-7.130	-7.176	-0.046	(0)
BaCl+	3.916e-08	3.521e-08	-7.407	-7.453	-0.046	(0)
BaCO3	2.664e-09	2.670e-09	-8.575	-8.573	0.001	-10.70
BaNO3+	7.619e-11	6.850e-11	-10.118	-10.164	-0.046	(0)
BaOH+	1.554e-12	1.401e-12	-11.809	-11.854	-0.045	(0)
Br	8.891e-06					
Br-	8.891e-06	7.962e-06	-5.051	-5.099	-0.048	24.63
C(4)	3.367e-03					
HCO3-	2.944e-03	2.657e-03	-2.531	-2.576	-0.045	24.78
CO2	3.757e-04	3.766e-04	-3.425	-3.424	0.001	34.44
CaHCO3+	2.858e-05	2.584e-05	-4.544	-4.588	-0.044	9.73
NaHCO3	8.024e-06	8.043e-06	-5.096	-5.095	0.001	1.80
MgHCO3+	4.546e-06	4.085e-06	-5.342	-5.389	-0.046	5.54

CO3-2	2.983e-06	1.978e-06	-5.525	-5.704	-0.178	-4.99
CaCO3	2.527e-06	2.534e-06	-5.597	-5.596	0.001	-14.60
MgCO3	2.476e-07	2.482e-07	-6.606	-6.605	0.001	-17.09
NaCO3-	2.215e-07	1.992e-07	-6.655	-6.701	-0.046	-0.91
BaHCO3+	7.409e-08	6.661e-08	-7.130	-7.176	-0.046	(0)
BaCO3	2.664e-09	2.670e-09	-8.575	-8.573	0.001	-10.70
(CO2)2	2.604e-09	2.611e-09	-8.584	-8.583	0.001	68.87
Ca	1.223e-03					
Ca+2	1.149e-03	7.613e-04	-2.940	-3.118	-0.179	-17.92
CaSO4	4.276e-05	4.287e-05	-4.369	-4.368	0.001	7.50
CaHCO3+	2.858e-05	2.584e-05	-4.544	-4.588	-0.044	9.73
CaCO3	2.527e-06	2.534e-06	-5.597	-5.596	0.001	-14.60
CaHPO4	2.933e-07	2.940e-07	-6.533	-6.532	0.001	(0)
CaH2PO4+	1.544e-08	1.394e-08	-7.811	-7.856	-0.045	(0)
CaPO4-	1.223e-08	1.104e-08	-7.912	-7.957	-0.045	(0)
CaOH+	2.227e-09	2.002e-09	-8.652	-8.699	-0.046	(0)
CaHSO4+	1.980e-11	1.780e-11	-10.703	-10.750	-0.046	(0)
Cl	4.911e-03					
Cl-	4.773e-03	4.285e-03	-2.321	-2.368	-0.047	18.14
NaCl	1.379e-04	1.382e-04	-3.861	-3.860	0.001	(0)
BaCl+	3.916e-08	3.521e-08	-7.407	-7.453	-0.046	(0)
F	3.687e-06					
F-	3.645e-06	3.269e-06	-5.438	-5.486	-0.047	-1.25
MgF+	3.157e-08	2.841e-08	-7.501	-7.546	-0.046	-10.52
NaF	1.011e-08	1.013e-08	-7.995	-7.994	0.001	7.26
HF	3.091e-10	3.098e-10	-9.510	-9.509	0.001	12.50
HF2-	4.326e-15	3.889e-15	-14.364	-14.410	-0.046	22.13
H(0)	8.662e-19					
H2	4.331e-19	4.342e-19	-18.363	-18.362	0.001	28.61
K	1.100e-04					
K+	1.098e-04	9.852e-05	-3.959	-4.006	-0.047	9.07
KSO4-	2.431e-07	2.194e-07	-6.614	-6.659	-0.045	34.17
KHPO4-	1.497e-10	1.351e-10	-9.825	-9.869	-0.045	38.18
Mg	2.115e-04					
Mg+2	1.969e-04	1.313e-04	-3.706	-3.882	-0.176	-21.61
MgSO4	9.739e-06	9.764e-06	-5.011	-5.010	0.001	5.84
MgHCO3+	4.546e-06	4.085e-06	-5.342	-5.389	-0.046	5.54
MgCO3	2.476e-07	2.482e-07	-6.606	-6.605	0.001	-17.09
MgHPO4	6.841e-08	6.857e-08	-7.165	-7.164	0.001	(0)
MgF+	3.157e-08	2.841e-08	-7.501	-7.546	-0.046	-10.52
MgOH+	8.408e-09	7.611e-09	-8.075	-8.119	-0.043	(0)
MgH2PO4+	3.393e-09	3.062e-09	-8.469	-8.514	-0.045	(0)
MgPO4-	2.847e-09	2.569e-09	-8.546	-8.590	-0.045	(0)
N(3)	4.286e-06					
NO2-	4.286e-06	3.838e-06	-5.368	-5.416	-0.048	25.04
N(5)	2.329e-04					
NO3-	2.329e-04	2.086e-04	-3.633	-3.681	-0.048	29.57
BaNO3+	7.619e-11	6.850e-11	-10.118	-10.164	-0.046	(0)
Na	6.137e-03					
Na+	5.981e-03	5.386e-03	-2.223	-2.269	-0.045	-1.37
NaCl	1.379e-04	1.382e-04	-3.861	-3.860	0.001	(0)
NaSO4-	9.472e-06	8.547e-06	-5.024	-5.068	-0.045	14.35
NaHCO3	8.024e-06	8.043e-06	-5.096	-5.095	0.001	1.80
NaCO3-	2.215e-07	1.992e-07	-6.655	-6.701	-0.046	-0.91
NaF	1.011e-08	1.013e-08	-7.995	-7.994	0.001	7.26
NaHPO4-	8.185e-09	7.386e-09	-8.087	-8.132	-0.045	34.24
NaOH	8.669e-20	8.691e-20	-19.062	-19.061	0.001	(0)
O(0)	0.000e+00					
O2	0.000e+00	0.000e+00	-55.631	-55.630	0.001	30.41
P	2.261e-06					
HPO4-2	1.066e-06	7.032e-07	-5.972	-6.153	-0.181	6.98
H2PO4-	7.916e-07	7.143e-07	-6.101	-6.146	-0.045	33.28
CaHPO4	2.933e-07	2.940e-07	-6.533	-6.532	0.001	(0)
MgHPO4	6.841e-08	6.857e-08	-7.165	-7.164	0.001	(0)
CaH2PO4+	1.544e-08	1.394e-08	-7.811	-7.856	-0.045	(0)
CaPO4-	1.223e-08	1.104e-08	-7.912	-7.957	-0.045	(0)
NaHPO4-	8.185e-09	7.386e-09	-8.087	-8.132	-0.045	34.24
MgH2PO4+	3.393e-09	3.062e-09	-8.469	-8.514	-0.045	(0)

MgPO4-	2.847e-09	2.569e-09	-8.546	-8.590	-0.045	(0)
KHPO4-	1.497e-10	1.351e-10	-9.825	-9.869	-0.045	38.18
PO4-3	1.319e-11	5.033e-12	-10.880	-11.298	-0.418	-22.65
H3PO4	6.626e-12	6.642e-12	-11.179	-11.178	0.001	47.41
S(6)	5.427e-04					
SO4-2	4.800e-04	3.164e-04	-3.319	-3.500	-0.181	14.79
CaSO4	4.276e-05	4.287e-05	-4.369	-4.368	0.001	7.50
MgSO4	9.739e-06	9.764e-06	-5.011	-5.010	0.001	5.84
NaSO4-	9.472e-06	8.547e-06	-5.024	-5.068	-0.045	14.35
BaSO4	4.128e-07	4.138e-07	-6.384	-6.383	0.001	(0)
KSO4-	2.431e-07	2.194e-07	-6.614	-6.659	-0.045	34.17
HSO4-	2.163e-09	1.945e-09	-8.665	-8.711	-0.046	40.35
CaHSO4+	1.980e-11	1.780e-11	-10.703	-10.750	-0.046	(0)

----------Distribution of alkalinity----------

Total alkalinity (eq/kgw) = 2.999e-03

Species	Alkalinity	Molality	Alk/Mol
HCO3-	2.944e-03	2.944e-03	1.00
CaHCO3+	2.858e-05	2.858e-05	1.00
NaHCO3	8.024e-06	8.024e-06	1.00
CO3-2	5.966e-06	2.983e-06	2.00
CaCO3	5.055e-06	2.527e-06	2.00
MgHCO3+	4.546e-06	4.546e-06	1.00
HPO4-2	1.066e-06	1.066e-06	1.00
MgCO3	4.952e-07	2.476e-07	2.00
NaCO3-	4.431e-07	2.215e-07	2.00
CaHPO4	2.933e-07	2.933e-07	1.00
OH-	1.799e-07	1.799e-07	1.00
BaHCO3+	7.409e-08	7.409e-08	1.00
H+	-6.925e-08	6.925e-08	-1.00
MgHPO4	6.841e-08	6.841e-08	1.00
CaPO4-	2.447e-08	1.223e-08	2.00
MgOH+	8.408e-09	8.408e-09	1.00
NaHPO4-	8.185e-09	8.185e-09	1.00
MgPO4-	5.695e-09	2.847e-09	2.00
BaCO3	5.327e-09	2.664e-09	2.00
CaOH+	2.227e-09	2.227e-09	1.00
HSO4-	-2.163e-09	2.163e-09	-1.00
HF	-3.091e-10	3.091e-10	-1.00
KHPO4-	1.497e-10	1.497e-10	1.00
PO4-3	2.638e-11	1.319e-11	2.00
CaHSO4+	-1.980e-11	1.980e-11	-1.00
H3PO4	-6.626e-12	6.626e-12	-1.00
BaOH+	1.554e-12	1.554e-12	1.00
HF2-	-4.326e-15	4.326e-15	-1.00
NaOH	8.669e-20	8.669e-20	1.00

----------Saturation indices----------

Phase	SI**	log IAP	log K(298 K, 1 atm)	
Anhydrite	-2.34	-6.62	-4.28	CaSO4
Aragonite	-0.49	-8.82	-8.34	CaCO3
BaCl2	-12.55	-10.32	2.23	BaCl2
BaCl2:2H2O	-10.53	-10.32	0.21	BaCl2:2H2O
BaCl2:H2O	-11.14	-10.32	0.82	BaCl2:H2O
Barite	0.76	-9.08	-9.84	BaSO4
Calcite	-0.34	-8.82	-8.48	CaCO3
CO2(g)	-1.95	-3.42	-1.47	CO2
Dolomite	-1.32	-18.41	-17.09	CaMg(CO3)2
Fluorite	-3.49	-14.09	-10.60	CaF2
Gypsum	-2.04	-6.62	-4.58	CaSO4:2H2O
H2(g)	-15.26	-18.36	-3.10	H2
H2O(g)	-1.50	-0.00	1.50	H2O
Halite	-6.21	-4.64	1.57	NaCl

Hydroxyapatite	-1.82	-5.25	-3.43	Ca5(PO4)3OH
O2(g)	-52.74	-55.63	-2.89	O2
Sylvite	-7.27	-6.37	0.90	KCl
Witherite	-2.73	-11.29	-8.56	BaCO3

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
For ideal gases, phi = 1.

Initial solution 15.

-----------------------------Solution composition------------------------------

Elements	Molality	Moles
Alkalinity	4.414e-03	4.414e-03
Ba	9.994e-06	9.994e-06
Br	4.238e-05	4.238e-05
Ca	8.446e-03	8.446e-03
Cl	2.685e-02	2.685e-02
F	1.055e-06	1.055e-06
K	4.151e-04	4.151e-04
Mg	3.542e-03	3.542e-03
N(5)	1.044e-04	1.044e-04
Na	8.433e-03	8.433e-03
P	6.469e-07	6.469e-07
S(6)	5.799e-04	5.799e-04

----------------------------Description of solution----------------------------

pH	= 5.900
pe	= 0.454
Specific Conductance (µS/cm, 26°C)	= 3405
Density (g/cm³)	= 0.99845
Volume (L)	= 1.00390
Activity of water	= 0.999
Ionic strength (mol/kgw)	= 4.306e-02
Mass of water (kg)	= 1.000e+00
Total carbon (mol/kg)	= 1.395e-02
Total CO2 (mol/kg)	= 1.395e-02
Temperature (°C)	= 25.89
Electrical balance (eq)	= 2.758e-04
Percent error, 100*(Cat-|An|)/(Cat+|An|)	= 0.44
Iterations	= 9 (153 overall)
Total H	= 1.110168e+02
Total O	= 5.554118e+01

----------------------------Distribution of species----------------------------

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma	mole V cm³/mol
H+	1.464e-06	1.259e-06	-5.834	-5.900	-0.066	0.00
OH-	1.046e-08	8.593e-09	-7.980	-8.066	-0.086	-3.86
H2O	5.551e+01	9.990e-01	1.744	-0.000	0.000	18.07
Ba	9.994e-06					
Ba+2	9.084e-06	4.283e-06	-5.042	-5.368	-0.327	-12.19
BaSO4	3.814e-07	3.852e-07	-6.419	-6.414	0.004	(0)
BaCl+	3.530e-07	2.928e-07	-6.452	-6.533	-0.081	(0)
BaHCO3+	1.749e-07	1.451e-07	-6.757	-6.838	-0.081	(0)
BaCO3	2.906e-10	2.935e-10	-9.537	-9.532	0.004	-10.69
BaNO3+	5.543e-11	4.598e-11	-10.256	-10.337	-0.081	(0)
BaOH+	1.381e-13	1.152e-13	-12.860	-12.939	-0.079	(0)
Br	4.238e-05					
Br-	4.238e-05	3.461e-05	-4.373	-4.461	-0.088	24.76
C(4)	1.395e-02					
CO2	9.537e-03	9.632e-03	-2.021	-2.016	0.004	34.48
HCO3-	4.107e-03	3.436e-03	-2.386	-2.464	-0.077	25.01
CaHCO3+	2.102e-04	1.768e-04	-3.677	-3.752	-0.075	9.82

MgHCO3+	8.304e-05	6.855e-05	-4.081	-4.164	-0.083	5.63
NaHCO3	1.206e-05	1.218e-05	-4.919	-4.914	0.004	1.80
(CO2)2	1.736e-06	1.753e-06	-5.760	-5.756	0.004	68.95
CaCO3	8.783e-07	8.870e-07	-6.056	-6.052	0.004	-14.60
CO3-2	2.659e-07	1.303e-07	-6.575	-6.885	-0.310	-4.52
MgCO3	2.119e-07	2.140e-07	-6.674	-6.670	0.004	-17.09
BaHCO3+	1.749e-07	1.451e-07	-6.757	-6.838	-0.081	(0)
NaCO3-	1.937e-08	1.607e-08	-7.713	-7.794	-0.081	-0.59
BaCO3	2.906e-10	2.935e-10	-9.537	-9.532	0.004	-10.69
Ca	8.446e-03					
Ca+2	8.109e-03	3.980e-03	-2.091	-2.400	-0.309	-17.64
CaHCO3+	2.102e-04	1.768e-04	-3.677	-3.752	-0.075	9.82
CaSO4	1.266e-04	1.279e-04	-3.898	-3.893	0.004	7.53
CaCO3	8.783e-07	8.870e-07	-6.056	-6.052	0.004	-14.60
CaH2PO4+	4.819e-08	4.032e-08	-7.317	-7.395	-0.077	(0)
CaHPO4	4.238e-08	4.280e-08	-7.373	-7.369	0.004	(0)
CaHSO4+	1.292e-09	1.072e-09	-8.889	-8.970	-0.081	(0)
CaOH+	6.318e-10	5.241e-10	-9.199	-9.281	-0.081	(0)
CaPO4-	9.776e-11	8.179e-11	-10.010	-10.087	-0.077	(0)
Cl	2.685e-02					
Cl-	2.604e-02	2.145e-02	-1.584	-1.669	-0.084	18.26
NaCl	8.098e-04	8.179e-04	-3.092	-3.087	0.004	(0)
BaCl+	3.530e-07	2.928e-07	-6.452	-6.533	-0.081	(0)
F	1.055e-06					
F-	9.439e-07	7.751e-07	-6.025	-6.111	-0.086	-1.14
MgF+	1.065e-07	8.837e-08	-6.973	-7.054	-0.081	-10.45
NaF	2.797e-09	2.825e-09	-8.553	-8.549	0.004	7.29
HF	1.472e-09	1.487e-09	-8.832	-8.828	0.004	12.54
HF2-	5.368e-15	4.453e-15	-14.270	-14.351	-0.081	22.27
H(0)	2.722e-16					
H2	1.361e-16	1.375e-16	-15.866	-15.862	0.004	28.61
K	4.151e-04					
K+	4.146e-04	3.409e-04	-3.382	-3.467	-0.085	9.18
KSO4-	5.218e-07	4.366e-07	-6.282	-6.360	-0.077	34.29
KHPO4-	1.533e-11	1.282e-11	-10.815	-10.892	-0.077	38.26
Mg	3.542e-03					
Mg+2	3.386e-03	1.698e-03	-2.470	-2.770	-0.300	-21.38
MgHCO3+	8.304e-05	6.855e-05	-4.081	-4.164	-0.083	5.63
MgSO4	7.237e-05	7.309e-05	-4.140	-4.136	0.004	5.87
MgCO3	2.119e-07	2.140e-07	-6.674	-6.670	0.004	-17.09
MgF+	1.065e-07	8.837e-08	-6.973	-7.054	-0.081	-10.45
MgH2PO4+	2.619e-08	2.191e-08	-7.582	-7.659	-0.077	(0)
MgHPO4	2.445e-08	2.469e-08	-7.612	-7.607	0.004	(0)
MgOH+	6.277e-09	5.301e-09	-8.202	-8.276	-0.073	(0)
MgPO4-	5.627e-11	4.708e-11	-10.250	-10.327	-0.077	(0)
N(5)	1.044e-04					
NO3-	1.044e-04	8.528e-05	-3.981	-4.069	-0.088	29.74
BaNO3+	5.543e-11	4.598e-11	-10.256	-10.337	-0.081	(0)
Na	8.433e-03					
Na+	7.604e-03	6.333e-03	-2.119	-2.198	-0.079	-1.19
NaCl	8.098e-04	8.179e-04	-3.092	-3.087	0.004	(0)
NaHCO3	1.206e-05	1.218e-05	-4.919	-4.914	0.004	1.80
NaSO4-	6.847e-06	5.728e-06	-5.165	-5.242	-0.077	15.27
NaCO3-	1.937e-08	1.607e-08	-7.713	-7.794	-0.081	-0.59
NaF	2.797e-09	2.825e-09	-8.553	-8.549	0.004	7.29
NaHPO4-	2.848e-10	2.382e-10	-9.546	-9.623	-0.077	36.62
NaOH	5.389e-21	5.442e-21	-20.269	-20.264	0.004	(0)
O(0)	0.000e+00					
O2	0.000e+00	0.000e+00	-60.375	-60.371	0.004	30.47
P	6.469e-07					
H2PO4-	4.652e-07	3.892e-07	-6.332	-6.410	-0.077	33.40
CaH2PO4+	4.819e-08	4.032e-08	-7.317	-7.395	-0.077	(0)
CaHPO4	4.238e-08	4.280e-08	-7.373	-7.369	0.004	(0)
HPO4-2	3.995e-08	1.929e-08	-7.398	-7.715	-0.316	7.35
MgH2PO4+	2.619e-08	2.191e-08	-7.582	-7.659	-0.077	(0)
MgHPO4	2.445e-08	2.469e-08	-7.612	-7.607	0.004	(0)
NaHPO4-	2.848e-10	2.382e-10	-9.546	-9.623	-0.077	36.62
CaPO4-	9.776e-11	8.179e-11	-10.010	-10.087	-0.077	(0)

H3PO4	7.219e-11	7.291e-11	-10.142	-10.137	0.004	47.46
MgPO4-	5.627e-11	4.708e-11	-10.250	-10.327	-0.077	(0)
KHPO4-	1.533e-11	1.282e-11	-10.815	-10.892	-0.077	38.26
PO4-3	3.950e-14	7.032e-15	-13.403	-14.153	-0.750	-21.86
S(6)	5.799e-04					
SO4-2	3.731e-04	1.795e-04	-3.428	-3.746	-0.318	15.29
CaSO4	1.266e-04	1.279e-04	-3.898	-3.893	0.004	7.53
MgSO4	7.237e-05	7.309e-05	-4.140	-4.136	0.004	5.87
NaSO4-	6.847e-06	5.728e-06	-5.165	-5.242	-0.077	15.27
KSO4-	5.218e-07	4.366e-07	-6.282	-6.360	-0.077	34.29
BaSO4	3.814e-07	3.852e-07	-6.419	-6.414	0.004	(0)
HSO4-	2.700e-08	2.240e-08	-7.569	-7.650	-0.081	40.50
CaHSO4+	1.292e-09	1.072e-09	-8.889	-8.970	-0.081	(0)

----------Distribution of alkalinity----------

Total alkalinity (eq/kgw) = 4.414e-03

Species	Alkalinity	Molality	Alk/Mol
HCO3-	4.107e-03	4.107e-03	1.00
CaHCO3+	2.102e-04	2.102e-04	1.00
MgHCO3+	8.304e-05	8.304e-05	1.00
NaHCO3	1.206e-05	1.206e-05	1.00
CaCO3	1.757e-06	8.783e-07	2.00
H+	-1.464e-06	1.464e-06	-1.00
CO3-2	5.319e-07	2.659e-07	2.00
MgCO3	4.238e-07	2.119e-07	2.00
BaHCO3+	1.749e-07	1.749e-07	1.00
CaHPO4	4.238e-08	4.238e-08	1.00
HPO4-2	3.995e-08	3.995e-08	1.00
NaCO3-	3.874e-08	1.937e-08	2.00
HSO4-	-2.700e-08	2.700e-08	-1.00
MgHPO4	2.445e-08	2.445e-08	1.00
OH-	1.046e-08	1.046e-08	1.00
MgOH+	6.277e-09	6.277e-09	1.00
HF	-1.472e-09	1.472e-09	-1.00
CaHSO4+	-1.292e-09	1.292e-09	-1.00
CaOH+	6.318e-10	6.318e-10	1.00
BaCO3	5.812e-10	2.906e-10	2.00
NaHPO4-	2.848e-10	2.848e-10	1.00
CaPO4-	1.955e-10	9.776e-11	2.00
MgPO4-	1.125e-10	5.627e-11	2.00
H3PO4	-7.219e-11	7.219e-11	-1.00
KHPO4-	1.533e-11	1.533e-11	1.00
BaOH+	1.381e-13	1.381e-13	1.00
PO4-3	7.900e-14	3.950e-14	2.00
HF2-	-5.368e-15	5.368e-15	-1.00
NaOH	5.389e-21	5.389e-21	1.00

----------Saturation indices----------

Phase	SI**	log IAP	log K(299 K, 1 atm)	
Anhydrite	-1.86	-6.15	-4.29	CaSO4
Aragonite	-0.94	-9.29	-8.34	CaCO3
BaCl2	-10.93	-8.71	2.22	BaCl2
BaCl2:2H2O	-8.92	-8.71	0.22	BaCl2:2H2O
BaCl2:H2O	-9.53	-8.71	0.83	BaCl2:H2O
Barite	0.72	-9.11	-9.84	BaSO4
Calcite	-0.80	-9.29	-8.48	CaCO3
CO2(g)	-0.54	-2.02	-1.48	CO2
Dolomite	-1.83	-18.94	-17.11	CaMg(CO3)2
Fluorite	-4.03	-14.62	-10.59	CaF2
Gypsum	-1.56	-6.15	-4.58	CaSO4:2H2O
H2(g)	-12.76	-15.86	-3.10	H2
H2O(g)	-1.48	-0.00	1.48	H2O
Halite	-5.44	-3.87	1.57	NaCl

Hydroxyapatite	-8.05	-11.55	-3.50	Ca5(PO4)3OH
O2(g)	-57.47	-60.37	-2.90	O2
Sylvite	-6.04	-5.14	0.90	KCl
Witherite	-3.69	-12.25	-8.56	BaCO3

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
For ideal gases, phi = 1.

Initial solution 16.

----------Solution composition----------

Elements	Molality	Moles
Al	6.505e-07	6.505e-07
Alkalinity	9.500e-04	9.500e-04
B	1.087e-05	1.087e-05
Ba	2.046e-05	2.046e-05
Ca	2.271e-04	2.271e-04
Cd	8.186e-09	8.186e-09
Cl	2.708e-04	2.708e-04
Cu	1.445e-07	1.445e-07
F	5.633e-05	5.633e-05
Fe	1.526e-05	1.526e-05
K	6.394e-05	6.394e-05
Mg	9.626e-05	9.626e-05
Mn	3.168e-07	3.168e-07
N(5)	2.542e-04	2.542e-04
Na	5.829e-04	5.829e-04
P	2.583e-07	2.583e-07
Pb	4.055e-09	4.055e-09
S(6)	4.477e-05	4.477e-05

----------Description of solution----------

pH	= 5.200
pe	= 0.276
Specific Conductance (µS/cm, 25°C)	= 157
Density (g/cm³)	= 0.99738
Volume (L)	= 1.00332
Activity of water	= 1.000
Ionic strength (mol/kgw)	= 1.884e-03
Mass of water (kg)	= 1.000e+00
Total carbon (mol/kg)	= 1.393e-02
Total CO2 (mol/kg)	= 1.393e-02
Temperature (°C)	= 24.52
Electrical balance (eq)	= -2.534e-04
Percent error, 100*(Cat-|An|)/(Cat+|An|)	= -8.51
Iterations	= 12 (165 overall)
Total H	= 1.110134e+02
Total O	= 5.553600e+01

----------Distribution of species----------

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma	mole V cm³/mol
H+	6.601e-06	6.310e-06	-5.180	-5.200	-0.020	0.00
OH-	1.623e-09	1.546e-09	-8.790	-8.811	-0.021	-4.11
H2O	5.551e+01	9.997e-01	1.744	-0.000	0.000	18.07
Al	6.505e-07					
AlF2+	3.882e-07	3.703e-07	-6.411	-6.431	-0.021	(0)
AlF3	2.396e-07	2.397e-07	-6.620	-6.620	0.000	(0)
AlF+2	1.739e-08	1.439e-08	-7.760	-7.842	-0.082	(0)
AlF4-	5.151e-09	4.910e-09	-8.288	-8.309	-0.021	(0)
Al(OH)2+	5.343e-11	5.096e-11	-10.272	-10.293	-0.021	(0)
AlOH+2	5.171e-11	4.280e-11	-10.286	-10.369	-0.082	-27.70
Al+3	4.212e-11	2.806e-11	-10.376	-10.552	-0.176	-42.17

AlSO4+	3.248e-12	3.096e-12	-11.488	-11.509	-0.021	(0)
Al(OH)3	1.148e-12	1.148e-12	-11.940	-11.940	0.000	(0)
Al(OH)4-	3.574e-13	3.407e-13	-12.447	-12.468	-0.021	(0)
Al(SO4)2-	3.598e-15	3.430e-15	-14.444	-14.465	-0.021	(0)
AlHSO4+2	2.091e-18	1.725e-18	-17.680	-17.763	-0.084	(0)
B	1.087e-05					
H3BO3	1.087e-05	1.087e-05	-4.964	-4.964	0.000	39.19
H2BO3-	1.032e-09	9.831e-10	-8.987	-9.007	-0.021	(0)
BF(OH)3-	2.326e-10	2.216e-10	-9.633	-9.654	-0.021	(0)
BF2(OH)2-	8.097e-12	7.716e-12	-11.092	-11.113	-0.021	(0)
BF3OH-	2.908e-15	2.772e-15	-14.536	-14.557	-0.021	(0)
BF4-	3.850e-18	3.669e-18	-17.415	-17.435	-0.021	(0)
Ba	2.046e-05					
Ba+2	2.001e-05	1.651e-05	-4.699	-4.782	-0.083	-12.73
BaSO4	2.904e-07	2.906e-07	-6.537	-6.537	0.000	(0)
BaHCO3+	1.486e-07	1.416e-07	-6.828	-6.849	-0.021	(0)
BaCl+	1.392e-08	1.326e-08	-7.856	-7.877	-0.021	(0)
BaNO3+	5.280e-10	5.032e-10	-9.277	-9.298	-0.021	(0)
BaCO3	5.647e-11	5.649e-11	-10.248	-10.248	0.000	-10.70
BaOH+	9.297e-14	8.865e-14	-13.032	-13.052	-0.021	(0)
C(4)	1.393e-02					
CO2	1.296e-02	1.297e-02	-1.887	-1.887	0.000	34.41
HCO3-	9.524e-04	9.084e-04	-3.021	-3.042	-0.021	24.66
(CO2)2	3.037e-06	3.038e-06	-5.518	-5.517	0.000	68.82
CaHCO3+	2.232e-06	2.129e-06	-5.651	-5.672	-0.020	9.66
FeHCO3+	1.111e-06	1.059e-06	-5.954	-5.975	-0.021	(0)
MgHCO3+	8.713e-07	8.303e-07	-6.060	-6.081	-0.021	5.47
NaHCO3	2.839e-07	2.841e-07	-6.547	-6.547	0.000	1.80
BaHCO3+	1.486e-07	1.416e-07	-6.828	-6.849	-0.021	(0)
MnHCO3+	2.070e-08	1.973e-08	-7.684	-7.705	-0.021	(0)
CO3-2	8.079e-09	6.687e-09	-8.093	-8.175	-0.082	-5.26
CaCO3	2.058e-09	2.059e-09	-8.686	-8.686	0.000	-14.60
FeCO3	1.868e-09	1.869e-09	-8.729	-8.728	0.000	(0)
PbHCO3+	1.445e-09	1.377e-09	-8.840	-8.861	-0.021	(0)
MgCO3	4.956e-10	4.958e-10	-9.305	-9.305	0.000	-17.09
CuHCO3+	2.312e-10	2.204e-10	-9.636	-9.657	-0.021	(0)
PbCO3	2.217e-10	2.218e-10	-9.654	-9.654	0.000	(0)
CdHCO3+	1.928e-10	1.838e-10	-9.715	-9.736	-0.021	(0)
MnCO3	1.294e-10	1.295e-10	-9.888	-9.888	0.000	(0)
NaCO3-	7.072e-11	6.739e-11	-10.150	-10.171	-0.021	-1.06
BaCO3	5.647e-11	5.649e-11	-10.248	-10.248	0.000	-10.70
CuCO3	1.737e-11	1.738e-11	-10.760	-10.760	0.000	(0)
CdCO3	3.396e-14	3.397e-14	-13.469	-13.469	0.000	(0)
Pb(CO3)2-2	4.517e-15	3.726e-15	-14.345	-14.429	-0.084	(0)
Cu(CO3)2-2	1.774e-16	1.463e-16	-15.751	-15.835	-0.084	(0)
Cd(CO3)2-2	8.710e-19	7.184e-19	-18.060	-18.144	-0.084	(0)
Ca	2.271e-04					
Ca+2	2.237e-04	1.851e-04	-3.650	-3.733	-0.082	-18.11
CaHCO3+	2.232e-06	2.129e-06	-5.651	-5.672	-0.020	9.66
CaSO4	1.151e-06	1.151e-06	-5.939	-5.939	0.000	7.48
CaCO3	2.058e-09	2.059e-09	-8.686	-8.686	0.000	-14.60
CaH2PO4+	1.180e-09	1.125e-09	-8.928	-8.949	-0.021	(0)
CaHPO4	2.366e-10	2.367e-10	-9.626	-9.626	0.000	(0)
CaHSO4+	4.977e-11	4.743e-11	-10.303	-10.324	-0.021	(0)
CaOH+	5.107e-12	4.867e-12	-11.292	-11.313	-0.021	(0)
CaPO4-	9.222e-14	8.796e-14	-13.035	-13.056	-0.021	(0)
Cd	8.186e-09					
Cd+2	7.755e-09	6.396e-09	-8.110	-8.194	-0.084	-18.73
CdHCO3+	1.928e-10	1.838e-10	-9.715	-9.736	-0.021	(0)
CdCl+	1.646e-10	1.569e-10	-9.784	-9.805	-0.021	5.72
CdSO4	6.456e-11	6.458e-11	-10.190	-10.190	0.000	78.29
CdF+	4.348e-12	4.143e-12	-11.362	-11.383	-0.021	(0)
CdNO3+	4.139e-12	3.945e-12	-11.383	-11.404	-0.021	17.55
CdCl2	1.678e-13	1.679e-13	-12.775	-12.775	0.000	23.14
CdOH+	8.536e-14	8.135e-14	-13.069	-13.090	-0.021	(0)
CdCO3	3.396e-14	3.397e-14	-13.469	-13.469	0.000	(0)
Cd(SO4)2-2	3.023e-14	2.494e-14	-13.519	-13.603	-0.084	-105.92
CdOHCl	1.016e-14	1.016e-14	-13.993	-13.993	0.000	(0)

CdF2	5.353e-16	5.355e-16	-15.271	-15.271	0.000	(0)
CdCl3-	2.838e-17	2.705e-17	-16.547	-16.568	-0.021	69.67
Cd(CO3)2-2	8.710e-19	7.184e-19	-18.060	-18.144	-0.084	(0)
Cd(OH)2	7.170e-19	7.173e-19	-18.144	-18.144	0.000	(0)
Cd2OH+3	3.954e-21	2.564e-21	-20.403	-20.591	-0.188	(0)
Cd(OH)3-	1.338e-26	1.275e-26	-25.873	-25.894	-0.021	(0)
Cd(OH)4-2	2.183e-35	1.801e-35	-34.661	-34.745	-0.084	(0)
Cl	2.708e-04					
Cl-	2.699e-04	2.572e-04	-3.569	-3.590	-0.021	18.07
NaCl	8.502e-07	8.506e-07	-6.070	-6.070	0.000	(0)
BaCl+	1.392e-08	1.326e-08	-7.856	-7.877	-0.021	(0)
FeCl+	4.341e-09	4.137e-09	-8.362	-8.383	-0.021	(0)
CuCl2-	2.943e-09	2.805e-09	-8.531	-8.552	-0.021	(0)
MnCl+	2.678e-10	2.554e-10	-9.572	-9.593	-0.021	-3.20
CdCl+	1.646e-10	1.569e-10	-9.784	-9.805	-0.021	5.72
PbCl+	2.027e-11	1.931e-11	-10.693	-10.714	-0.021	7.94
CuCl3-2	1.380e-12	1.141e-12	-11.860	-11.943	-0.083	(0)
CuCl+	3.434e-13	3.273e-13	-12.464	-12.485	-0.021	0.77
CdCl2	1.678e-13	1.679e-13	-12.775	-12.775	0.000	23.14
MnCl2	2.866e-14	2.867e-14	-13.543	-13.543	0.000	86.48
CdOHCl	1.016e-14	1.016e-14	-13.993	-13.993	0.000	(0)
PbCl2	7.940e-15	7.944e-15	-14.100	-14.100	0.000	34.93
CuCl2	4.495e-17	4.497e-17	-16.347	-16.347	0.000	30.46
CdCl3-	2.838e-17	2.705e-17	-16.547	-16.568	-0.021	69.67
MnCl3-	2.130e-18	2.031e-18	-17.672	-17.692	-0.021	43.38
PbCl3-	1.698e-18	1.618e-18	-17.770	-17.791	-0.021	65.90
FeCl+2	1.893e-20	1.565e-20	-19.723	-19.805	-0.083	(0)
PbCl4-2	2.406e-22	1.984e-22	-21.619	-21.702	-0.084	101.32
CuCl3-	4.269e-23	4.069e-23	-22.370	-22.391	-0.021	(0)
FeCl2+	1.915e-23	1.826e-23	-22.718	-22.739	-0.021	(0)
FeCl3	4.694e-28	4.696e-28	-27.328	-27.328	0.000	(0)
CuCl4-2	6.273e-29	5.186e-29	-28.203	-28.285	-0.083	(0)
Cu(1)	1.436e-07					
Cu+	1.407e-07	1.339e-07	-6.852	-6.873	-0.021	(0)
CuCl2-	2.943e-09	2.805e-09	-8.531	-8.552	-0.021	(0)
CuCl3-2	1.380e-12	1.141e-12	-11.860	-11.943	-0.083	(0)
Cu(2)	8.379e-10					
Cu+2	5.840e-10	4.840e-10	-9.234	-9.315	-0.082	-26.57
CuHCO3+	2.312e-10	2.204e-10	-9.636	-9.657	-0.021	(0)
CuCO3	1.737e-11	1.738e-11	-10.760	-10.760	0.000	(0)
CuSO4	3.457e-12	3.458e-12	-11.461	-11.461	0.000	13.03
CuOH+	8.048e-13	7.669e-13	-12.094	-12.115	-0.021	(0)
CuF+	4.734e-13	4.512e-13	-12.325	-12.346	-0.021	(0)
CuCl+	3.434e-13	3.273e-13	-12.464	-12.485	-0.021	0.77
Cu(OH)2	2.538e-13	2.539e-13	-12.596	-12.595	0.000	(0)
Cu(CO3)2-2	1.774e-16	1.463e-16	-15.751	-15.835	-0.084	(0)
CuCl2	4.495e-17	4.497e-17	-16.347	-16.347	0.000	30.46
Cu2(OH)2+2	2.975e-19	2.454e-19	-18.527	-18.610	-0.084	(0)
Cu(OH)3-	2.544e-21	2.424e-21	-20.595	-20.615	-0.021	(0)
CuCl3-	4.269e-23	4.069e-23	-22.370	-22.391	-0.021	(0)
Cu(OH)4-2	9.291e-29	7.663e-29	-28.032	-28.116	-0.084	(0)
CuCl4-2	6.273e-29	5.186e-29	-28.203	-28.285	-0.083	(0)
F	5.633e-05					
F-	5.401e-05	5.145e-05	-4.268	-4.289	-0.021	-1.31
HF	4.825e-07	4.827e-07	-6.317	-6.316	0.000	12.48
AlF2+	3.882e-07	3.703e-07	-6.411	-6.431	-0.021	(0)
MgF+	2.767e-07	2.638e-07	-6.558	-6.579	-0.021	-10.56
AlF3	2.396e-07	2.397e-07	-6.620	-6.620	0.000	(0)
AlF+2	1.739e-08	1.439e-08	-7.760	-7.842	-0.082	(0)
NaF	1.641e-08	1.642e-08	-7.785	-7.785	0.000	7.24
FeF+	6.291e-09	5.995e-09	-8.201	-8.222	-0.021	(0)
AlF4-	5.151e-09	4.910e-09	-8.288	-8.309	-0.021	(0)
BF(OH)3-	2.326e-10	2.216e-10	-9.633	-9.654	-0.021	(0)
HF2-	9.962e-11	9.494e-11	-10.002	-10.023	-0.021	22.05
MnF+	9.099e-11	8.676e-11	-10.041	-10.062	-0.021	(0)
BF2(OH)2-	8.097e-12	7.716e-12	-11.092	-11.113	-0.021	(0)
CdF+	4.348e-12	4.143e-12	-11.362	-11.383	-0.021	(0)
PbF+	1.833e-12	1.747e-12	-11.737	-11.758	-0.021	(0)

CuF+	4.734e-13	4.512e-13	-12.325	-12.346	-0.021	(0)
BF3OH-	2.908e-15	2.772e-15	-14.536	-14.557	-0.021	(0)
PbF2	1.834e-15	1.835e-15	-14.737	-14.736	0.000	(0)
CdF2	5.353e-16	5.355e-16	-15.271	-15.271	0.000	(0)
FeF2+	3.538e-16	3.374e-16	-15.451	-15.472	-0.021	(0)
FeF+2	2.003e-16	1.656e-16	-15.698	-15.781	-0.083	(0)
FeF3	2.745e-17	2.747e-17	-16.561	-16.561	0.000	(0)
BF4-	3.850e-18	3.669e-18	-17.415	-17.435	-0.021	(0)
PbF3-	7.177e-19	6.839e-19	-18.144	-18.165	-0.021	(0)
PbF4-2	2.042e-23	1.684e-23	-22.690	-22.774	-0.084	(0)
Fe(2)	1.526e-05					
Fe+2	1.406e-05	1.165e-05	-4.852	-4.934	-0.082	-22.13
FeHCO3+	1.111e-06	1.059e-06	-5.954	-5.975	-0.021	(0)
FeSO4	7.209e-08	7.212e-08	-7.142	-7.142	0.000	19.48
FeF+	6.291e-09	5.995e-09	-8.201	-8.222	-0.021	(0)
FeCl+	4.341e-09	4.137e-09	-8.362	-8.383	-0.021	(0)
FeCO3	1.868e-09	1.869e-09	-8.729	-8.728	0.000	(0)
FeH2PO4+	1.469e-09	1.401e-09	-8.833	-8.854	-0.021	(0)
FeOH+	5.907e-10	5.632e-10	-9.229	-9.249	-0.021	(0)
FeHPO4	1.091e-10	1.092e-10	-9.962	-9.962	0.000	(0)
FeHSO4+	3.133e-12	2.986e-12	-11.504	-11.525	-0.021	(0)
Fe(OH)2	7.282e-16	7.285e-16	-15.138	-15.138	0.000	(0)
Fe(OH)3-	4.476e-21	4.268e-21	-20.349	-20.370	-0.021	(0)
Fe(3)	1.151e-13					
Fe(OH)2+	1.099e-13	1.048e-13	-12.959	-12.979	-0.021	(0)
FeOH+2	2.461e-15	2.035e-15	-14.609	-14.691	-0.083	(0)
Fe(OH)3	2.095e-15	2.096e-15	-14.679	-14.679	0.000	(0)
FeF2+	3.538e-16	3.374e-16	-15.451	-15.472	-0.021	(0)
FeF+2	2.003e-16	1.656e-16	-15.698	-15.781	-0.083	(0)
FeF3	2.745e-17	2.747e-17	-16.561	-16.561	0.000	(0)
Fe+3	3.072e-18	2.046e-18	-17.513	-17.689	-0.176	(0)
FeSO4+	8.174e-19	7.795e-19	-18.088	-18.108	-0.021	(0)
Fe(OH)4-	3.114e-19	2.970e-19	-18.507	-18.527	-0.021	(0)
FeH2PO4+2	1.596e-19	1.321e-19	-18.797	-18.879	-0.082	(0)
FeCl+2	1.893e-20	1.565e-20	-19.723	-19.805	-0.083	(0)
FeHPO4+	1.338e-21	1.276e-21	-20.873	-20.894	-0.021	(0)
Fe(SO4)2-	6.271e-22	5.977e-22	-21.203	-21.224	-0.021	(0)
FeCl2+	1.915e-23	1.826e-23	-22.718	-22.739	-0.021	(0)
FeHSO4+2	1.597e-23	1.317e-23	-22.797	-22.880	-0.084	(0)
FeCl3	4.694e-28	4.696e-28	-27.328	-27.328	0.000	(0)
Fe2(OH)2+4	2.457e-28	1.137e-28	-27.610	-27.944	-0.335	(0)
Fe3(OH)4+5	8.677e-39	2.603e-39	-38.062	-38.584	-0.523	(0)
H(0)	1.588e-14					
H2	7.941e-15	7.945e-15	-14.100	-14.100	0.000	28.61
K	6.394e-05					
K+	6.393e-05	6.090e-05	-4.194	-4.215	-0.021	9.00
KSO4-	1.562e-08	1.490e-08	-7.806	-7.827	-0.021	34.10
KHPO4-	2.931e-13	2.795e-13	-12.533	-12.554	-0.021	38.16
Mg	9.626e-05					
Mg+2	9.447e-05	7.828e-05	-4.025	-4.106	-0.082	-21.77
MgHCO3+	8.713e-07	8.303e-07	-6.060	-6.081	-0.021	5.47
MgSO4	6.361e-07	6.364e-07	-6.196	-6.196	0.000	5.82
MgF+	2.767e-07	2.638e-07	-6.558	-6.579	-0.021	-10.56
MgH2PO4+	6.355e-10	6.061e-10	-9.197	-9.217	-0.021	(0)
MgCO3	4.956e-10	4.958e-10	-9.305	-9.305	0.000	-17.09
MgHPO4	1.353e-10	1.354e-10	-9.869	-9.868	0.000	(0)
MgOH+	4.518e-11	4.312e-11	-10.345	-10.365	-0.020	(0)
MgPO4-	5.262e-14	5.019e-14	-13.279	-13.299	-0.021	(0)
Mn(2)	3.168e-07					
Mn+2	2.941e-07	2.437e-07	-6.532	-6.613	-0.082	-20.75
MnHCO3+	2.070e-08	1.973e-08	-7.684	-7.705	-0.021	(0)
MnSO4	1.507e-09	1.508e-09	-8.822	-8.822	0.000	22.76
MnCl+	2.678e-10	2.554e-10	-9.572	-9.593	-0.021	-3.20
MnCO3	1.294e-10	1.295e-10	-9.888	-9.888	0.000	(0)
MnF+	9.099e-11	8.676e-11	-10.041	-10.062	-0.021	(0)
MnOH+	1.001e-12	9.545e-13	-12.000	-12.020	-0.021	(0)
Mn(NO3)2	5.690e-14	5.692e-14	-13.245	-13.245	0.000	41.17
MnCl2	2.866e-14	2.867e-14	-13.543	-13.543	0.000	86.48

MnCl3-	2.130e-18	2.031e-18	-17.672	-17.692	-0.021	43.38
Mn(OH)3-	1.611e-26	1.537e-26	-25.793	-25.813	-0.021	(0)
Mn(3)	1.990e-32					
Mn+3	1.990e-32	1.326e-32	-31.701	-31.878	-0.176	(0)
N(5)	2.542e-04					
NO3-	2.542e-04	2.421e-04	-3.595	-3.616	-0.021	29.45
BaNO3+	5.280e-10	5.032e-10	-9.277	-9.298	-0.021	(0)
PbNO3+	7.172e-12	6.835e-12	-11.144	-11.165	-0.021	(0)
CdNO3+	4.139e-12	3.945e-12	-11.383	-11.404	-0.021	17.55
Mn(NO3)2	5.690e-14	5.692e-14	-13.245	-13.245	0.000	41.17
Na	5.829e-04					
Na+	5.817e-04	5.545e-04	-3.235	-3.256	-0.021	-1.49
NaCl	8.502e-07	8.506e-07	-6.070	-6.070	0.000	(0)
NaHCO3	2.839e-07	2.841e-07	-6.547	-6.547	0.000	1.80
NaSO4-	1.020e-07	9.729e-08	-6.991	-7.012	-0.021	13.85
NaF	1.641e-08	1.642e-08	-7.785	-7.785	0.000	7.24
NaCO3-	7.072e-11	6.739e-11	-10.150	-10.171	-0.021	-1.06
NaHPO4-	2.668e-12	2.545e-12	-11.574	-11.594	-0.021	33.58
NaOH	8.569e-23	8.573e-23	-22.067	-22.067	0.000	(0)
O(0)	0.000e+00					
O2	0.000e+00	0.000e+00	-64.336	-64.336	0.000	30.36
P	2.583e-07					
H2PO4-	2.515e-07	2.399e-07	-6.600	-6.620	-0.021	33.23
HPO4-2	2.847e-09	2.354e-09	-8.546	-8.628	-0.083	6.77
FeH2PO4+	1.469e-09	1.401e-09	-8.833	-8.854	-0.021	(0)
CaH2PO4+	1.180e-09	1.125e-09	-8.928	-8.949	-0.021	(0)
MgH2PO4+	6.355e-10	6.061e-10	-9.197	-9.217	-0.021	(0)
CaHPO4	2.366e-10	2.367e-10	-9.626	-9.626	0.000	(0)
H3PO4	2.214e-10	2.215e-10	-9.655	-9.655	0.000	47.38
MgHPO4	1.353e-10	1.354e-10	-9.869	-9.868	0.000	(0)
FeHPO4	1.091e-10	1.092e-10	-9.962	-9.962	0.000	(0)
NaHPO4-	2.668e-12	2.545e-12	-11.574	-11.594	-0.021	33.58
KHPO4-	2.931e-13	2.795e-13	-12.533	-12.554	-0.021	38.16
CaPO4-	9.222e-14	8.796e-14	-13.035	-13.056	-0.021	(0)
MgPO4-	5.262e-14	5.019e-14	-13.279	-13.299	-0.021	(0)
PO4-3	2.570e-16	1.666e-16	-15.590	-15.778	-0.188	-23.10
FeH2PO4+2	1.596e-19	1.321e-19	-18.797	-18.879	-0.082	(0)
FeHPO4+	1.338e-21	1.276e-21	-20.873	-20.894	-0.021	(0)
Pb	4.055e-09					
Pb+2	2.314e-09	1.909e-09	-8.636	-8.719	-0.084	-15.50
PbHCO3+	1.445e-09	1.377e-09	-8.840	-8.861	-0.021	(0)
PbCO3	2.217e-10	2.218e-10	-9.654	-9.654	0.000	(0)
PbSO4	3.768e-11	3.769e-11	-10.424	-10.424	0.000	(0)
PbCl+	2.027e-11	1.931e-11	-10.693	-10.714	-0.021	7.94
PbNO3+	7.172e-12	6.835e-12	-11.144	-11.165	-0.021	(0)
PbOH+	6.188e-12	5.897e-12	-11.208	-11.229	-0.021	(0)
PbF+	1.833e-12	1.747e-12	-11.737	-11.758	-0.021	(0)
Pb(SO4)2-2	8.421e-15	6.946e-15	-14.075	-14.158	-0.084	(0)
PbCl2	7.940e-15	7.944e-15	-14.100	-14.100	0.000	34.93
Pb(CO3)2-2	4.517e-15	3.726e-15	-14.345	-14.429	-0.084	(0)
PbF2	1.834e-15	1.835e-15	-14.737	-14.736	0.000	(0)
Pb(OH)2	3.634e-16	3.635e-16	-15.440	-15.439	0.000	(0)
PbCl3-	1.698e-18	1.618e-18	-17.770	-17.791	-0.021	65.90
PbF3-	7.177e-19	6.839e-19	-18.144	-18.165	-0.021	(0)
Pb2OH+3	3.887e-19	2.520e-19	-18.410	-18.599	-0.188	(0)
Pb(OH)3-	6.940e-22	6.614e-22	-21.159	-21.180	-0.021	(0)
PbCl4-2	2.406e-22	1.984e-22	-21.619	-21.702	-0.084	101.32
PbF4-2	2.042e-23	1.684e-23	-22.690	-22.774	-0.084	(0)
Pb(OH)4-2	2.911e-28	2.401e-28	-27.536	-27.620	-0.084	(0)
Pb3(OH)4+2	6.519e-30	5.377e-30	-29.186	-29.269	-0.084	(0)
S(6)	4.477e-05					
SO4-2	4.247e-05	3.511e-05	-4.372	-4.455	-0.083	14.50
CaSO4	1.151e-06	1.151e-06	-5.939	-5.939	0.000	7.48
MgSO4	6.361e-07	6.364e-07	-6.196	-6.196	0.000	5.82
BaSO4	2.904e-07	2.906e-07	-6.537	-6.537	0.000	(0)
NaSO4-	1.020e-07	9.729e-08	-6.991	-7.012	-0.021	13.85
FeSO4	7.209e-08	7.212e-08	-7.142	-7.142	0.000	19.48
HSO4-	2.237e-08	2.132e-08	-7.650	-7.671	-0.021	40.26

KSO4-	1.562e-08	1.490e-08	-7.806	-7.827	-0.021	34.10
MnSO4	1.507e-09	1.508e-09	-8.822	-8.822	0.000	22.76
CdSO4	6.456e-11	6.458e-11	-10.190	-10.190	0.000	78.29
CaHSO4+	4.977e-11	4.743e-11	-10.303	-10.324	-0.021	(0)
PbSO4	3.768e-11	3.769e-11	-10.424	-10.424	0.000	(0)
CuSO4	3.457e-12	3.458e-12	-11.461	-11.461	0.000	13.03
AlSO4+	3.248e-12	3.096e-12	-11.488	-11.509	-0.021	(0)
FeHSO4+	3.133e-12	2.986e-12	-11.504	-11.525	-0.021	(0)
Cd(SO4)2-2	3.023e-14	2.494e-14	-13.519	-13.603	-0.084	-105.92
Pb(SO4)2-2	8.421e-15	6.946e-15	-14.075	-14.158	-0.084	(0)
Al(SO4)2-	3.598e-15	3.430e-15	-14.444	-14.465	-0.021	(0)
AlHSO4+2	2.091e-18	1.725e-18	-17.680	-17.763	-0.084	(0)
FeSO4+	8.174e-19	7.795e-19	-18.088	-18.108	-0.021	(0)
Fe(SO4)2-	6.271e-22	5.977e-22	-21.203	-21.224	-0.021	(0)
FeHSO4+2	1.597e-23	1.317e-23	-22.797	-22.880	-0.084	(0)

----------Distribution of alkalinity----------

Total alkalinity (eq/kgw) = 9.500e-04

Species	Alkalinity	Molality	Alk/Mol
HCO3-	9.524e-04	9.524e-04	1.00
H+	-6.601e-06	6.601e-06	-1.00
CaHCO3+	2.232e-06	2.232e-06	1.00
FeHCO3+	1.111e-06	1.111e-06	1.00
MgHCO3+	8.713e-07	8.713e-07	1.00
HF	-4.825e-07	4.825e-07	-1.00
NaHCO3	2.839e-07	2.839e-07	1.00
BaHCO3+	1.486e-07	1.486e-07	1.00
HSO4-	-2.237e-08	2.237e-08	-1.00
MnHCO3+	2.070e-08	2.070e-08	1.00
CO3-2	1.616e-08	8.079e-09	2.00
CaCO3	4.117e-09	2.058e-09	2.00
FeCO3	3.736e-09	1.868e-09	2.00
HPO4-2	2.847e-09	2.847e-09	1.00
OH-	1.623e-09	1.623e-09	1.00
PbHCO3+	1.445e-09	1.445e-09	1.00
H2BO3-	1.032e-09	1.032e-09	1.00
MgCO3	9.912e-10	4.956e-10	2.00
FeOH+	5.907e-10	5.907e-10	1.00
PbCO3	4.434e-10	2.217e-10	2.00
MnCO3	2.588e-10	1.294e-10	2.00
CaHPO4	2.366e-10	2.366e-10	1.00
CuHCO3+	2.312e-10	2.312e-10	1.00
H3PO4	-2.214e-10	2.214e-10	-1.00
CdHCO3+	1.928e-10	1.928e-10	1.00
NaCO3-	1.414e-10	7.072e-11	2.00
MgHPO4	1.353e-10	1.353e-10	1.00
BaCO3	1.129e-10	5.647e-11	2.00
FeHPO4	1.091e-10	1.091e-10	1.00
Al(OH)2+	1.069e-10	5.343e-11	2.00
HF2-	-9.962e-11	9.962e-11	-1.00
AlOH+2	5.171e-11	5.171e-11	1.00
CaHSO4+	-4.977e-11	4.977e-11	-1.00
MgOH+	4.518e-11	4.518e-11	1.00
CuCO3	3.475e-11	1.737e-11	2.00
BF2(OH)2-	-8.097e-12	8.097e-12	-1.00
PbOH+	6.188e-12	6.188e-12	1.00
CaOH+	5.107e-12	5.107e-12	1.00
Al(OH)3	3.444e-12	1.148e-12	3.00
FeHSO4+	-3.133e-12	3.133e-12	-1.00
NaHPO4-	2.668e-12	2.668e-12	1.00
Al(OH)4-	1.430e-12	3.574e-13	4.00
MnOH+	1.001e-12	1.001e-12	1.00
CuOH+	8.048e-13	8.048e-13	1.00
Cu(OH)2	5.075e-13	2.538e-13	2.00
KHPO4-	2.931e-13	2.931e-13	1.00

CaPO4-	1.844e-13	9.222e-14	2.00
MgPO4-	1.052e-13	5.262e-14	2.00
BaOH+	9.297e-14	9.297e-14	1.00
CdOH+	8.536e-14	8.536e-14	1.00
CdCO3	6.792e-14	3.396e-14	2.00
Pb(CO3)2-2	1.807e-14	4.517e-15	4.00
CdOHCl	1.016e-14	1.016e-14	1.00
BF3OH-	-5.817e-15	2.908e-15	-2.00
FeOH+2	-2.461e-15	2.461e-15	-1.00
Fe(OH)3	2.095e-15	2.095e-15	1.00
Fe(OH)2	1.456e-15	7.282e-16	2.00
Pb(OH)2	7.268e-16	3.634e-16	2.00
Cu(CO3)2-2	7.096e-16	1.774e-16	4.00
FeF2+	-7.076e-16	3.538e-16	-2.00
PO4-3	5.140e-16	2.570e-16	2.00
FeF+2	-4.007e-16	2.003e-16	-2.00
FeF3	-5.491e-17	2.745e-17	-2.00
BF4-	-1.155e-17	3.850e-18	-3.00
Fe+3	-6.144e-18	3.072e-18	-2.00
Cd(CO3)2-2	3.484e-18	8.710e-19	4.00
AlHSO4+2	-2.091e-18	2.091e-18	-1.00
FeSO4+	-1.635e-18	8.174e-19	-2.00
Cd(OH)2	1.434e-18	7.170e-19	2.00
Fe(OH)4-	6.228e-19	3.114e-19	2.00
Cu2(OH)2+2	5.950e-19	2.975e-19	2.00
Pb2OH+3	3.887e-19	3.887e-19	1.00
FeH2PO4+2	-3.192e-19	1.596e-19	-2.00
FeCl+2	-3.786e-20	1.893e-20	-2.00
Fe(OH)3-	1.343e-20	4.476e-21	3.00
Cu(OH)3-	7.631e-21	2.544e-21	3.00
Cd2OH+3	3.954e-21	3.954e-21	1.00
Pb(OH)3-	2.082e-21	6.940e-22	3.00
FeHPO4+	-1.338e-21	1.338e-21	-1.00
Fe(SO4)2-	-1.254e-21	6.271e-22	-2.00
NaOH	8.569e-23	8.569e-23	1.00
FeHSO4+2	-4.791e-23	1.597e-23	-3.00
FeCl2+	-3.830e-23	1.915e-23	-2.00
Mn(OH)3-	4.834e-26	1.611e-26	3.00
Cd(OH)3-	4.014e-26	1.338e-26	3.00
Pb(OH)4-2	1.164e-27	2.911e-28	4.00
FeCl3	-9.388e-28	4.694e-28	-2.00
Fe2(OH)2+4	-4.913e-28	2.457e-28	-2.00
Cu(OH)4-2	3.716e-28	9.291e-29	4.00
Pb3(OH)4+2	2.608e-29	6.519e-30	4.00
Cd(OH)4-2	8.733e-35	2.183e-35	4.00
Fe3(OH)4+5	-1.735e-38	8.677e-39	-2.00

-------------------------------Saturation indices--------------------------------

Phase	SI**	log IAP	log K(297 K, 1 atm)	
Al(OH)3(a)	-5.78	5.05	10.83	Al(OH)3
Alunite	-12.24	-13.58	-1.34	KAl3(SO4)2(OH)6
Anglesite	-5.38	-13.17	-7.79	PbSO4
Anhydrite	-3.91	-8.19	-4.27	CaSO4
Aragonite	-3.57	-11.91	-8.33	CaCO3
BaCl2	-14.19	-11.96	2.23	BaCl2
BaCl2:2H2O	-12.17	-11.96	0.20	BaCl2:2H2O
BaCl2:H2O	-12.79	-11.96	0.82	BaCl2:H2O
Barite	0.61	-9.24	-9.85	BaSO4
Calcite	-3.43	-11.91	-8.48	CaCO3
Cd(OH)2	-11.44	2.21	13.65	Cd(OH)2
CdSO4	-12.57	-12.65	-0.08	CdSO4
Cerussite	-3.76	-16.89	-13.14	PbCO3
CO2(g)	-0.42	-1.89	-1.46	CO2
Dolomite	-7.11	-24.19	-17.08	CaMg(CO3)2
Fe(OH)3(a)	-6.98	-2.09	4.89	Fe(OH)3
Fluorite	-1.70	-12.31	-10.61	CaF2

Gibbsite	-3.09	5.05	8.14	Al(OH)3
Goethite	-1.11	-2.09	-0.98	FeOOH
Gypsum	-3.61	-8.19	-4.58	CaSO4:2H2O
H2(g)	-11.00	-14.10	-3.10	H2
H2O(g)	-1.52	-0.00	1.52	H2O
Halite	-8.42	-6.85	1.57	NaCl
Hausmannite	-38.84	22.31	61.15	Mn3O4
Hematite	-0.21	-4.18	-3.97	Fe2O3
Hydroxyapatite	-20.37	-23.75	-3.38	Ca5(PO4)3OH
Jarosite-K	-25.82	-34.99	-9.17	KFe3(SO4)2(OH)6
Manganite	-16.08	9.26	25.34	MnOOH
Melanterite	-7.17	-9.39	-2.22	FeSO4:7H2O
O2(g)	-61.45	-64.34	-2.89	O2
Otavite	-4.27	-16.37	-12.10	CdCO3
Pb(OH)2	-6.49	1.68	8.17	Pb(OH)2
Pyrochroite	-11.41	3.79	15.20	Mn(OH)2
Pyrolusite	-26.72	14.74	41.46	MnO2:H2O
Rhodochrosite	-3.66	-14.79	-11.13	MnCO3
Siderite	-2.22	-13.11	-10.89	FeCO3
Sylvite	-8.70	-7.81	0.90	KCl
Vivianite	-10.36	-46.36	-36.00	Fe3(PO4)2:8H2O
Witherite	-4.39	-12.96	-8.56	BaCO3

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
For ideal gases, phi = 1.

Initial solution 17.

-----------------------------Solution composition-----------------------------

Elements	Molality	Moles
Al	3.179e-05	3.179e-05
Alkalinity	5.570e-04	5.570e-04
B	1.564e-05	1.564e-05
Ba	1.311e-05	1.311e-05
Br	4.256e-06	4.256e-06
Ca	3.319e-04	3.319e-04
Cd	1.157e-08	1.157e-08
Cl	1.777e-03	1.777e-03
Cu	8.436e-08	8.436e-08
F	6.265e-05	6.265e-05
Fe	4.311e-07	4.311e-07
K	2.097e-04	2.097e-04
Mg	3.106e-04	3.106e-04
Mn	1.457e-06	1.457e-06
N(5)	2.038e-03	2.038e-03
Na	8.919e-04	8.919e-04
P	1.970e-06	1.970e-06
Pb	1.429e-08	1.429e-08
S(6)	2.811e-05	2.811e-05
Zn	3.996e-06	3.996e-06

----------------------------Description of solution----------------------------

pH	= 4.200
pe	= 0.145
Specific Conductance (µS/cm, 24°C)	= 436
Density (g/cm³)	= 0.99816
Volume (L)	= 1.00579
Activity of water	= 0.998
Ionic strength (mol/kgw)	= 4.194e-03
Mass of water (kg)	= 1.000e+00
Total carbon (mol/kg)	= 8.369e-02
Total CO2 (mol/kg)	= 8.369e-02
Temperature (°C)	= 24.48
Electrical balance (eq)	= -1.977e-03
Percent error, 100*(Cat-|An|)/(Cat+|An|)	= -28.22

Iterations = 11 (176 overall)
Total H = 1.110132e+02
Total O = 5.568051e+01

----------Distribution of species----------

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma	mole V cm³/mol
H+	6.725e-05	6.310e-05	-4.172	-4.200	-0.028	0.00
OH-	1.652e-10	1.539e-10	-9.782	-9.813	-0.031	-4.09
H2O	5.551e+01	9.985e-01	1.744	-0.001	0.000	18.07
Al	3.179e-05					
AlF2+	2.121e-05	1.982e-05	-4.673	-4.703	-0.030	(0)
AlF+2	8.869e-06	6.753e-06	-5.052	-5.171	-0.118	(0)
AlF3	1.462e-06	1.464e-06	-5.835	-5.835	0.000	(0)
Al+3	2.048e-07	1.154e-07	-6.689	-6.938	-0.249	-42.04
AlOH+2	2.303e-08	1.753e-08	-7.638	-7.756	-0.118	-27.64
AlSO4+	7.615e-09	7.105e-09	-8.118	-8.148	-0.030	(0)
AlF4-	3.666e-09	3.421e-09	-8.436	-8.466	-0.030	(0)
Al(OH)2+	2.224e-09	2.078e-09	-8.653	-8.682	-0.030	(0)
Al(SO4)2-	4.710e-12	4.394e-12	-11.327	-11.357	-0.030	(0)
Al(OH)3	4.658e-12	4.662e-12	-11.332	-11.331	0.000	(0)
Al(OH)4-	1.480e-13	1.381e-13	-12.830	-12.860	-0.030	(0)
AlHSO4+2	5.233e-14	3.957e-14	-13.281	-13.403	-0.121	(0)
B	1.564e-05					
H3BO3	1.564e-05	1.565e-05	-4.806	-4.805	0.000	39.19
H2BO3-	1.516e-10	1.414e-10	-9.819	-9.850	-0.030	(0)
BF(OH)3-	3.902e-11	3.638e-11	-10.409	-10.439	-0.030	(0)
BF2(OH)2-	1.552e-12	1.447e-12	-11.809	-11.839	-0.030	(0)
BF3OH-	6.374e-16	5.944e-16	-15.196	-15.226	-0.030	(0)
BF4-	9.640e-19	8.989e-19	-18.016	-18.046	-0.030	(0)
Ba	1.311e-05					
Ba+2	1.290e-05	9.762e-06	-4.889	-5.010	-0.121	-12.67
BaSO4	9.583e-08	9.592e-08	-7.018	-7.018	0.000	(0)
BaHCO3+	5.723e-08	5.337e-08	-7.242	-7.273	-0.030	(0)
BaCl+	5.387e-08	5.024e-08	-7.269	-7.299	-0.030	(0)
BaNO3+	2.501e-09	2.332e-09	-8.602	-8.632	-0.030	(0)
BaCO3	2.126e-12	2.128e-12	-11.672	-11.672	0.000	-10.70
BaOH+	5.607e-15	5.235e-15	-14.251	-14.281	-0.030	(0)
Br	4.256e-06					
Br-	4.256e-06	3.962e-06	-5.371	-5.402	-0.031	24.57
CdBr+	4.784e-12	4.461e-12	-11.320	-11.351	-0.030	(0)
ZnBr+	3.181e-12	2.966e-12	-11.497	-11.528	-0.030	(0)
PbBr+	1.832e-12	1.708e-12	-11.737	-11.767	-0.030	(0)
CdBr2	9.461e-17	9.471e-17	-16.024	-16.024	0.000	(0)
ZnBr2	4.675e-18	4.679e-18	-17.330	-17.330	0.000	(0)
PbBr2	3.190e-18	3.193e-18	-17.496	-17.496	0.000	(0)
C(4)	8.369e-02					
CO2	8.282e-02	8.290e-02	-1.082	-1.081	0.000	34.41
HCO3-	6.206e-04	5.797e-04	-3.207	-3.237	-0.030	24.68
(CO2)2	1.239e-04	1.240e-04	-3.907	-3.907	0.000	68.81
CaHCO3+	1.965e-06	1.837e-06	-5.707	-5.736	-0.029	9.68
MgHCO3+	1.705e-06	1.589e-06	-5.768	-5.799	-0.030	5.49
NaHCO3	2.693e-07	2.695e-07	-6.570	-6.569	0.000	1.80
ZnHCO3+	2.227e-07	2.077e-07	-6.652	-6.683	-0.030	(0)
MnHCO3+	5.863e-08	5.474e-08	-7.232	-7.262	-0.030	(0)
BaHCO3+	5.723e-08	5.337e-08	-7.242	-7.273	-0.030	(0)
FeHCO3+	1.944e-08	1.813e-08	-7.711	-7.742	-0.030	(0)
PbHCO3+	3.646e-09	3.400e-09	-8.438	-8.469	-0.030	(0)
CO3-2	5.600e-10	4.264e-10	-9.252	-9.370	-0.118	-5.19
ZnCO3	2.419e-10	2.421e-10	-9.616	-9.616	0.000	(0)
CaCO3	1.773e-10	1.775e-10	-9.751	-9.751	0.000	-14.60
CdHCO3+	1.493e-10	1.392e-10	-9.826	-9.856	-0.030	(0)
MgCO3	9.470e-11	9.479e-11	-10.024	-10.023	0.000	-17.09
PbCO3	5.465e-11	5.471e-11	-10.262	-10.262	0.000	(0)
MnCO3	3.584e-11	3.588e-11	-10.446	-10.445	0.000	(0)
CuHCO3+	3.505e-11	3.268e-11	-10.455	-10.486	-0.030	(0)

NaCO3-	6.837e-12	6.375e-12	-11.165	-11.195	-0.030	-1.03
FeCO3	3.195e-12	3.198e-12	-11.495	-11.495	0.000	(0)
BaCO3	2.126e-12	2.128e-12	-11.672	-11.672	0.000	-10.70
CuCO3	2.573e-13	2.575e-13	-12.590	-12.589	0.000	(0)
Zn(CO3)2-2	2.919e-15	2.207e-15	-14.535	-14.656	-0.121	(0)
CdCO3	2.569e-15	2.572e-15	-14.590	-14.590	0.000	(0)
Pb(CO3)2-2	7.749e-17	5.859e-17	-16.111	-16.232	-0.121	(0)
Cu(CO3)2-2	1.828e-19	1.382e-19	-18.738	-18.859	-0.121	(0)
Cd(CO3)2-2	4.586e-21	3.467e-21	-20.339	-20.460	-0.121	(0)
Ca	3.319e-04					
Ca+2	3.290e-04	2.504e-04	-3.483	-3.601	-0.119	-18.04
CaHCO3+	1.965e-06	1.837e-06	-5.707	-5.736	-0.029	9.68
CaSO4	8.688e-07	8.696e-07	-6.061	-6.061	0.000	7.48
CaH2PO4+	1.220e-08	1.140e-08	-7.914	-7.943	-0.030	(0)
CaHSO4+	3.839e-10	3.580e-10	-9.416	-9.446	-0.030	(0)
CaHPO4	2.394e-10	2.397e-10	-9.621	-9.620	0.000	(0)
CaCO3	1.773e-10	1.775e-10	-9.751	-9.751	0.000	-14.60
CaOH+	7.052e-13	6.576e-13	-12.152	-12.182	-0.030	(0)
CaPO4-	9.526e-15	8.898e-15	-14.021	-14.051	-0.030	(0)
Cd	1.157e-08					
Cd+2	1.004e-08	7.594e-09	-7.998	-8.120	-0.121	-18.67
CdCl+	1.280e-09	1.194e-09	-8.893	-8.923	-0.030	5.75
CdHCO3+	1.493e-10	1.392e-10	-9.826	-9.856	-0.030	(0)
CdSO4	4.276e-11	4.280e-11	-10.369	-10.369	0.000	78.31
CdNO3+	3.941e-11	3.675e-11	-10.404	-10.435	-0.030	17.57
CdCl2	8.181e-12	8.189e-12	-11.087	-11.087	0.000	23.14
CdBr+	4.784e-12	4.461e-12	-11.320	-11.351	-0.030	(0)
CdF+	6.019e-13	5.612e-13	-12.220	-12.251	-0.030	(0)
Cd(SO4)2-2	1.221e-14	9.230e-15	-13.913	-14.035	-0.121	-105.88
CdOH+	1.031e-14	9.616e-15	-13.987	-14.017	-0.030	(0)
CdCl3-	9.064e-15	8.453e-15	-14.043	-14.073	-0.030	69.72
CdOHCl	7.708e-15	7.716e-15	-14.113	-14.113	0.000	(0)
CdCO3	2.569e-15	2.572e-15	-14.590	-14.590	0.000	(0)
CdBr2	9.461e-17	9.471e-17	-16.024	-16.024	0.000	(0)
CdF2	8.269e-18	8.277e-18	-17.083	-17.082	0.000	(0)
Cd(OH)2	8.486e-21	8.494e-21	-20.071	-20.071	0.000	(0)
Cd(CO3)2-2	4.586e-21	3.467e-21	-20.339	-20.460	-0.121	(0)
Cd2OH+3	6.752e-22	3.600e-22	-21.171	-21.444	-0.273	(0)
Cd(OH)3-	1.617e-29	1.508e-29	-28.791	-28.822	-0.030	(0)
Cd(OH)4-2	2.813e-39	2.127e-39	-38.551	-38.672	-0.121	(0)
Cl	1.777e-03					
Cl-	1.769e-03	1.649e-03	-2.752	-2.783	-0.031	18.09
NaCl	8.097e-06	8.104e-06	-5.092	-5.091	0.000	(0)
BaCl+	5.387e-08	5.024e-08	-7.269	-7.299	-0.030	(0)
CuCl2-	3.884e-08	3.621e-08	-7.411	-7.441	-0.030	(0)
ZnCl+	1.324e-08	1.234e-08	-7.878	-7.909	-0.030	-14.40
MnCl+	7.622e-09	7.116e-09	-8.118	-8.148	-0.030	-3.19
CdCl+	1.280e-09	1.194e-09	-8.893	-8.923	-0.030	5.75
FeCl+	7.633e-10	7.118e-10	-9.117	-9.148	-0.030	(0)
PbCl+	5.131e-10	4.785e-10	-9.290	-9.320	-0.030	7.96
CuCl3-2	1.243e-10	9.444e-11	-9.906	-10.025	-0.119	(0)
ZnCl2	2.125e-11	2.127e-11	-10.673	-10.672	0.000	103.05
CdCl2	8.181e-12	8.189e-12	-11.087	-11.087	0.000	23.14
MnCl2	5.117e-12	5.122e-12	-11.291	-11.291	0.000	86.53
ZnOHCl	2.457e-12	2.459e-12	-11.610	-11.609	0.000	(0)
PbCl2	1.261e-12	1.263e-12	-11.899	-11.899	0.000	34.93
CuCl+	5.219e-13	4.866e-13	-12.282	-12.313	-0.030	0.80
ZnCl3-	4.207e-14	3.922e-14	-13.376	-13.406	-0.030	16.94
CdCl3-	9.064e-15	8.453e-15	-14.043	-14.073	-0.030	69.72
CdOHCl	7.708e-15	7.716e-15	-14.113	-14.113	0.000	(0)
MnCl3-	2.491e-15	2.326e-15	-14.604	-14.633	-0.030	43.41
PbCl3-	1.768e-15	1.648e-15	-14.753	-14.783	-0.030	65.92
CuCl2	4.280e-16	4.285e-16	-15.369	-15.368	0.000	30.41
ZnCl4-2	4.249e-17	3.228e-17	-16.372	-16.491	-0.119	145.23
PbCl4-2	1.713e-18	1.296e-18	-17.766	-17.888	-0.121	101.39
CuCl3-	2.664e-21	2.484e-21	-20.575	-20.605	-0.030	(0)
FeCl+2	2.613e-21	1.985e-21	-20.583	-20.702	-0.119	(0)
FeCl2+	1.592e-23	1.486e-23	-22.798	-22.828	-0.030	(0)

CuCl4-2	2.669e-26	2.028e-26	-25.574	-25.693	-0.119	(0)
FeCl3	2.448e-27	2.451e-27	-26.611	-26.611	0.000	(0)
Cu(1)	8.418e-08					
Cu+	4.522e-08	4.207e-08	-7.345	-7.376	-0.031	(0)
CuCl2-	3.884e-08	3.621e-08	-7.411	-7.441	-0.030	(0)
CuCl3-2	1.243e-10	9.444e-11	-9.906	-10.025	-0.119	(0)
Cu(2)	1.836e-10					
Cu+2	1.473e-10	1.125e-10	-9.832	-9.949	-0.117	-26.50
CuHCO3+	3.505e-11	3.268e-11	-10.455	-10.486	-0.030	(0)
CuCl+	5.219e-13	4.866e-13	-12.282	-12.313	-0.030	0.80
CuSO4	4.482e-13	4.486e-13	-12.349	-12.348	0.000	13.03
CuCO3	2.573e-13	2.575e-13	-12.590	-12.589	0.000	(0)
CuOH+	1.909e-14	1.780e-14	-13.719	-13.750	-0.030	(0)
CuF+	1.282e-14	1.196e-14	-13.892	-13.922	-0.030	(0)
Cu(OH)2	5.879e-16	5.885e-16	-15.231	-15.230	0.000	(0)
CuCl2	4.280e-16	4.285e-16	-15.369	-15.368	0.000	30.41
Cu(CO3)2-2	1.828e-19	1.382e-19	-18.738	-18.859	-0.121	(0)
CuCl3-	2.664e-21	2.484e-21	-20.575	-20.605	-0.030	(0)
Cu2(OH)2+2	1.741e-22	1.316e-22	-21.759	-21.881	-0.121	(0)
Cu(OH)3-	6.018e-25	5.612e-25	-24.221	-24.251	-0.030	(0)
CuCl4-2	2.669e-26	2.028e-26	-25.574	-25.693	-0.119	(0)
Cu(OH)4-2	2.343e-33	1.772e-33	-32.630	-32.752	-0.121	(0)
F	6.265e-05					
AlF2+	2.121e-05	1.982e-05	-4.673	-4.703	-0.030	(0)
AlF+2	8.869e-06	6.753e-06	-5.052	-5.171	-0.118	(0)
F-	6.301e-06	5.871e-06	-5.201	-5.231	-0.031	-1.29
AlF3	1.462e-06	1.464e-06	-5.835	-5.835	0.000	(0)
HF	5.498e-07	5.504e-07	-6.260	-6.259	0.000	12.48
MgF+	9.673e-08	9.025e-08	-7.014	-7.045	-0.030	-10.55
AlF4-	3.666e-09	3.421e-09	-8.436	-8.466	-0.030	(0)
NaF	2.782e-09	2.785e-09	-8.556	-8.555	0.000	7.24
ZnF+	2.515e-10	2.345e-10	-9.600	-9.630	-0.030	(0)
MnF+	4.609e-11	4.303e-11	-10.336	-10.366	-0.030	(0)
BF(OH)3-	3.902e-11	3.638e-11	-10.409	-10.439	-0.030	(0)
FeF+	1.969e-11	1.836e-11	-10.706	-10.736	-0.030	(0)
HF2-	1.324e-11	1.235e-11	-10.878	-10.908	-0.030	22.07
BF2(OH)2-	1.552e-12	1.447e-12	-11.809	-11.839	-0.030	(0)
PbF+	8.267e-13	7.709e-13	-12.083	-12.113	-0.030	(0)
CdF+	6.019e-13	5.612e-13	-12.220	-12.251	-0.030	(0)
CuF+	1.282e-14	1.196e-14	-13.892	-13.922	-0.030	(0)
BF3OH-	6.374e-16	5.944e-16	-15.196	-15.226	-0.030	(0)
PbF2	9.231e-17	9.240e-17	-16.035	-16.034	0.000	(0)
CdF2	8.269e-18	8.277e-18	-17.083	-17.082	0.000	(0)
BF4-	9.640e-19	8.989e-19	-18.016	-18.046	-0.030	(0)
FeF+2	4.924e-19	3.741e-19	-18.308	-18.427	-0.119	(0)
FeF2+	9.308e-20	8.690e-20	-19.031	-19.061	-0.030	(0)
PbF3-	4.214e-21	3.930e-21	-20.375	-20.406	-0.030	(0)
FeF3	8.064e-22	8.072e-22	-21.093	-21.093	0.000	(0)
PbF4-2	1.460e-26	1.104e-26	-25.835	-25.957	-0.121	(0)
Fe(2)	4.311e-07					
Fe+2	4.095e-07	3.127e-07	-6.388	-6.505	-0.117	-22.06
FeHCO3+	1.944e-08	1.813e-08	-7.711	-7.742	-0.030	(0)
FeSO4	1.079e-09	1.080e-09	-8.967	-8.967	0.000	19.52
FeCl+	7.633e-10	7.118e-10	-9.117	-9.148	-0.030	(0)
FeH2PO4+	3.014e-10	2.816e-10	-9.521	-9.550	-0.030	(0)
FeF+	1.969e-11	1.836e-11	-10.706	-10.736	-0.030	(0)
FeCO3	3.195e-12	3.198e-12	-11.495	-11.495	0.000	(0)
FeHPO4	2.192e-12	2.194e-12	-11.659	-11.659	0.000	(0)
FeOH+	1.612e-12	1.505e-12	-11.793	-11.822	-0.030	(0)
FeHSO4+	4.794e-13	4.471e-13	-12.319	-12.350	-0.030	(0)
Fe(OH)2	1.936e-19	1.938e-19	-18.713	-18.713	0.000	(0)
Fe(OH)3-	1.214e-25	1.133e-25	-24.916	-24.946	-0.030	(0)
Fe(3)	2.811e-17					
Fe(OH)2+	2.209e-17	2.063e-17	-16.656	-16.685	-0.030	(0)
FeOH+2	5.286e-18	4.016e-18	-17.277	-17.396	-0.119	(0)
FeF+2	4.924e-19	3.741e-19	-18.308	-18.427	-0.119	(0)
FeF2+	9.308e-20	8.690e-20	-19.031	-19.061	-0.030	(0)
Fe+3	7.195e-20	4.053e-20	-19.143	-19.392	-0.249	(0)

Fe(OH)3	4.108e-20	4.112e-20	-19.386	-19.386	0.000	(0)
FeH2PO4+2	2.574e-20	1.960e-20	-19.589	-19.708	-0.118	(0)
FeSO4+	9.225e-21	8.612e-21	-20.035	-20.065	-0.030	(0)
FeCl+2	2.613e-21	1.985e-21	-20.583	-20.702	-0.119	(0)
FeF3	8.064e-22	8.072e-22	-21.093	-21.093	0.000	(0)
FeHPO4+	2.025e-23	1.890e-23	-22.694	-22.723	-0.030	(0)
FeCl2+	1.592e-23	1.486e-23	-22.798	-22.828	-0.030	(0)
Fe(SO4)2-	3.953e-24	3.687e-24	-23.403	-23.433	-0.030	(0)
FeHSO4+2	1.925e-24	1.455e-24	-23.716	-23.837	-0.121	(0)
Fe(OH)4-	6.221e-25	5.811e-25	-24.206	-24.236	-0.030	(0)
FeCl3	2.448e-27	2.451e-27	-26.611	-26.611	0.000	(0)
Fe2(OH)2+4	1.357e-33	4.435e-34	-32.867	-33.353	-0.486	(0)
Fe3(OH)4+5	0.000e+00	0.000e+00	-46.939	-47.698	-0.759	(0)
H(0)	2.903e-12					
H2	1.452e-12	1.453e-12	-11.838	-11.838	0.000	28.61
K	2.097e-04					
K+	2.097e-04	1.954e-04	-3.678	-3.709	-0.031	9.02
KSO4-	2.856e-08	2.668e-08	-7.544	-7.574	-0.030	34.12
KHPO4-	7.190e-13	6.717e-13	-12.143	-12.173	-0.030	38.18
Mg	3.106e-04					
Mg+2	3.077e-04	2.349e-04	-3.512	-3.629	-0.117	-21.70
MgHCO3+	1.705e-06	1.589e-06	-5.768	-5.799	-0.030	5.49
MgSO4	1.064e-06	1.065e-06	-5.973	-5.973	0.000	5.82
MgF+	9.673e-08	9.025e-08	-7.014	-7.045	-0.030	-10.55
MgH2PO4+	1.457e-08	1.361e-08	-7.837	-7.866	-0.030	(0)
MgHPO4	3.036e-10	3.039e-10	-9.518	-9.517	0.000	(0)
MgCO3	9.470e-11	9.479e-11	-10.024	-10.023	0.000	-17.09
MgOH+	1.376e-11	1.287e-11	-10.861	-10.890	-0.029	(0)
MgPO4-	1.205e-14	1.126e-14	-13.919	-13.949	-0.030	(0)
Mn(2)	1.457e-06					
Mn+2	1.387e-06	1.059e-06	-5.858	-5.975	-0.117	-20.35
MnHCO3+	5.863e-08	5.474e-08	-7.232	-7.262	-0.030	(0)
MnCl+	7.622e-09	7.116e-09	-8.118	-8.148	-0.030	-3.19
MnSO4	3.654e-09	3.657e-09	-8.437	-8.437	0.000	22.77
MnF+	4.609e-11	4.303e-11	-10.336	-10.366	-0.030	(0)
MnCO3	3.584e-11	3.588e-11	-10.446	-10.445	0.000	(0)
Mn(NO3)2	1.519e-11	1.520e-11	-10.818	-10.818	0.000	41.18
MnCl2	5.117e-12	5.122e-12	-11.291	-11.291	0.000	86.53
MnOH+	4.424e-13	4.130e-13	-12.354	-12.384	-0.030	(0)
MnCl3-	2.491e-15	2.326e-15	-14.604	-14.633	-0.030	43.41
Mn(OH)3-	7.127e-29	6.654e-29	-28.147	-28.177	-0.030	(0)
Mn(3)	7.522e-32					
Mn+3	7.522e-32	4.237e-32	-31.124	-31.373	-0.249	(0)
N(5)	2.038e-03					
NO3-	2.038e-03	1.897e-03	-2.691	-2.722	-0.031	29.47
BaNO3+	2.501e-09	2.332e-09	-8.602	-8.632	-0.030	(0)
PbNO3+	2.222e-10	2.072e-10	-9.653	-9.684	-0.030	(0)
CdNO3+	3.941e-11	3.675e-11	-10.404	-10.435	-0.030	17.57
Mn(NO3)2	1.519e-11	1.520e-11	-10.818	-10.818	0.000	41.18
Na	8.919e-04					
Na+	8.834e-04	8.244e-04	-3.054	-3.084	-0.030	-1.46
NaCl	8.097e-06	8.104e-06	-5.092	-5.091	0.000	(0)
NaHCO3	2.693e-07	2.695e-07	-6.570	-6.569	0.000	1.80
NaSO4-	8.643e-08	8.074e-08	-7.063	-7.093	-0.030	14.03
NaF	2.782e-09	2.785e-09	-8.556	-8.555	0.000	7.24
NaCO3-	6.837e-12	6.375e-12	-11.165	-11.195	-0.030	-1.03
NaHPO4-	3.033e-12	2.833e-12	-11.518	-11.548	-0.030	33.76
NaOH	1.268e-23	1.269e-23	-22.897	-22.897	0.000	(0)
O(0)	0.000e+00					
O2	0.000e+00	0.000e+00	-68.874	-68.874	0.000	30.36
P	1.970e-06					
H2PO4-	1.923e-06	1.797e-06	-5.716	-5.746	-0.030	33.25
H3PO4	1.657e-08	1.659e-08	-7.781	-7.780	0.000	47.38
MgH2PO4+	1.457e-08	1.361e-08	-7.837	-7.866	-0.030	(0)
CaH2PO4+	1.220e-08	1.140e-08	-7.914	-7.943	-0.030	(0)
HPO4-2	2.320e-09	1.763e-09	-8.635	-8.754	-0.119	6.85
MgHPO4	3.036e-10	3.039e-10	-9.518	-9.517	0.000	(0)
FeH2PO4+	3.014e-10	2.816e-10	-9.521	-9.550	-0.030	(0)

CaHPO4	2.394e-10	2.397e-10	-9.621	-9.620	0.000	(0)
NaHPO4-	3.033e-12	2.833e-12	-11.518	-11.548	-0.030	33.76
FeHPO4	2.192e-12	2.194e-12	-11.659	-11.659	0.000	(0)
KHPO4-	7.190e-13	6.717e-13	-12.143	-12.173	-0.030	38.18
MgPO4-	1.205e-14	1.126e-14	-13.919	-13.949	-0.030	(0)
CaPO4-	9.526e-15	8.898e-15	-14.021	-14.051	-0.030	(0)
PO4-3	2.341e-17	1.246e-17	-16.631	-16.904	-0.274	-22.92
FeH2PO4+2	2.574e-20	1.960e-20	-19.589	-19.708	-0.118	(0)
FeHPO4+	2.025e-23	1.890e-23	-22.694	-22.723	-0.030	(0)
Pb	1.429e-08					
Pb+2	9.765e-09	7.384e-09	-8.010	-8.132	-0.121	-15.43
PbHCO3+	3.646e-09	3.400e-09	-8.438	-8.469	-0.030	(0)
PbCl+	5.131e-10	4.785e-10	-9.290	-9.320	-0.030	7.96
PbNO3+	2.222e-10	2.072e-10	-9.653	-9.684	-0.030	(0)
PbSO4	8.133e-11	8.140e-11	-10.090	-10.089	0.000	(0)
PbCO3	5.465e-11	5.471e-11	-10.262	-10.262	0.000	(0)
PbOH+	2.443e-12	2.278e-12	-11.612	-11.642	-0.030	(0)
PbBr+	1.832e-12	1.708e-12	-11.737	-11.767	-0.030	(0)
PbCl2	1.261e-12	1.263e-12	-11.899	-11.899	0.000	34.93
PbF+	8.267e-13	7.709e-13	-12.083	-12.113	-0.030	(0)
Pb(SO4)2-2	1.108e-14	8.376e-15	-13.956	-14.077	-0.121	(0)
PbCl3-	1.768e-15	1.648e-15	-14.753	-14.783	-0.030	65.92
PbF2	9.231e-17	9.240e-17	-16.035	-16.034	0.000	(0)
Pb(CO3)2-2	7.749e-17	5.859e-17	-16.111	-16.232	-0.121	(0)
Pb(OH)2	1.401e-17	1.403e-17	-16.853	-16.853	0.000	(0)
PbBr2	3.190e-18	3.193e-18	-17.496	-17.496	0.000	(0)
PbCl4-2	1.713e-18	1.296e-18	-17.766	-17.888	-0.121	101.39
Pb2OH+3	7.064e-19	3.766e-19	-18.151	-18.424	-0.273	(0)
PbF3-	4.214e-21	3.930e-21	-20.375	-20.406	-0.030	(0)
Pb(OH)3-	2.733e-24	2.549e-24	-23.563	-23.594	-0.030	(0)
PbF4-2	1.460e-26	1.104e-26	-25.835	-25.957	-0.121	(0)
Pb(OH)4-2	1.222e-31	9.239e-32	-30.913	-31.034	-0.121	(0)
Pb3(OH)4+2	4.070e-32	3.078e-32	-31.390	-31.512	-0.121	(0)
S(6)	2.811e-05					
SO4-2	2.581e-05	1.961e-05	-4.588	-4.708	-0.119	14.57
MgSO4	1.064e-06	1.065e-06	-5.973	-5.973	0.000	5.82
CaSO4	8.688e-07	8.696e-07	-6.061	-6.061	0.000	7.48
HSO4-	1.275e-07	1.189e-07	-6.894	-6.925	-0.030	40.27
BaSO4	9.583e-08	9.592e-08	-7.018	-7.018	0.000	(0)
NaSO4-	8.643e-08	8.074e-08	-7.063	-7.093	-0.030	14.03
KSO4-	2.856e-08	2.668e-08	-7.544	-7.574	-0.030	34.12
ZnSO4	1.302e-08	1.303e-08	-7.886	-7.885	0.000	21.80
AlSO4+	7.615e-09	7.105e-09	-8.118	-8.148	-0.030	(0)
MnSO4	3.654e-09	3.657e-09	-8.437	-8.437	0.000	22.77
FeSO4	1.079e-09	1.080e-09	-8.967	-8.967	0.000	19.52
CaHSO4+	3.839e-10	3.580e-10	-9.416	-9.446	-0.030	(0)
PbSO4	8.133e-11	8.140e-11	-10.090	-10.089	0.000	(0)
CdSO4	4.276e-11	4.280e-11	-10.369	-10.369	0.000	78.31
Al(SO4)2-	4.710e-12	4.394e-12	-11.327	-11.357	-0.030	(0)
Zn(SO4)2-2	2.757e-12	2.085e-12	-11.560	-11.681	-0.121	-13.43
FeHSO4+	4.794e-13	4.471e-13	-12.319	-12.350	-0.030	(0)
CuSO4	4.482e-13	4.486e-13	-12.349	-12.348	0.000	13.03
AlHSO4+2	5.233e-14	3.957e-14	-13.281	-13.403	-0.121	(0)
Cd(SO4)2-2	1.221e-14	9.230e-15	-13.913	-14.035	-0.121	-105.88
Pb(SO4)2-2	1.108e-14	8.376e-15	-13.956	-14.077	-0.121	(0)
FeSO4+	9.225e-21	8.612e-21	-20.035	-20.065	-0.030	(0)
Fe(SO4)2-	3.953e-24	3.687e-24	-23.403	-23.433	-0.030	(0)
FeHSO4+2	1.925e-24	1.455e-24	-23.716	-23.837	-0.121	(0)
Zn	3.996e-06					
Zn+2	3.746e-06	2.846e-06	-5.426	-5.546	-0.119	-25.22
ZnHCO3+	2.227e-07	2.077e-07	-6.652	-6.683	-0.030	(0)
ZnCl+	1.324e-08	1.234e-08	-7.878	-7.909	-0.030	-14.40
ZnSO4	1.302e-08	1.303e-08	-7.886	-7.885	0.000	21.80
ZnF+	2.515e-10	2.345e-10	-9.600	-9.630	-0.030	(0)
ZnCO3	2.419e-10	2.421e-10	-9.616	-9.616	0.000	(0)
ZnOH+	5.091e-11	4.747e-11	-10.293	-10.324	-0.030	(0)
ZnCl2	2.125e-11	2.127e-11	-10.673	-10.672	0.000	103.05
ZnBr+	3.181e-12	2.966e-12	-11.497	-11.528	-0.030	(0)

Zn(SO4)2-2	2.757e-12	2.085e-12	-11.560	-11.681	-0.121	-13.43
ZnOHCl	2.457e-12	2.459e-12	-11.610	-11.609	0.000	(0)
ZnCl3-	4.207e-14	3.922e-14	-13.376	-13.406	-0.030	16.94
Zn(OH)2	8.964e-15	8.973e-15	-14.047	-14.047	0.000	(0)
Zn(CO3)2-2	2.919e-15	2.207e-15	-14.535	-14.656	-0.121	(0)
ZnCl4-2	4.249e-17	3.228e-17	-16.372	-16.491	-0.119	145.23
ZnBr2	4.675e-18	4.679e-18	-17.330	-17.330	0.000	(0)
Zn(OH)3-	4.815e-22	4.490e-22	-21.317	-21.348	-0.030	(0)
Zn(OH)4-2	1.489e-30	1.126e-30	-29.827	-29.948	-0.121	(0)

----------Distribution of alkalinity----------

Total alkalinity (eq/kgw) = 5.570e-04

Species	Alkalinity	Molality	Alk/Mol
HCO3-	6.206e-04	6.206e-04	1.00
H+	-6.725e-05	6.725e-05	-1.00
CaHCO3+	1.965e-06	1.965e-06	1.00
MgHCO3+	1.705e-06	1.705e-06	1.00
HF	-5.498e-07	5.498e-07	-1.00
NaHCO3	2.693e-07	2.693e-07	1.00
ZnHCO3+	2.227e-07	2.227e-07	1.00
HSO4-	-1.275e-07	1.275e-07	-1.00
MnHCO3+	5.863e-08	5.863e-08	1.00
BaHCO3+	5.723e-08	5.723e-08	1.00
AlOH+2	2.303e-08	2.303e-08	1.00
FeHCO3+	1.944e-08	1.944e-08	1.00
H3PO4	-1.657e-08	1.657e-08	-1.00
Al(OH)2+	4.449e-09	2.224e-09	2.00
PbHCO3+	3.646e-09	3.646e-09	1.00
HPO4-2	2.320e-09	2.320e-09	1.00
CO3-2	1.120e-09	5.600e-10	2.00
ZnCO3	4.838e-10	2.419e-10	2.00
CaHSO4+	-3.839e-10	3.839e-10	-1.00
CaCO3	3.547e-10	1.773e-10	2.00
MgHPO4	3.036e-10	3.036e-10	1.00
CaHPO4	2.394e-10	2.394e-10	1.00
MgCO3	1.894e-10	9.470e-11	2.00
OH-	1.652e-10	1.652e-10	1.00
H2BO3-	1.516e-10	1.516e-10	1.00
CdHCO3+	1.493e-10	1.493e-10	1.00
PbCO3	1.093e-10	5.465e-11	2.00
MnCO3	7.169e-11	3.584e-11	2.00
ZnOH+	5.091e-11	5.091e-11	1.00
CuHCO3+	3.505e-11	3.505e-11	1.00
Al(OH)3	1.397e-11	4.658e-12	3.00
MgOH+	1.376e-11	1.376e-11	1.00
NaCO3-	1.367e-11	6.837e-12	2.00
HF2-	-1.324e-11	1.324e-11	-1.00
FeCO3	6.391e-12	3.195e-12	2.00
BaCO3	4.252e-12	2.126e-12	2.00
NaHPO4-	3.033e-12	3.033e-12	1.00
ZnOHCl	2.457e-12	2.457e-12	1.00
PbOH+	2.443e-12	2.443e-12	1.00
FeHPO4	2.192e-12	2.192e-12	1.00
FeOH+	1.612e-12	1.612e-12	1.00
BF2(OH)2-	-1.552e-12	1.552e-12	-1.00
KHPO4-	7.190e-13	7.190e-13	1.00
CaOH+	7.052e-13	7.052e-13	1.00
Al(OH)4-	5.920e-13	1.480e-13	4.00
CuCO3	5.146e-13	2.573e-13	2.00
FeHSO4+	-4.794e-13	4.794e-13	-1.00
MnOH+	4.424e-13	4.424e-13	1.00
AlHSO4+2	-5.233e-14	5.233e-14	-1.00
MgPO4-	2.411e-14	1.205e-14	2.00
CuOH+	1.909e-14	1.909e-14	1.00
CaPO4-	1.905e-14	9.526e-15	2.00

Zn(OH)2	1.793e-14	8.964e-15	2.00
Zn(CO3)2-2	1.168e-14	2.919e-15	4.00
CdOH+	1.031e-14	1.031e-14	1.00
CdOHCl	7.708e-15	7.708e-15	1.00
BaOH+	5.607e-15	5.607e-15	1.00
CdCO3	5.138e-15	2.569e-15	2.00
BF3OH-	-1.275e-15	6.374e-16	-2.00
Cu(OH)2	1.176e-15	5.879e-16	2.00
Pb(CO3)2-2	3.099e-16	7.749e-17	4.00
PO4-3	4.682e-17	2.341e-17	2.00
Pb(OH)2	2.803e-17	1.401e-17	2.00
FeOH+2	-5.286e-18	5.286e-18	-1.00
BF4-	-2.892e-18	9.640e-19	-3.00
FeF+2	-9.848e-19	4.924e-19	-2.00
Cu(CO3)2-2	7.313e-19	1.828e-19	4.00
Pb2OH+3	7.064e-19	7.064e-19	1.00
Fe(OH)2	3.871e-19	1.936e-19	2.00
FeF2+	-1.862e-19	9.308e-20	-2.00
Fe+3	-1.439e-19	7.195e-20	-2.00
FeH2PO4+2	-5.148e-20	2.574e-20	-2.00
Fe(OH)3	4.108e-20	4.108e-20	1.00
FeSO4+	-1.845e-20	9.225e-21	-2.00
Cd(CO3)2-2	1.834e-20	4.586e-21	4.00
Cd(OH)2	1.697e-20	8.486e-21	2.00
FeCl+2	-5.225e-21	2.613e-21	-2.00
FeF3	-1.613e-21	8.064e-22	-2.00
Zn(OH)3-	1.445e-21	4.815e-22	3.00
Cd2OH+3	6.752e-22	6.752e-22	1.00
Cu2(OH)2+2	3.482e-22	1.741e-22	2.00
FeCl2+	-3.184e-23	1.592e-23	-2.00
FeHPO4+	-2.025e-23	2.025e-23	-1.00
NaOH	1.268e-23	1.268e-23	1.00
Pb(OH)3-	8.199e-24	2.733e-24	3.00
Fe(SO4)2-	-7.907e-24	3.953e-24	-2.00
FeHSO4+2	-5.775e-24	1.925e-24	-3.00
Cu(OH)3-	1.805e-24	6.018e-25	3.00
Fe(OH)4-	1.244e-24	6.221e-25	2.00
Fe(OH)3-	3.642e-25	1.214e-25	3.00
FeCl3	-4.897e-27	2.448e-27	-2.00
Mn(OH)3-	2.138e-28	7.127e-29	3.00
Cd(OH)3-	4.852e-29	1.617e-29	3.00
Zn(OH)4-2	5.958e-30	1.489e-30	4.00
Pb(OH)4-2	4.888e-31	1.222e-31	4.00
Pb3(OH)4+2	1.628e-31	4.070e-32	4.00
Cu(OH)4-2	9.373e-33	2.343e-33	4.00
Fe2(OH)2+4	-2.714e-33	1.357e-33	-2.00
Cd(OH)4-2	1.125e-38	2.813e-39	4.00
Fe3(OH)4+5	-0.000e+00	0.000e+00	-2.00

-------------------------------Saturation indices-------------------------------

Phase	SI**	log IAP	log K(297 K, 1 atm)	
Al(OH)3(a)	-5.17	5.66	10.83	Al(OH)3
Alunite	-7.41	-8.74	-1.34	KAl3(SO4)2(OH)6
Anglesite	-5.05	-12.84	-7.79	PbSO4
Anhydrite	-4.04	-8.31	-4.27	CaSO4
Aragonite	-4.64	-12.97	-8.33	CaCO3
BaCl2	-12.81	-10.58	2.23	BaCl2
BaCl2:2H2O	-10.78	-10.58	0.20	BaCl2:2H2O
BaCl2:H2O	-11.40	-10.58	0.82	BaCl2:H2O
Barite	0.13	-9.72	-9.85	BaSO4
Calcite	-4.49	-12.97	-8.48	CaCO3
Cd(OH)2	-13.37	0.28	13.65	Cd(OH)2
CdSO4	-12.75	-12.83	-0.08	CdSO4
Cerussite	-4.37	-17.50	-13.14	PbCO3
CO2(g)	0.38	-1.08	-1.46	CO2
Dolomite	-8.89	-25.97	-17.08	CaMg(CO3)2

Fe(OH)3(a)	-11.69	-6.79	4.89	Fe(OH)3
Fluorite	-3.46	-14.06	-10.61	CaF2
Gibbsite	-2.48	5.66	8.14	Al(OH)3
Goethite	-5.81	-6.79	-0.98	FeOOH
Gypsum	-3.73	-8.31	-4.58	CaSO4:2H2O
H2(g)	-8.74	-11.84	-3.10	H2
H2O(g)	-1.52	-0.00	1.52	H2O
Halite	-7.44	-5.87	1.57	NaCl
Hausmannite	-45.20	15.96	61.16	Mn3O4
Hematite	-9.62	-13.59	-3.97	Fe2O3
Hydroxyapatite	-24.09	-27.47	-3.37	Ca5(PO4)3OH
Jarosite-K	-36.94	-46.10	-9.17	KFe3(SO4)2(OH)6
Manganite	-18.57	6.77	25.34	MnOOH
Melanterite	-9.00	-11.22	-2.22	FeSO4:7H2O
O2(g)	-65.99	-68.87	-2.89	O2
Otavite	-5.39	-17.49	-12.10	CdCO3
Pb(OH)2	-7.90	0.27	8.17	Pb(OH)2
Pyrochroite	-12.78	2.42	15.20	Mn(OH)2
Pyrolusite	-30.35	11.11	41.46	MnO2:H2O
Rhodochrosite	-4.22	-15.35	-11.13	MnCO3
Siderite	-4.99	-15.88	-10.89	FeCO3
Smithsonite	-4.92	-14.92	-9.99	ZnCO3
Sylvite	-7.39	-6.49	0.90	KCl
Vivianite	-17.33	-53.33	-36.00	Fe3(PO4)2:8H2O
Witherite	-5.82	-14.38	-8.56	BaCO3
Zn(OH)2(e)	-8.65	2.85	11.50	Zn(OH)2

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
For ideal gases, phi = 1.

Initial solution 18.

-----------------------------Solution composition-----------------------------

Elements	Molality	Moles
Al	1.076e-06	1.076e-06
Alkalinity	4.309e-03	4.309e-03
B	1.299e-05	1.299e-05
Ba	1.100e-05	1.100e-05
Br	5.508e-06	5.508e-06
Ca	7.438e-04	7.438e-04
Cd	7.387e-09	7.387e-09
Cl	5.051e-04	5.051e-04
Cu	4.187e-08	4.187e-08
F	6.529e-05	6.529e-05
Fe	5.752e-07	5.752e-07
K	8.187e-05	8.187e-05
Mg	2.773e-04	2.773e-04
Mn	1.176e-07	1.176e-07
N(5)	3.285e-05	3.285e-05
Na	2.711e-03	2.711e-03
P	4.618e-06	4.618e-06
Pb	2.559e-09	2.559e-09
S(6)	3.020e-05	3.020e-05
Zn	2.361e-06	2.361e-06

----------------------------Description of solution----------------------------

pH	=	6.500
pe	=	0.269
Specific Conductance (µS/cm, 26°C)	=	464
Density (g/cm³)	=	0.99716
Volume (L)	=	1.00337
Activity of water	=	1.000
Ionic strength (mol/kgw)	=	5.881e-03
Mass of water (kg)	=	1.000e+00
Total carbon (mol/kg)	=	7.074e-03

Total CO2 (mol/kg) = 7.074e-03
Temperature (°C) = 25.80
Electrical balance (eq) = -1.164e-04
Percent error, 100*(Cat-|An|)/(Cat+|An|) = -1.20
Iterations = 13 (189 overall)
Total H = 1.110168e+02
Total O = 5.552495e+01

----------Distribution of species----------

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma	mole V cm³/mol
H+	3.404e-07	3.162e-07	-6.468	-6.500	-0.032	0.00
OH-	3.694e-08	3.401e-08	-7.432	-7.468	-0.036	-4.03
H2O	5.551e+01	9.998e-01	1.744	-0.000	0.000	18.07
Al	1.076e-06					
AlF2+	5.480e-07	5.061e-07	-6.261	-6.296	-0.034	(0)
AlF3	3.642e-07	3.647e-07	-6.439	-6.438	0.001	(0)
Al(OH)4-	8.679e-08	8.004e-08	-7.062	-7.097	-0.035	(0)
Al(OH)2+	2.912e-08	2.690e-08	-7.536	-7.570	-0.034	(0)
AlF+2	2.416e-08	1.759e-08	-7.617	-7.755	-0.138	(0)
Al(OH)3	1.327e-08	1.328e-08	-7.877	-7.877	0.001	(0)
AlF4-	9.004e-09	8.303e-09	-8.046	-8.081	-0.035	(0)
AlOH+2	1.391e-09	1.013e-09	-8.857	-8.995	-0.138	-27.65
Al+3	5.932e-11	3.061e-11	-10.227	-10.514	-0.287	-42.05
AlSO4+	2.085e-12	1.923e-12	-11.681	-11.716	-0.035	(0)
Al(SO4)2-	1.302e-15	1.200e-15	-14.886	-14.921	-0.035	(0)
AlHSO4+2	7.530e-20	5.431e-20	-19.123	-19.265	-0.142	(0)
B	1.299e-05					
H3BO3	1.297e-05	1.298e-05	-4.887	-4.887	0.001	39.29
H2BO3-	2.601e-08	2.397e-08	-7.585	-7.620	-0.035	(0)
BF(OH)3-	3.234e-10	2.981e-10	-9.490	-9.526	-0.035	(0)
BF2(OH)2-	6.262e-13	5.770e-13	-12.203	-12.239	-0.035	(0)
BF3OH-	1.224e-17	1.128e-17	-16.912	-16.948	-0.035	(0)
BF4-	9.007e-22	8.301e-22	-21.045	-21.081	-0.035	(0)
Ba	1.100e-05					
Ba+2	1.059e-05	7.645e-06	-4.975	-5.117	-0.141	-12.56
BaHCO3+	3.208e-07	2.957e-07	-6.494	-6.529	-0.035	(0)
BaSO4	7.524e-08	7.534e-08	-7.124	-7.123	0.001	(0)
BaCl+	1.212e-08	1.117e-08	-7.917	-7.952	-0.035	(0)
BaCO3	2.376e-09	2.380e-09	-8.624	-8.624	0.001	-10.69
BaNO3+	3.155e-11	2.908e-11	-10.501	-10.536	-0.035	(0)
BaOH+	8.873e-13	8.190e-13	-12.052	-12.087	-0.035	(0)
Br	5.508e-06					
Br-	5.508e-06	5.065e-06	-5.259	-5.295	-0.036	24.64
CdBr+	3.793e-12	3.496e-12	-11.421	-11.456	-0.035	(0)
ZnBr+	1.668e-12	1.537e-12	-11.778	-11.813	-0.035	(0)
PbBr+	5.524e-14	5.091e-14	-13.258	-13.293	-0.035	(0)
CdBr2	9.531e-17	9.544e-17	-16.021	-16.020	0.001	(0)
ZnBr2	3.095e-18	3.099e-18	-17.509	-17.509	0.001	(0)
PbBr2	1.189e-19	1.191e-19	-18.925	-18.924	0.001	(0)
C(4)	7.074e-03					
HCO3-	4.260e-03	3.935e-03	-2.371	-2.405	-0.034	24.79
CO2	2.767e-03	2.771e-03	-2.558	-2.557	0.001	34.47
CaHCO3+	2.849e-05	2.634e-05	-4.545	-4.579	-0.034	9.74
MgHCO3+	9.731e-06	8.965e-06	-5.012	-5.047	-0.036	5.54
NaHCO3	5.475e-06	5.482e-06	-5.262	-5.261	0.001	1.80
CO3-2	8.145e-07	5.929e-07	-6.089	-6.227	-0.138	-5.04
ZnHCO3+	6.200e-07	5.714e-07	-6.208	-6.243	-0.035	(0)
CaCO3	5.242e-07	5.249e-07	-6.281	-6.280	0.001	-14.60
BaHCO3+	3.208e-07	2.957e-07	-6.494	-6.529	-0.035	(0)
(CO2)2	1.445e-07	1.447e-07	-6.840	-6.840	0.001	68.94
ZnCO3	1.363e-07	1.365e-07	-6.866	-6.865	0.001	(0)
FeHCO3+	1.350e-07	1.244e-07	-6.870	-6.905	-0.035	(0)
MgCO3	1.110e-07	1.111e-07	-6.955	-6.954	0.001	-17.09
NaCO3-	3.104e-08	2.861e-08	-7.508	-7.544	-0.035	-0.89
MnHCO3+	2.481e-08	2.290e-08	-7.605	-7.640	-0.035	(0)

FeCO3	4.490e-09	4.496e-09	-8.348	-8.347	0.001	(0)
MnCO3	3.072e-09	3.076e-09	-8.513	-8.512	0.001	(0)
Zn(CO3)2-2	2.398e-09	1.730e-09	-8.620	-8.762	-0.142	(0)
BaCO3	2.376e-09	2.380e-09	-8.624	-8.624	0.001	-10.69
PbCO3	1.734e-09	1.736e-09	-8.761	-8.760	0.001	(0)
CdHCO3+	6.322e-10	5.826e-10	-9.199	-9.235	-0.035	(0)
PbHCO3+	5.714e-10	5.265e-10	-9.243	-9.279	-0.035	(0)
CuCO3	3.948e-10	3.953e-10	-9.404	-9.403	0.001	(0)
CuHCO3+	2.657e-10	2.448e-10	-9.576	-9.611	-0.035	(0)
Pb(CO3)2-2	3.584e-12	2.585e-12	-11.446	-11.588	-0.142	(0)
CdCO3	2.202e-12	2.205e-12	-11.657	-11.657	0.001	(0)
Cu(CO3)2-2	4.091e-13	2.950e-13	-12.388	-12.530	-0.142	(0)
Cd(CO3)2-2	5.733e-15	4.135e-15	-14.242	-14.384	-0.142	(0)
Ca	7.438e-04					
Ca+2	7.127e-04	5.185e-04	-3.147	-3.285	-0.138	-17.99
CaHCO3+	2.849e-05	2.634e-05	-4.545	-4.579	-0.034	9.74
CaSO4	1.821e-06	1.824e-06	-5.740	-5.739	0.001	7.53
CaCO3	5.242e-07	5.249e-07	-6.281	-6.280	0.001	-14.60
CaHPO4	1.793e-07	1.796e-07	-6.746	-6.746	0.001	(0)
CaH2PO4+	4.602e-08	4.251e-08	-7.337	-7.372	-0.034	(0)
CaPO4-	1.476e-09	1.364e-09	-8.831	-8.865	-0.034	(0)
CaOH+	2.952e-10	2.721e-10	-9.530	-9.565	-0.035	(0)
CaHSO4+	4.162e-12	3.835e-12	-11.381	-11.416	-0.035	(0)
Cd	7.387e-09					
Cd+2	6.493e-09	4.683e-09	-8.188	-8.329	-0.142	-18.57
CdHCO3+	6.322e-10	5.826e-10	-9.199	-9.235	-0.035	(0)
CdCl+	2.232e-10	2.057e-10	-9.651	-9.687	-0.035	6.11
CdSO4	2.665e-11	2.669e-11	-10.574	-10.574	0.001	77.66
CdBr+	3.793e-12	3.496e-12	-11.421	-11.456	-0.035	(0)
CdF+	3.658e-12	3.371e-12	-11.437	-11.472	-0.035	(0)
CdCO3	2.202e-12	2.205e-12	-11.657	-11.657	0.001	(0)
CdOH+	1.418e-12	1.307e-12	-11.848	-11.884	-0.035	(0)
CdCl2	3.941e-13	3.946e-13	-12.404	-12.404	0.001	23.14
CdNO3+	3.767e-13	3.471e-13	-12.424	-12.460	-0.035	17.54
CdOHCl	2.729e-13	2.733e-13	-12.564	-12.563	0.001	(0)
Cd(SO4)2-2	7.939e-15	5.726e-15	-14.100	-14.242	-0.142	-105.01
Cd(CO3)2-2	5.733e-15	4.135e-15	-14.242	-14.384	-0.142	(0)
CdF2	4.836e-16	4.842e-16	-15.316	-15.315	0.001	(0)
Cd(OH)2	2.088e-16	2.091e-16	-15.680	-15.680	0.001	(0)
CdCl3-	1.254e-16	1.156e-16	-15.902	-15.937	-0.035	68.80
CdBr2	9.531e-17	9.544e-17	-16.021	-16.020	0.001	(0)
Cd2OH+3	6.189e-20	2.967e-20	-19.208	-19.528	-0.319	(0)
Cd(OH)3-	8.049e-23	7.418e-23	-22.094	-22.130	-0.035	(0)
Cd(OH)4-2	2.898e-30	2.090e-30	-29.538	-29.680	-0.142	(0)
Cl	5.051e-04					
Cl-	4.982e-04	4.588e-04	-3.303	-3.338	-0.036	18.14
NaCl	6.863e-06	6.872e-06	-5.164	-5.163	0.001	(0)
BaCl+	1.212e-08	1.117e-08	-7.917	-7.952	-0.035	(0)
CuCl2-	2.548e-09	2.347e-09	-8.594	-8.629	-0.036	(0)
ZnCl+	1.601e-09	1.475e-09	-8.796	-8.831	-0.036	-13.11
CdCl+	2.232e-10	2.057e-10	-9.651	-9.687	-0.035	6.11
FeCl+	2.172e-10	2.002e-10	-9.663	-9.699	-0.035	(0)
MnCl+	1.322e-10	1.221e-10	-9.879	-9.913	-0.035	-2.86
ZnOHCl	5.533e-11	5.540e-11	-10.257	-10.256	0.001	(0)
PbCl+	3.406e-12	3.139e-12	-11.468	-11.503	-0.035	8.02
CuCl3-2	2.359e-12	1.712e-12	-11.627	-11.766	-0.139	(0)
ZnCl2	7.101e-13	7.111e-13	-12.149	-12.148	0.001	100.48
CdCl2	3.941e-13	3.946e-13	-12.404	-12.404	0.001	23.14
CdOHCl	2.729e-13	2.733e-13	-12.564	-12.563	0.001	(0)
CuCl+	1.730e-13	1.594e-13	-12.762	-12.797	-0.036	0.47
MnCl2	2.441e-14	2.445e-14	-13.612	-13.612	0.001	84.92
PbCl2	2.245e-15	2.248e-15	-14.649	-14.648	0.001	35.04
ZnCl3-	3.992e-16	3.678e-16	-15.399	-15.434	-0.036	17.06
CdCl3-	1.254e-16	1.156e-16	-15.902	-15.937	-0.035	68.80
CuCl2	3.956e-17	3.962e-17	-16.403	-16.402	0.001	31.93
MnCl3-	3.346e-18	3.089e-18	-17.475	-17.510	-0.035	43.37
PbCl3-	8.935e-19	8.234e-19	-18.049	-18.084	-0.035	66.09
ZnCl4-2	1.172e-19	8.510e-20	-18.931	-19.070	-0.139	145.45

FeCl+2	1.147e-21	8.326e-22	-20.940	-21.080	-0.139	(0)
PbCl4-2	2.522e-22	1.819e-22	-21.598	-21.740	-0.142	101.64
CuCl3-	7.099e-23	6.541e-23	-22.149	-22.184	-0.036	(0)
FeCl2+	1.802e-24	1.664e-24	-23.744	-23.779	-0.035	(0)
CuCl4-2	2.111e-28	1.532e-28	-27.676	-27.815	-0.139	(0)
FeCl3	7.622e-29	7.633e-29	-28.118	-28.117	0.001	(0)
Cu(1)	4.101e-08					
Cu+	3.846e-08	3.533e-08	-7.415	-7.452	-0.037	(0)
CuCl2-	2.548e-09	2.347e-09	-8.594	-8.629	-0.036	(0)
CuCl3-2	2.359e-12	1.712e-12	-11.627	-11.766	-0.139	(0)
Cu(2)	8.616e-10					
CuCO3	3.948e-10	3.953e-10	-9.404	-9.403	0.001	(0)
CuHCO3+	2.657e-10	2.448e-10	-9.576	-9.611	-0.035	(0)
Cu+2	1.698e-10	1.242e-10	-9.770	-9.906	-0.136	-26.48
Cu(OH)2	2.589e-11	2.593e-11	-10.587	-10.586	0.001	(0)
CuOH+	4.260e-12	3.925e-12	-11.371	-11.406	-0.036	(0)
CuSO4	5.005e-13	5.012e-13	-12.301	-12.300	0.001	13.19
Cu(CO3)2-2	4.091e-13	2.950e-13	-12.388	-12.530	-0.142	(0)
CuCl+	1.730e-13	1.594e-13	-12.762	-12.797	-0.036	0.47
CuF+	1.412e-13	1.301e-13	-12.850	-12.886	-0.035	(0)
CuCl2	3.956e-17	3.962e-17	-16.403	-16.402	0.001	31.93
Cu2(OH)2+2	1.012e-17	7.298e-18	-16.995	-17.137	-0.142	(0)
Cu(OH)3-	5.360e-18	4.940e-18	-17.271	-17.306	-0.035	(0)
CuCl3-	7.099e-23	6.541e-23	-22.149	-22.184	-0.036	(0)
Cu(OH)4-2	4.320e-24	3.116e-24	-23.364	-23.506	-0.142	(0)
CuCl4-2	2.111e-28	1.532e-28	-27.676	-27.815	-0.139	(0)
F	6.529e-05					
F-	6.213e-05	5.718e-05	-4.207	-4.243	-0.036	-1.27
MgF+	8.065e-07	7.438e-07	-6.093	-6.129	-0.035	-10.54
AlF2+	5.480e-07	5.061e-07	-6.261	-6.296	-0.034	(0)
AlF3	3.642e-07	3.647e-07	-6.439	-6.438	0.001	(0)
NaF	8.179e-08	8.190e-08	-7.087	-7.087	0.001	7.29
HF	2.748e-08	2.751e-08	-7.561	-7.560	0.001	12.54
AlF+2	2.416e-08	1.759e-08	-7.617	-7.755	-0.138	(0)
AlF4-	9.004e-09	8.303e-09	-8.046	-8.081	-0.035	(0)
ZnF+	1.021e-09	9.411e-10	-8.991	-9.026	-0.035	(0)
BF(OH)3-	3.234e-10	2.981e-10	-9.490	-9.526	-0.035	(0)
FeF+	1.962e-10	1.808e-10	-9.707	-9.743	-0.035	(0)
MnF+	2.799e-11	2.584e-11	-10.553	-10.588	-0.035	(0)
HF2-	6.591e-12	6.074e-12	-11.181	-11.217	-0.035	22.14
CdF+	3.658e-12	3.371e-12	-11.437	-11.472	-0.035	(0)
BF2(OH)2-	6.262e-13	5.770e-13	-12.203	-12.239	-0.035	(0)
PbF+	1.859e-13	1.713e-13	-12.731	-12.766	-0.035	(0)
CuF+	1.412e-13	1.301e-13	-12.850	-12.886	-0.035	(0)
CdF2	4.836e-16	4.842e-16	-15.316	-15.315	0.001	(0)
PbF2	1.998e-16	2.000e-16	-15.699	-15.699	0.001	(0)
FeF2+	1.338e-17	1.235e-17	-16.873	-16.908	-0.035	(0)
BF3OH-	1.224e-17	1.128e-17	-16.912	-16.948	-0.035	(0)
FeF+2	7.406e-18	5.376e-18	-17.130	-17.270	-0.139	(0)
FeF3	1.121e-18	1.123e-18	-17.950	-17.950	0.001	(0)
PbF3-	8.992e-20	8.286e-20	-19.046	-19.082	-0.035	(0)
BF4-	9.007e-22	8.301e-22	-21.045	-21.081	-0.035	(0)
PbF4-2	3.144e-24	2.268e-24	-23.502	-23.644	-0.142	(0)
Fe(2)	5.752e-07					
Fe+2	4.325e-07	3.161e-07	-6.364	-6.500	-0.136	-21.95
FeHCO3+	1.350e-07	1.244e-07	-6.870	-6.905	-0.035	(0)
FeCO3	4.490e-09	4.496e-09	-8.348	-8.347	0.001	(0)
FeSO4	1.120e-09	1.122e-09	-8.951	-8.950	0.001	18.14
FeHPO4	7.821e-10	7.832e-10	-9.107	-9.106	0.001	(0)
FeH2PO4+	5.412e-10	4.999e-10	-9.267	-9.301	-0.034	(0)
FeOH+	3.635e-10	3.355e-10	-9.440	-9.474	-0.035	(0)
FeCl+	2.172e-10	2.002e-10	-9.663	-9.699	-0.035	(0)
FeF+	1.962e-10	1.808e-10	-9.707	-9.743	-0.035	(0)
Fe(OH)2	9.664e-15	9.677e-15	-14.015	-14.014	0.001	(0)
FeHSO4+	2.537e-15	2.338e-15	-14.596	-14.631	-0.035	(0)
Fe(OH)3-	1.241e-18	1.146e-18	-17.906	-17.941	-0.035	(0)
Fe(3)	2.038e-12					
Fe(OH)2+	1.465e-12	1.353e-12	-11.834	-11.869	-0.034	(0)

Fe(OH)3	5.697e-13	5.705e-13	-12.244	-12.244	0.001	(0)
Fe(OH)4-	1.839e-15	1.699e-15	-14.735	-14.770	-0.034	(0)
FeOH+2	1.727e-15	1.254e-15	-14.763	-14.902	-0.139	(0)
FeF2+	1.338e-17	1.235e-17	-16.873	-16.908	-0.035	(0)
FeF+2	7.406e-18	5.376e-18	-17.130	-17.270	-0.139	(0)
FeF3	1.121e-18	1.123e-18	-17.950	-17.950	0.001	(0)
Fe+3	1.136e-19	5.859e-20	-18.945	-19.232	-0.287	(0)
FeH2PO4+2	6.836e-20	4.976e-20	-19.165	-19.303	-0.138	(0)
FeSO4+	1.393e-20	1.286e-20	-19.856	-19.891	-0.035	(0)
FeHPO4+	1.091e-20	1.007e-20	-19.962	-19.997	-0.035	(0)
FeCl+2	1.147e-21	8.326e-22	-20.940	-21.080	-0.139	(0)
Fe(SO4)2-	6.021e-24	5.549e-24	-23.220	-23.256	-0.035	(0)
FeCl2+	1.802e-24	1.664e-24	-23.744	-23.779	-0.035	(0)
FeHSO4+2	1.509e-26	1.089e-26	-25.821	-25.963	-0.142	(0)
Fe2(OH)2+4	1.512e-28	4.093e-29	-27.820	-28.388	-0.568	(0)
FeCl3	7.622e-29	7.633e-29	-28.118	-28.117	0.001	(0)
Fe3(OH)4+5	8.283e-38	1.075e-38	-37.082	-37.969	-0.887	(0)
H(0)	4.064e-17					
H2	2.032e-17	2.035e-17	-16.692	-16.691	0.001	28.61
K	8.187e-05					
K+	8.185e-05	7.536e-05	-4.087	-4.123	-0.036	9.07
KSO4-	1.143e-08	1.056e-08	-7.942	-7.976	-0.034	34.17
KHPO4-	9.899e-11	9.144e-11	-10.004	-10.039	-0.034	38.10
Mg	2.773e-04					
Mg+2	2.656e-04	1.940e-04	-3.576	-3.712	-0.136	-21.71
MgHCO3+	9.731e-06	8.965e-06	-5.012	-5.047	-0.036	5.54
MgSO4	9.118e-07	9.130e-07	-6.040	-6.040	0.001	5.87
MgF+	8.065e-07	7.438e-07	-6.093	-6.129	-0.035	-10.54
MgCO3	1.110e-07	1.111e-07	-6.955	-6.954	0.001	-17.09
MgHPO4	9.073e-08	9.085e-08	-7.042	-7.042	0.001	(0)
MgH2PO4+	2.193e-08	2.026e-08	-7.659	-7.693	-0.034	(0)
MgOH+	2.587e-09	2.394e-09	-8.587	-8.621	-0.034	(0)
MgPO4-	7.453e-10	6.885e-10	-9.128	-9.162	-0.034	(0)
Mn(2)	1.176e-07					
Mn+2	8.935e-08	6.531e-08	-7.049	-7.185	-0.136	-20.15
MnHCO3+	2.481e-08	2.290e-08	-7.605	-7.640	-0.035	(0)
MnCO3	3.072e-09	3.076e-09	-8.513	-8.512	0.001	(0)
MnSO4	2.316e-10	2.319e-10	-9.635	-9.635	0.001	22.19
MnCl+	1.322e-10	1.221e-10	-9.879	-9.913	-0.035	-2.86
MnF+	2.799e-11	2.584e-11	-10.553	-10.588	-0.035	(0)
MnOH+	6.137e-12	5.664e-12	-11.212	-11.247	-0.035	(0)
MnCl2	2.441e-14	2.445e-14	-13.612	-13.612	0.001	84.92
Mn(NO3)2	2.366e-16	2.369e-16	-15.626	-15.625	0.001	40.83
MnCl3-	3.346e-18	3.089e-18	-17.475	-17.510	-0.035	43.37
Mn(OH)3-	3.544e-23	3.271e-23	-22.450	-22.485	-0.035	(0)
Mn(3)	8.164e-33					
Mn+3	8.164e-33	4.213e-33	-32.088	-32.375	-0.287	(0)
N(5)	3.285e-05					
NO3-	3.285e-05	3.021e-05	-4.483	-4.520	-0.036	29.61
BaNO3+	3.155e-11	2.908e-11	-10.501	-10.536	-0.035	(0)
CdNO3+	3.767e-13	3.471e-13	-12.424	-12.460	-0.035	17.54
PbNO3+	8.169e-14	7.528e-14	-13.088	-13.123	-0.035	(0)
Mn(NO3)2	2.366e-16	2.369e-16	-15.626	-15.625	0.001	40.83
Na	2.711e-03					
Na+	2.698e-03	2.489e-03	-2.569	-2.604	-0.035	-1.37
NaCl	6.863e-06	6.872e-06	-5.164	-5.163	0.001	(0)
NaHCO3	5.475e-06	5.482e-06	-5.262	-5.261	0.001	1.80
NaSO4-	2.669e-07	2.465e-07	-6.574	-6.608	-0.034	14.10
NaF	8.179e-08	8.190e-08	-7.087	-7.087	0.001	7.29
NaCO3-	3.104e-08	2.861e-08	-7.508	-7.544	-0.035	-0.89
NaHPO4-	3.270e-09	3.020e-09	-8.486	-8.520	-0.034	33.86
NaOH	8.453e-21	8.464e-21	-20.073	-20.072	0.001	(0)
O(0)	0.000e+00					
O2	0.000e+00	0.000e+00	-58.740	-58.740	0.001	30.46
P	4.618e-06					
H2PO4-	3.416e-06	3.155e-06	-5.466	-5.501	-0.034	33.24
HPO4-2	8.573e-07	6.223e-07	-6.067	-6.206	-0.139	6.85
CaHPO4	1.793e-07	1.796e-07	-6.746	-6.746	0.001	(0)

MgHPO4	9.073e-08	9.085e-08	-7.042	-7.042	0.001	(0)
CaH2PO4+	4.602e-08	4.251e-08	-7.337	-7.372	-0.034	(0)
MgH2PO4+	2.193e-08	2.026e-08	-7.659	-7.693	-0.034	(0)
NaHPO4-	3.270e-09	3.020e-09	-8.486	-8.520	-0.034	33.86
CaPO4-	1.476e-09	1.364e-09	-8.831	-8.865	-0.034	(0)
FeHPO4	7.821e-10	7.832e-10	-9.107	-9.106	0.001	(0)
MgPO4-	7.453e-10	6.885e-10	-9.128	-9.162	-0.034	(0)
FeH2PO4+	5.412e-10	4.999e-10	-9.267	-9.301	-0.034	(0)
H3PO4	1.481e-10	1.483e-10	-9.829	-9.829	0.001	47.45
KHPO4-	9.899e-11	9.144e-11	-10.004	-10.039	-0.034	38.10
PO4-3	1.884e-12	9.014e-13	-11.725	-12.045	-0.320	-22.93
FeH2PO4+2	6.836e-20	4.976e-20	-19.165	-19.303	-0.138	(0)
FeHPO4+	1.091e-20	1.007e-20	-19.962	-19.997	-0.035	(0)
Pb	2.559e-09					
PbCO3	1.734e-09	1.736e-09	-8.761	-8.760	0.001	(0)
PbHCO3+	5.714e-10	5.265e-10	-9.243	-9.279	-0.035	(0)
Pb+2	2.336e-10	1.685e-10	-9.632	-9.773	-0.142	-15.41
PbOH+	1.127e-11	1.039e-11	-10.948	-10.984	-0.035	(0)
Pb(CO3)2-2	3.584e-12	2.585e-12	-11.446	-11.588	-0.142	(0)
PbCl+	3.406e-12	3.139e-12	-11.468	-11.503	-0.035	8.02
PbSO4	1.860e-12	1.863e-12	-11.730	-11.730	0.001	(0)
PbF+	1.859e-13	1.713e-13	-12.731	-12.766	-0.035	(0)
PbNO3+	8.169e-14	7.528e-14	-13.088	-13.123	-0.035	(0)
PbBr+	5.524e-14	5.091e-14	-13.258	-13.293	-0.035	(0)
Pb(OH)2	1.276e-14	1.278e-14	-13.894	-13.894	0.001	(0)
PbCl2	2.245e-15	2.248e-15	-14.649	-14.648	0.001	35.04
Pb(SO4)2-2	2.666e-16	1.923e-16	-15.574	-15.716	-0.142	(0)
PbF2	1.998e-16	2.000e-16	-15.699	-15.699	0.001	(0)
PbCl3-	8.935e-19	8.234e-19	-18.049	-18.084	-0.035	66.09
Pb(OH)3-	5.032e-19	4.638e-19	-18.298	-18.334	-0.035	(0)
PbBr2	1.189e-19	1.191e-19	-18.925	-18.924	0.001	(0)
PbF3-	8.992e-20	8.286e-20	-19.046	-19.082	-0.035	(0)
Pb2OH+3	8.171e-20	3.917e-20	-19.088	-19.407	-0.319	(0)
PbCl4-2	2.522e-22	1.819e-22	-21.598	-21.740	-0.142	101.64
Pb(OH)4-2	4.657e-24	3.359e-24	-23.332	-23.474	-0.142	(0)
PbF4-2	3.144e-24	2.268e-24	-23.502	-23.644	-0.142	(0)
Pb3(OH)4+2	9.844e-28	7.100e-28	-27.007	-27.149	-0.142	(0)
S(6)	3.020e-05					
SO4-2	2.710e-05	1.966e-05	-4.567	-4.706	-0.139	14.78
CaSO4	1.821e-06	1.824e-06	-5.740	-5.739	0.001	7.53
MgSO4	9.118e-07	9.130e-07	-6.040	-6.040	0.001	5.87
NaSO4-	2.669e-07	2.465e-07	-6.574	-6.608	-0.034	14.10
BaSO4	7.524e-08	7.534e-08	-7.124	-7.123	0.001	(0)
KSO4-	1.143e-08	1.056e-08	-7.942	-7.976	-0.034	34.17
ZnSO4	5.343e-09	5.350e-09	-8.272	-8.272	0.001	21.59
FeSO4	1.120e-09	1.122e-09	-8.951	-8.950	0.001	18.14
HSO4-	6.676e-10	6.152e-10	-9.175	-9.211	-0.035	40.37
MnSO4	2.316e-10	2.319e-10	-9.635	-9.635	0.001	22.19
CdSO4	2.665e-11	2.669e-11	-10.574	-10.574	0.001	77.66
CaHSO4+	4.162e-12	3.835e-12	-11.381	-11.416	-0.035	(0)
AlSO4+	2.085e-12	1.923e-12	-11.681	-11.716	-0.035	(0)
PbSO4	1.860e-12	1.863e-12	-11.730	-11.730	0.001	(0)
Zn(SO4)2-2	1.178e-12	8.499e-13	-11.929	-12.071	-0.142	-12.26
CuSO4	5.005e-13	5.012e-13	-12.301	-12.300	0.001	13.19
Cd(SO4)2-2	7.939e-15	5.726e-15	-14.100	-14.242	-0.142	-105.01
FeHSO4+	2.537e-15	2.338e-15	-14.596	-14.631	-0.035	(0)
Al(SO4)2-	1.302e-15	1.200e-15	-14.886	-14.921	-0.035	(0)
Pb(SO4)2-2	2.666e-16	1.923e-16	-15.574	-15.716	-0.142	(0)
AlHSO4+2	7.530e-20	5.431e-20	-19.123	-19.265	-0.142	(0)
FeSO4+	1.393e-20	1.286e-20	-19.856	-19.891	-0.035	(0)
Fe(SO4)2-	6.021e-24	5.549e-24	-23.220	-23.256	-0.035	(0)
FeHSO4+2	1.509e-26	1.089e-26	-25.821	-25.963	-0.142	(0)
Zn	2.361e-06					
Zn+2	1.589e-06	1.154e-06	-5.799	-5.938	-0.139	-25.27
ZnHCO3+	6.200e-07	5.714e-07	-6.208	-6.243	-0.035	(0)
ZnCO3	1.363e-07	1.365e-07	-6.866	-6.865	0.001	(0)
ZnSO4	5.343e-09	5.350e-09	-8.272	-8.272	0.001	21.59
ZnOH+	4.610e-09	4.248e-09	-8.336	-8.372	-0.035	(0)

Zn(CO3)2-2	2.398e-09	1.730e-09	-8.620	-8.762	-0.142	(0)
ZnCl+	1.601e-09	1.475e-09	-8.796	-8.831	-0.036	-13.11
ZnF+	1.021e-09	9.411e-10	-8.991	-9.026	-0.035	(0)
Zn(OH)2	1.450e-10	1.452e-10	-9.839	-9.838	0.001	(0)
ZnOHCl	5.533e-11	5.540e-11	-10.257	-10.256	0.001	(0)
ZnBr+	1.668e-12	1.537e-12	-11.778	-11.813	-0.035	(0)
Zn(SO4)2-2	1.178e-12	8.499e-13	-11.929	-12.071	-0.142	-12.26
ZnCl2	7.101e-13	7.111e-13	-12.149	-12.148	0.001	100.48
Zn(OH)3-	1.575e-15	1.451e-15	-14.803	-14.838	-0.035	(0)
ZnCl3-	3.992e-16	3.678e-16	-15.399	-15.434	-0.036	17.06
ZnBr2	3.095e-18	3.099e-18	-17.509	-17.509	0.001	(0)
ZnCl4-2	1.172e-19	8.510e-20	-18.931	-19.070	-0.139	145.45
Zn(OH)4-2	1.008e-21	7.273e-22	-20.996	-21.138	-0.142	(0)

----------Distribution of alkalinity----------

Total alkalinity (eq/kgw) = 4.309e-03

Species	Alkalinity	Molality	Alk/Mol
HCO3-	4.260e-03	4.260e-03	1.00
CaHCO3+	2.849e-05	2.849e-05	1.00
MgHCO3+	9.731e-06	9.731e-06	1.00
NaHCO3	5.475e-06	5.475e-06	1.00
CO3-2	1.629e-06	8.145e-07	2.00
CaCO3	1.048e-06	5.242e-07	2.00
HPO4-2	8.573e-07	8.573e-07	1.00
ZnHCO3+	6.200e-07	6.200e-07	1.00
Al(OH)4-	3.472e-07	8.679e-08	4.00
H+	-3.404e-07	3.404e-07	-1.00
BaHCO3+	3.208e-07	3.208e-07	1.00
ZnCO3	2.725e-07	1.363e-07	2.00
MgCO3	2.220e-07	1.110e-07	2.00
CaHPO4	1.793e-07	1.793e-07	1.00
FeHCO3+	1.350e-07	1.350e-07	1.00
MgHPO4	9.073e-08	9.073e-08	1.00
NaCO3-	6.208e-08	3.104e-08	2.00
Al(OH)2+	5.823e-08	2.912e-08	2.00
Al(OH)3	3.980e-08	1.327e-08	3.00
OH-	3.694e-08	3.694e-08	1.00
HF	-2.748e-08	2.748e-08	-1.00
H2BO3-	2.601e-08	2.601e-08	1.00
MnHCO3+	2.481e-08	2.481e-08	1.00
Zn(CO3)2-2	9.593e-09	2.398e-09	4.00
FeCO3	8.980e-09	4.490e-09	2.00
MnCO3	6.143e-09	3.072e-09	2.00
BaCO3	4.753e-09	2.376e-09	2.00
ZnOH+	4.610e-09	4.610e-09	1.00
PbCO3	3.467e-09	1.734e-09	2.00
NaHPO4-	3.270e-09	3.270e-09	1.00
CaPO4-	2.953e-09	1.476e-09	2.00
MgOH+	2.587e-09	2.587e-09	1.00
MgPO4-	1.491e-09	7.453e-10	2.00
AlOH+2	1.391e-09	1.391e-09	1.00
CuCO3	7.895e-10	3.948e-10	2.00
FeHPO4	7.821e-10	7.821e-10	1.00
HSO4-	-6.676e-10	6.676e-10	-1.00
CdHCO3+	6.322e-10	6.322e-10	1.00
PbHCO3+	5.714e-10	5.714e-10	1.00
FeOH+	3.635e-10	3.635e-10	1.00
CaOH+	2.952e-10	2.952e-10	1.00
Zn(OH)2	2.899e-10	1.450e-10	2.00
CuHCO3+	2.657e-10	2.657e-10	1.00
H3PO4	-1.481e-10	1.481e-10	-1.00
KHPO4-	9.899e-11	9.899e-11	1.00
ZnOHCl	5.533e-11	5.533e-11	1.00
Cu(OH)2	5.179e-11	2.589e-11	2.00
Pb(CO3)2-2	1.434e-11	3.584e-12	4.00

PbOH+	1.127e-11	1.127e-11	1.00
HF2-	-6.591e-12	6.591e-12	-1.00
MnOH+	6.137e-12	6.137e-12	1.00
CdCO3	4.405e-12	2.202e-12	2.00
CuOH+	4.260e-12	4.260e-12	1.00
CaHSO4+	-4.162e-12	4.162e-12	-1.00
PO4-3	3.769e-12	1.884e-12	2.00
Cu(CO3)2-2	1.636e-12	4.091e-13	4.00
CdOH+	1.418e-12	1.418e-12	1.00
BaOH+	8.873e-13	8.873e-13	1.00
BF2(OH)2-	-6.262e-13	6.262e-13	-1.00
Fe(OH)3	5.697e-13	5.697e-13	1.00
CdOHCl	2.729e-13	2.729e-13	1.00
Pb(OH)2	2.552e-14	1.276e-14	2.00
Cd(CO3)2-2	2.293e-14	5.733e-15	4.00
Fe(OH)2	1.933e-14	9.664e-15	2.00
Zn(OH)3-	4.725e-15	1.575e-15	3.00
Fe(OH)4-	3.678e-15	1.839e-15	2.00
FeHSO4+	-2.537e-15	2.537e-15	-1.00
FeOH+2	-1.727e-15	1.727e-15	-1.00
Cd(OH)2	4.176e-16	2.088e-16	2.00
FeF2+	-2.677e-17	1.338e-17	-2.00
BF3OH-	-2.448e-17	1.224e-17	-2.00
Cu2(OH)2+2	2.024e-17	1.012e-17	2.00
Cu(OH)3-	1.608e-17	5.360e-18	3.00
FeF+2	-1.481e-17	7.406e-18	-2.00
Fe(OH)3-	3.724e-18	1.241e-18	3.00
FeF3	-2.242e-18	1.121e-18	-2.00
Pb(OH)3-	1.510e-18	5.032e-19	3.00
Fe+3	-2.271e-19	1.136e-19	-2.00
FeH2PO4+2	-1.367e-19	6.836e-20	-2.00
Pb2OH+3	8.171e-20	8.171e-20	1.00
AlHSO4+2	-7.530e-20	7.530e-20	-1.00
Cd2OH+3	6.189e-20	6.189e-20	1.00
FeSO4+	-2.786e-20	1.393e-20	-2.00
FeHPO4+	-1.091e-20	1.091e-20	-1.00
NaOH	8.453e-21	8.453e-21	1.00
Zn(OH)4-2	4.033e-21	1.008e-21	4.00
BF4-	-2.702e-21	9.007e-22	-3.00
FeCl+2	-2.294e-21	1.147e-21	-2.00
Cd(OH)3-	2.415e-22	8.049e-23	3.00
Mn(OH)3-	1.063e-22	3.544e-23	3.00
Pb(OH)4-2	1.863e-23	4.657e-24	4.00
Cu(OH)4-2	1.728e-23	4.320e-24	4.00
Fe(SO4)2-	-1.204e-23	6.021e-24	-2.00
FeCl2+	-3.605e-24	1.802e-24	-2.00
FeHSO4+2	-4.528e-26	1.509e-26	-3.00
Pb3(OH)4+2	3.938e-27	9.844e-28	4.00
Fe2(OH)2+4	-3.025e-28	1.512e-28	-2.00
FeCl3	-1.524e-28	7.622e-29	-2.00
Cd(OH)4-2	1.159e-29	2.898e-30	4.00
Fe3(OH)4+5	-1.657e-37	8.283e-38	-2.00

-------------------------------Saturation indices--------------------------------

Phase	SI**	log IAP	log K(298 K, 1 atm)	
Al(OH)3(a)	-1.76	8.99	10.75	Al(OH)3
Alunite	-4.58	-6.08	-1.50	KAl3(SO4)2(OH)6
Anglesite	-6.69	-14.48	-7.79	PbSO4
Anhydrite	-3.71	-7.99	-4.29	CaSO4
Aragonite	-1.17	-9.51	-8.34	CaCO3
BaCl2	-14.02	-11.79	2.22	BaCl2
BaCl2:2H2O	-12.01	-11.79	0.21	BaCl2:2H2O
BaCl2:H2O	-12.62	-11.79	0.83	BaCl2:H2O
Barite	0.01	-9.82	-9.84	BaSO4
Calcite	-1.03	-9.51	-8.48	CaCO3
Cd(OH)2	-8.98	4.67	13.65	Cd(OH)2

CdSO4	-12.91	-13.04	-0.13	CdSO4
Cerussite	-2.88	-16.00	-13.12	PbCO3
CO2(g)	-1.08	-2.56	-1.48	CO2
Dolomite	-2.34	-19.45	-17.11	CaMg(CO3)2
Fe(OH)3(a)	-4.62	0.27	4.89	Fe(OH)3
Fluorite	-1.18	-11.77	-10.59	CaF2
Gibbsite	0.92	8.99	8.07	Al(OH)3
Goethite	1.30	0.27	-1.03	FeOOH
Gypsum	-3.41	-7.99	-4.58	CaSO4:2H2O
H2(g)	-13.59	-16.69	-3.10	H2
H2O(g)	-1.48	-0.00	1.48	H2O
Halite	-7.51	-5.94	1.57	NaCl
Hausmannite	-29.85	30.98	60.83	Mn3O4
Hematite	4.60	0.54	-4.07	Fe2O3
Hydroxyapatite	-5.55	-9.04	-3.49	Ca5(PO4)3OH
Jarosite-K	-22.96	-32.23	-9.27	KFe3(SO4)2(OH)6
Manganite	-12.76	12.58	25.34	MnOOH
Melanterite	-9.01	-11.21	-2.20	FeSO4:7H2O
O2(g)	-55.84	-58.74	-2.90	O2
Otavite	-2.46	-14.56	-12.10	CdCO3
Pb(OH)2	-4.90	3.23	8.12	Pb(OH)2
Pyrochroite	-9.39	5.81	15.20	Mn(OH)2
Pyrolusite	-21.90	19.35	41.25	MnO2:H2O
Rhodochrosite	-2.28	-13.41	-11.13	MnCO3
Siderite	-1.83	-12.73	-10.89	FeCO3
Smithsonite	-2.16	-12.17	-10.01	ZnCO3
Sylvite	-8.37	-7.46	0.90	KCl
Vivianite	-7.59	-43.59	-36.00	Fe3(PO4)2:8H2O
Witherite	-2.78	-11.34	-8.56	BaCO3
Zn(OH)2(e)	-4.44	7.06	11.50	Zn(OH)2

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
For ideal gases, phi = 1.

Initial solution 19.

-----------------------------Solution composition-----------------------------

Elements	Molality	Moles
Al	1.946e-06	1.946e-06
Alkalinity	7.698e-04	7.698e-04
B	1.170e-05	1.170e-05
Ba	5.826e-06	5.826e-06
Br	2.128e-06	2.128e-06
Ca	2.146e-04	2.146e-04
Cd	7.830e-09	7.830e-09
Cl	2.595e-04	2.595e-04
Cu	3.195e-08	3.195e-08
F	5.685e-05	5.685e-05
Fe	7.068e-07	7.068e-07
K	6.394e-05	6.394e-05
Mg	1.156e-04	1.156e-04
Mn	9.202e-07	9.202e-07
N(3)	1.428e-06	1.428e-06
N(5)	3.299e-04	3.299e-04
Na	5.786e-04	5.786e-04
P	9.687e-08	9.687e-08
Pb	7.723e-10	7.723e-10
S(6)	1.353e-04	1.353e-04
Zn	1.687e-06	1.687e-06

----------------------------Description of solution----------------------------

pH = 4.400
pe = 0.227
Specific Conductance (µS/cm, 26°C) = 184
Density (g/cm³) = 0.99747

```
                              Volume (L)  =   1.00568
                       Activity of water  =   0.999
                  Ionic strength (mol/kgw)  =   1.988e-03
                        Mass of water (kg)  =   1.000e+00
                     Total carbon (mol/kg)  =   6.923e-02
                        Total CO2 (mol/kg)  =   6.923e-02
                          Temperature (°C)  =  26.22
                   Electrical balance (eq)  =  -3.633e-04
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  = -11.88
                                Iterations  =  10 (199 overall)
                                   Total H  = 1.110133e+02
                                   Total O  = 5.564707e+01
```

----------Redox couples----------

Redox couple	pe	Eh (volts)
N(3)/N(5)	11.0017	0.6535

----------Distribution of species----------

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma	mole V cm³/mol
H+	4.170e-05	3.981e-05	-4.380	-4.400	-0.020	0.00
OH-	2.928e-10	2.785e-10	-9.533	-9.555	-0.022	-4.05
H2O	5.551e+01	9.988e-01	1.744	-0.001	0.000	18.08
Al	1.946e-06					
AlF2+	1.200e-06	1.144e-06	-5.921	-5.942	-0.021	(0)
AlF3	6.735e-07	6.738e-07	-6.172	-6.171	0.000	(0)
AlF+2	5.891e-08	4.850e-08	-7.230	-7.314	-0.084	(0)
AlF4-	1.318e-08	1.254e-08	-7.880	-7.902	-0.021	(0)
Al+3	1.563e-10	1.030e-10	-9.806	-9.987	-0.181	-42.28
AlSO4+	3.675e-11	3.498e-11	-10.435	-10.456	-0.021	(0)
AlOH+2	3.374e-11	2.778e-11	-10.472	-10.556	-0.084	-27.76
Al(OH)2+	6.373e-12	6.071e-12	-11.196	-11.217	-0.021	(0)
Al(SO4)2-	1.236e-13	1.176e-13	-12.908	-12.929	-0.021	(0)
Al(OH)3	2.452e-14	2.453e-14	-13.611	-13.610	0.000	(0)
Al(OH)4-	1.239e-15	1.180e-15	-14.907	-14.928	-0.021	(0)
AlHSO4+2	1.522e-16	1.249e-16	-15.818	-15.904	-0.086	(0)
B	1.170e-05					
H3BO3	1.170e-05	1.171e-05	-4.932	-4.932	0.000	39.32
BF(OH)3-	2.319e-10	2.207e-10	-9.635	-9.656	-0.022	(0)
H2BO3-	1.818e-10	1.730e-10	-9.740	-9.762	-0.022	(0)
BF2(OH)2-	4.623e-11	4.400e-11	-10.335	-10.357	-0.022	(0)
BF3OH-	9.238e-14	8.792e-14	-13.034	-13.056	-0.022	(0)
BF4-	7.002e-16	6.663e-16	-15.155	-15.176	-0.022	(0)
Ba	5.826e-06					
Ba+2	5.544e-06	4.550e-06	-5.256	-5.342	-0.086	-12.64
BaSO4	2.410e-07	2.411e-07	-6.618	-6.618	0.000	(0)
BaHCO3+	3.681e-08	3.503e-08	-7.434	-7.456	-0.022	(0)
BaCl+	3.770e-09	3.588e-09	-8.424	-8.445	-0.022	(0)
BaNO3+	1.888e-10	1.797e-10	-9.724	-9.745	-0.022	(0)
BaCO3	2.246e-12	2.247e-12	-11.649	-11.648	0.000	-10.69
BaOH+	4.062e-15	3.868e-15	-14.391	-14.413	-0.021	(0)
Br	2.128e-06					
Br-	2.128e-06	2.023e-06	-5.672	-5.694	-0.022	24.62
CdBr+	1.881e-12	1.790e-12	-11.726	-11.747	-0.022	(0)
ZnBr+	7.014e-13	6.675e-13	-12.154	-12.176	-0.022	(0)
PbBr+	5.040e-14	4.796e-14	-13.298	-13.319	-0.022	(0)
CdBr2	1.955e-17	1.956e-17	-16.709	-16.709	0.000	(0)
ZnBr2	5.375e-19	5.377e-19	-18.270	-18.269	0.000	(0)
PbBr2	4.448e-20	4.450e-20	-19.352	-19.352	0.000	(0)
C(4)	6.923e-02					
CO2	6.824e-02	6.827e-02	-1.166	-1.166	0.000	34.49
HCO3-	8.116e-04	7.730e-04	-3.091	-3.112	-0.021	24.78
(CO2)2	8.901e-05	8.905e-05	-4.051	-4.050	0.000	68.98
CaHCO3+	1.817e-06	1.732e-06	-5.741	-5.762	-0.021	9.73

MgHCO3+	8.827e-07	8.400e-07	-6.054	-6.076	-0.022	5.52
NaHCO3	2.371e-07	2.372e-07	-6.625	-6.625	0.000	1.80
ZnHCO3+	1.283e-07	1.221e-07	-6.892	-6.913	-0.022	(0)
MnHCO3+	5.098e-08	4.855e-08	-7.293	-7.314	-0.021	(0)
FeHCO3+	4.369e-08	4.158e-08	-7.360	-7.381	-0.022	(0)
BaHCO3+	3.681e-08	3.503e-08	-7.434	-7.456	-0.022	(0)
CO3-2	1.133e-09	9.330e-10	-8.946	-9.030	-0.084	-5.14
CaCO3	2.769e-10	2.771e-10	-9.558	-9.557	0.000	-14.59
PbHCO3+	2.546e-10	2.423e-10	-9.594	-9.616	-0.022	(0)
ZnCO3	2.334e-10	2.335e-10	-9.632	-9.632	0.000	(0)
CdHCO3+	1.545e-10	1.470e-10	-9.811	-9.833	-0.022	(0)
MgCO3	8.373e-11	8.377e-11	-10.077	-10.077	0.000	-17.09
MnCO3	5.220e-11	5.222e-11	-10.282	-10.282	0.000	(0)
CuHCO3+	3.836e-11	3.651e-11	-10.416	-10.438	-0.022	(0)
FeCO3	1.203e-11	1.204e-11	-10.920	-10.919	0.000	(0)
NaCO3-	1.067e-11	1.015e-11	-10.972	-10.994	-0.022	-0.91
PbCO3	6.395e-12	6.398e-12	-11.194	-11.194	0.000	(0)
BaCO3	2.246e-12	2.247e-12	-11.649	-11.648	0.000	-10.69
CuCO3	4.719e-13	4.721e-13	-12.326	-12.326	0.000	(0)
Zn(CO3)2-2	5.677e-15	4.657e-15	-14.246	-14.332	-0.086	(0)
CdCO3	4.454e-15	4.456e-15	-14.351	-14.351	0.000	(0)
Pb(CO3)2-2	1.828e-17	1.499e-17	-16.738	-16.824	-0.086	(0)
Cu(CO3)2-2	6.761e-19	5.545e-19	-18.170	-18.256	-0.086	(0)
Cd(CO3)2-2	1.603e-20	1.315e-20	-19.795	-19.881	-0.086	(0)
Ca	2.146e-04					
Ca+2	2.095e-04	1.724e-04	-3.679	-3.763	-0.085	-18.09
CaSO4	3.270e-06	3.272e-06	-5.485	-5.485	0.000	7.55
CaHCO3+	1.817e-06	1.732e-06	-5.741	-5.762	-0.021	9.73
CaHSO4+	9.157e-10	8.715e-10	-9.038	-9.060	-0.022	(0)
CaH2PO4+	4.307e-10	4.103e-10	-9.366	-9.387	-0.021	(0)
CaCO3	2.769e-10	2.771e-10	-9.558	-9.557	0.000	-14.59
CaHPO4	1.379e-11	1.380e-11	-10.860	-10.860	0.000	(0)
CaOH+	7.543e-13	7.179e-13	-12.122	-12.144	-0.022	(0)
CaPO4-	8.806e-16	8.388e-16	-15.055	-15.076	-0.021	(0)
Cd	7.830e-09					
Cd+2	7.331e-09	6.013e-09	-8.135	-8.221	-0.086	-18.65
CdSO4	1.847e-10	1.848e-10	-9.734	-9.733	0.000	77.46
CdHCO3+	1.545e-10	1.470e-10	-9.811	-9.833	-0.022	(0)
CdCl+	1.491e-10	1.419e-10	-9.826	-9.848	-0.022	6.16
CdNO3+	4.804e-12	4.572e-12	-11.318	-11.340	-0.022	17.49
CdF+	3.719e-12	3.539e-12	-11.430	-11.451	-0.022	(0)
CdBr+	1.881e-12	1.790e-12	-11.726	-11.747	-0.022	(0)
Cd(SO4)2-2	2.592e-13	2.126e-13	-12.586	-12.672	-0.086	-104.85
CdCl2	1.462e-13	1.463e-13	-12.835	-12.835	0.000	23.14
CdOH+	1.443e-14	1.373e-14	-13.841	-13.862	-0.022	(0)
CdCO3	4.454e-15	4.456e-15	-14.351	-14.351	0.000	(0)
CdOHCl	1.509e-15	1.509e-15	-14.821	-14.821	0.000	(0)
CdF2	4.154e-16	4.156e-16	-15.382	-15.381	0.000	(0)
CdCl3-	2.431e-17	2.314e-17	-16.614	-16.636	-0.022	68.47
CdBr2	1.955e-17	1.956e-17	-16.709	-16.709	0.000	(0)
Cd(OH)2	1.690e-20	1.691e-20	-19.772	-19.772	0.000	(0)
Cd(CO3)2-2	1.603e-20	1.315e-20	-19.795	-19.881	-0.086	(0)
Cd2OH+3	6.221e-22	3.983e-22	-21.206	-21.400	-0.194	(0)
Cd(OH)3-	5.001e-29	4.759e-29	-28.301	-28.322	-0.022	(0)
Cd(OH)4-2	1.297e-38	1.064e-38	-37.887	-37.973	-0.086	(0)
Cl	2.595e-04					
Cl-	2.587e-04	2.461e-04	-3.587	-3.609	-0.022	18.12
NaCl	8.160e-07	8.164e-07	-6.088	-6.088	0.000	(0)
BaCl+	3.770e-09	3.588e-09	-8.424	-8.445	-0.022	(0)
ZnCl+	9.212e-10	8.767e-10	-9.036	-9.057	-0.022	-12.72
MnCl+	7.420e-10	7.066e-10	-9.130	-9.151	-0.021	-2.79
CuCl2-	5.954e-10	5.666e-10	-9.225	-9.247	-0.022	(0)
FeCl+	1.920e-10	1.827e-10	-9.717	-9.738	-0.022	(0)
CdCl+	1.491e-10	1.419e-10	-9.826	-9.848	-0.022	6.16
PbCl+	4.188e-12	3.985e-12	-11.378	-11.400	-0.022	8.01
CuCl3-2	2.700e-13	2.221e-13	-12.569	-12.654	-0.085	(0)
ZnOHCl	2.564e-13	2.565e-13	-12.591	-12.591	0.000	(0)
ZnCl2	2.270e-13	2.271e-13	-12.644	-12.644	0.000	99.69

CdCl2	1.462e-13	1.463e-13	-12.835	-12.835	0.000	23.14
MnCl2	7.589e-14	7.592e-14	-13.120	-13.120	0.000	84.42
CuCl+	6.962e-14	6.626e-14	-13.157	-13.179	-0.022	0.33
PbCl2	1.519e-15	1.520e-15	-14.818	-14.818	0.000	35.07
CdOHCl	1.509e-15	1.509e-15	-14.821	-14.821	0.000	(0)
ZnCl3-	6.638e-17	6.317e-17	-16.178	-16.199	-0.022	17.10
CdCl3-	2.431e-17	2.314e-17	-16.614	-16.636	-0.022	68.47
CuCl2	8.870e-18	8.874e-18	-17.052	-17.052	0.000	32.40
MnCl3-	5.405e-18	5.147e-18	-17.267	-17.288	-0.021	43.31
PbCl3-	3.146e-19	2.994e-19	-18.502	-18.524	-0.022	66.11
ZnCl4-2	9.568e-21	7.868e-21	-20.019	-20.104	-0.085	145.37
FeCl+2	8.698e-22	7.153e-22	-21.061	-21.146	-0.085	(0)
PbCl4-2	4.341e-23	3.560e-23	-22.362	-22.448	-0.086	101.58
CuCl3-	8.322e-24	7.919e-24	-23.080	-23.101	-0.022	(0)
FeCl2+	7.947e-25	7.568e-25	-24.100	-24.121	-0.021	(0)
FeCl3	1.862e-29	1.863e-29	-28.730	-28.730	0.000	(0)
CuCl4-2	1.222e-29	1.005e-29	-28.913	-28.998	-0.085	(0)
Cu(1)	3.179e-08					
Cu+	3.120e-08	2.966e-08	-7.506	-7.528	-0.022	(0)
CuCl2-	5.954e-10	5.666e-10	-9.225	-9.247	-0.022	(0)
CuCl3-2	2.700e-13	2.221e-13	-12.569	-12.654	-0.085	(0)
Cu(2)	1.554e-10					
Cu+2	1.143e-10	9.423e-11	-9.942	-10.026	-0.084	-26.58
CuHCO3+	3.836e-11	3.651e-11	-10.416	-10.438	-0.022	(0)
CuSO4	2.051e-12	2.052e-12	-11.688	-11.688	0.000	13.24
CuCO3	4.719e-13	4.721e-13	-12.326	-12.326	0.000	(0)
CuF+	8.518e-14	8.106e-14	-13.070	-13.091	-0.022	(0)
CuCl+	6.962e-14	6.626e-14	-13.157	-13.179	-0.022	0.33
CuOH+	2.484e-14	2.364e-14	-13.605	-13.626	-0.022	(0)
Cu(OH)2	1.239e-15	1.239e-15	-14.907	-14.907	0.000	(0)
CuCl2	8.870e-18	8.874e-18	-17.052	-17.052	0.000	32.40
Cu(CO3)2-2	6.761e-19	5.545e-19	-18.170	-18.256	-0.086	(0)
Cu2(OH)2+2	3.364e-22	2.759e-22	-21.473	-21.559	-0.086	(0)
CuCl3-	8.322e-24	7.919e-24	-23.080	-23.101	-0.022	(0)
Cu(OH)3-	1.969e-24	1.873e-24	-23.706	-23.727	-0.022	(0)
CuCl4-2	1.222e-29	1.005e-29	-28.913	-28.998	-0.085	(0)
Cu(OH)4-2	1.143e-32	9.378e-33	-31.942	-32.028	-0.086	(0)
F	5.685e-05					
F-	4.914e-05	4.675e-05	-4.309	-4.330	-0.022	-1.29
HF	2.852e-06	2.853e-06	-5.545	-5.545	0.000	12.55
AlF2+	1.200e-06	1.144e-06	-5.921	-5.942	-0.021	(0)
AlF3	6.735e-07	6.738e-07	-6.172	-6.171	0.000	(0)
MgF+	3.063e-07	2.916e-07	-6.514	-6.535	-0.021	-10.57
AlF+2	5.891e-08	4.850e-08	-7.230	-7.314	-0.084	(0)
NaF	1.478e-08	1.478e-08	-7.830	-7.830	0.000	7.31
AlF4-	1.318e-08	1.254e-08	-7.880	-7.902	-0.021	(0)
ZnF+	8.837e-10	8.410e-10	-9.054	-9.075	-0.022	(0)
HF2-	5.428e-10	5.166e-10	-9.265	-9.287	-0.022	22.13
FeF+	2.642e-10	2.514e-10	-9.578	-9.600	-0.022	(0)
MnF+	2.393e-10	2.279e-10	-9.621	-9.642	-0.021	(0)
BF(OH)3-	2.319e-10	2.207e-10	-9.635	-9.656	-0.022	(0)
BF2(OH)2-	4.623e-11	4.400e-11	-10.335	-10.357	-0.022	(0)
CdF+	3.719e-12	3.539e-12	-11.430	-11.451	-0.022	(0)
PbF+	3.447e-13	3.281e-13	-12.463	-12.484	-0.022	(0)
BF3OH-	9.238e-14	8.792e-14	-13.034	-13.056	-0.022	(0)
CuF+	8.518e-14	8.106e-14	-13.070	-13.091	-0.022	(0)
BF4-	7.002e-16	6.663e-16	-15.155	-15.176	-0.022	(0)
CdF2	4.154e-16	4.156e-16	-15.382	-15.381	0.000	(0)
PbF2	3.130e-16	3.132e-16	-15.504	-15.504	0.000	(0)
FeF2+	1.386e-17	1.320e-17	-16.858	-16.880	-0.021	(0)
FeF+2	8.499e-18	6.989e-18	-17.071	-17.156	-0.085	(0)
FeF3	9.814e-19	9.819e-19	-18.008	-18.008	0.000	(0)
PbF3-	1.114e-19	1.061e-19	-18.953	-18.974	-0.022	(0)
PbF4-2	2.893e-24	2.373e-24	-23.539	-23.625	-0.086	(0)
Fe(2)	7.068e-07					
Fe+2	6.523e-07	5.378e-07	-6.186	-6.269	-0.084	-22.02
FeHCO3+	4.369e-08	4.158e-08	-7.360	-7.381	-0.022	(0)
FeSO4	1.034e-08	1.034e-08	-7.986	-7.985	0.000	17.72

FeF+	2.642e-10	2.514e-10	-9.578	-9.600	-0.022	(0)
FeCl+	1.920e-10	1.827e-10	-9.717	-9.738	-0.022	(0)
FeH2PO4+	2.571e-11	2.449e-11	-10.590	-10.611	-0.021	(0)
FeCO3	1.203e-11	1.204e-11	-10.920	-10.919	0.000	(0)
FeOH+	4.907e-12	4.673e-12	-11.309	-11.330	-0.021	(0)
FeHSO4+	2.856e-12	2.718e-12	-11.544	-11.566	-0.022	(0)
FeHPO4	3.053e-13	3.054e-13	-12.515	-12.515	0.000	(0)
Fe(OH)2	1.108e-18	1.109e-18	-17.955	-17.955	0.000	(0)
Fe(OH)3-	1.099e-24	1.046e-24	-23.959	-23.980	-0.021	(0)
Fe(3)	1.908e-16					
Fe(OH)2+	1.471e-16	1.402e-16	-15.832	-15.853	-0.021	(0)
FeOH+2	1.959e-17	1.611e-17	-16.708	-16.793	-0.085	(0)
FeF2+	1.386e-17	1.320e-17	-16.858	-16.880	-0.021	(0)
FeF+2	8.499e-18	6.989e-18	-17.071	-17.156	-0.085	(0)
FeF3	9.814e-19	9.819e-19	-18.008	-18.008	0.000	(0)
Fe(OH)3	4.774e-19	4.776e-19	-18.321	-18.321	0.000	(0)
Fe+3	1.405e-19	9.259e-20	-18.852	-19.033	-0.181	(0)
FeSO4+	1.158e-19	1.103e-19	-18.936	-18.957	-0.021	(0)
FeH2PO4+2	2.750e-21	2.264e-21	-20.561	-20.645	-0.084	(0)
FeCl+2	8.698e-22	7.153e-22	-21.061	-21.146	-0.085	(0)
Fe(SO4)2-	2.694e-22	2.564e-22	-21.570	-21.591	-0.022	(0)
FeHSO4+2	1.433e-23	1.176e-23	-22.844	-22.930	-0.086	(0)
Fe(OH)4-	1.205e-23	1.148e-23	-22.919	-22.940	-0.021	(0)
FeHPO4+	3.884e-24	3.699e-24	-23.411	-23.432	-0.021	(0)
FeCl2+	7.947e-25	7.568e-25	-24.100	-24.121	-0.021	(0)
FeCl3	1.862e-29	1.863e-29	-28.730	-28.730	0.000	(0)
Fe2(OH)2+4	1.468e-32	6.644e-33	-31.833	-32.178	-0.344	(0)
Fe3(OH)4+5	0.000e+00	0.000e+00	-45.222	-45.760	-0.538	(0)
H(0)	7.791e-13					
H2	3.895e-13	3.897e-13	-12.409	-12.409	0.000	28.60
K	6.394e-05					
K+	6.389e-05	6.079e-05	-4.195	-4.216	-0.022	9.06
KSO4-	4.843e-08	4.613e-08	-7.315	-7.336	-0.021	34.15
KHPO4-	1.775e-14	1.691e-14	-13.751	-13.772	-0.021	38.04
Mg	1.156e-04					
Mg+2	1.120e-04	9.235e-05	-3.951	-4.035	-0.084	-21.83
MgSO4	2.361e-06	2.362e-06	-5.627	-5.627	0.000	5.88
MgHCO3+	8.827e-07	8.400e-07	-6.054	-6.076	-0.022	5.52
MgF+	3.063e-07	2.916e-07	-6.514	-6.535	-0.021	-10.57
MgH2PO4+	2.938e-10	2.798e-10	-9.532	-9.553	-0.021	(0)
MgCO3	8.373e-11	8.377e-11	-10.077	-10.077	0.000	-17.09
MgHPO4	9.985e-12	9.990e-12	-11.001	-11.000	0.000	(0)
MgOH+	9.848e-12	9.387e-12	-11.007	-11.027	-0.021	(0)
MgPO4-	6.362e-16	6.061e-16	-15.196	-15.217	-0.021	(0)
Mn(2)	9.202e-07					
Mn+2	8.546e-07	7.047e-07	-6.068	-6.152	-0.084	-20.70
MnHCO3+	5.098e-08	4.855e-08	-7.293	-7.314	-0.021	(0)
MnSO4	1.356e-08	1.356e-08	-7.868	-7.868	0.000	22.01
MnCl+	7.420e-10	7.066e-10	-9.130	-9.151	-0.021	-2.79
MnF+	2.393e-10	2.279e-10	-9.621	-9.642	-0.021	(0)
MnCO3	5.220e-11	5.222e-11	-10.282	-10.282	0.000	(0)
MnOH+	5.269e-13	5.017e-13	-12.278	-12.300	-0.021	(0)
Mn(NO3)2	2.752e-13	2.753e-13	-12.560	-12.560	0.000	40.72
MnCl2	7.589e-14	7.592e-14	-13.120	-13.120	0.000	84.42
MnCl3-	5.405e-18	5.147e-18	-17.267	-17.288	-0.021	43.31
Mn(OH)3-	1.852e-28	1.764e-28	-27.732	-27.754	-0.021	(0)
Mn(3)	6.657e-32					
Mn+3	6.657e-32	4.386e-32	-31.177	-31.358	-0.181	(0)
N(3)	1.428e-06					
NO2-	1.428e-06	1.358e-06	-5.845	-5.867	-0.022	25.04
N(5)	3.299e-04					
NO3-	3.299e-04	3.137e-04	-3.482	-3.503	-0.022	29.61
BaNO3+	1.888e-10	1.797e-10	-9.724	-9.745	-0.022	(0)
CdNO3+	4.804e-12	4.572e-12	-11.318	-11.340	-0.022	17.49
PbNO3+	1.924e-12	1.831e-12	-11.716	-11.737	-0.022	(0)
Mn(NO3)2	2.752e-13	2.753e-13	-12.560	-12.560	0.000	40.72
Na	5.786e-04					
Na+	5.772e-04	5.495e-04	-3.239	-3.260	-0.021	-1.40

NaCl	8.160e-07	8.164e-07	-6.088	-6.088	0.000	(0)
NaSO4-	3.081e-07	2.935e-07	-6.511	-6.532	-0.021	13.80
NaHCO3	2.371e-07	2.372e-07	-6.625	-6.625	0.000	1.80
NaF	1.478e-08	1.478e-08	-7.830	-7.830	0.000	7.31
NaCO3-	1.067e-11	1.015e-11	-10.972	-10.994	-0.022	-0.91
NaHPO4-	1.605e-13	1.529e-13	-12.795	-12.816	-0.021	33.54
NaOH	1.530e-23	1.531e-23	-22.815	-22.815	0.000	(0)
O(0)	0.000e+00					
O2	0.000e+00	0.000e+00	-67.171	-67.170	0.000	30.50
P	9.687e-08					
H2PO4-	9.538e-08	9.085e-08	-7.021	-7.042	-0.021	33.19
H3PO4	5.400e-10	5.403e-10	-9.268	-9.267	0.000	47.47
CaH2PO4+	4.307e-10	4.103e-10	-9.366	-9.387	-0.021	(0)
MgH2PO4+	2.938e-10	2.798e-10	-9.532	-9.553	-0.021	(0)
HPO4-2	1.735e-10	1.427e-10	-9.761	-9.846	-0.085	6.72
FeH2PO4+	2.571e-11	2.449e-11	-10.590	-10.611	-0.021	(0)
CaHPO4	1.379e-11	1.380e-11	-10.860	-10.860	0.000	(0)
MgHPO4	9.985e-12	9.990e-12	-11.001	-11.000	0.000	(0)
FeHPO4	3.053e-13	3.054e-13	-12.515	-12.515	0.000	(0)
NaHPO4-	1.605e-13	1.529e-13	-12.795	-12.816	-0.021	33.54
KHPO4-	1.775e-14	1.691e-14	-13.751	-13.772	-0.021	38.04
CaPO4-	8.806e-16	8.388e-16	-15.055	-15.076	-0.021	(0)
MgPO4-	6.362e-16	6.061e-16	-15.196	-15.217	-0.021	(0)
PO4-3	2.586e-18	1.655e-18	-17.587	-17.781	-0.194	-23.24
FeH2PO4+2	2.750e-21	2.264e-21	-20.561	-20.645	-0.084	(0)
FeHPO4+	3.884e-24	3.699e-24	-23.411	-23.432	-0.021	(0)
Pb	7.723e-10					
Pb+2	4.811e-10	3.946e-10	-9.318	-9.404	-0.086	-15.51
PbHCO3+	2.546e-10	2.423e-10	-9.594	-9.616	-0.022	(0)
PbSO4	2.346e-11	2.347e-11	-10.630	-10.630	0.000	(0)
PbCO3	6.395e-12	6.398e-12	-11.194	-11.194	0.000	(0)
PbCl+	4.188e-12	3.985e-12	-11.378	-11.400	-0.022	8.01
PbNO3+	1.924e-12	1.831e-12	-11.716	-11.737	-0.022	(0)
PbF+	3.447e-13	3.281e-13	-12.463	-12.484	-0.022	(0)
PbOH+	2.029e-13	1.930e-13	-12.693	-12.714	-0.022	(0)
PbBr+	5.040e-14	4.796e-14	-13.298	-13.319	-0.022	(0)
Pb(SO4)2-2	1.588e-14	1.302e-14	-13.799	-13.885	-0.086	(0)
PbCl2	1.519e-15	1.520e-15	-14.818	-14.818	0.000	35.07
PbF2	3.130e-16	3.132e-16	-15.504	-15.504	0.000	(0)
Pb(CO3)2-2	1.828e-17	1.499e-17	-16.738	-16.824	-0.086	(0)
Pb(OH)2	1.883e-18	1.884e-18	-17.725	-17.725	0.000	(0)
PbCl3-	3.146e-19	2.994e-19	-18.502	-18.524	-0.022	66.11
PbF3-	1.114e-19	1.061e-19	-18.953	-18.974	-0.022	(0)
PbBr2	4.448e-20	4.450e-20	-19.352	-19.352	0.000	(0)
Pb2OH+3	2.664e-21	1.706e-21	-20.575	-20.768	-0.194	(0)
PbCl4-2	4.341e-23	3.560e-23	-22.362	-22.448	-0.086	101.58
PbF4-2	2.893e-24	2.373e-24	-23.539	-23.625	-0.086	(0)
Pb(OH)3-	5.703e-25	5.428e-25	-24.244	-24.265	-0.022	(0)
Pb(OH)4-2	3.803e-32	3.120e-32	-31.420	-31.506	-0.086	(0)
Pb3(OH)4+2	4.695e-35	3.852e-35	-34.328	-34.414	-0.086	(0)
S(6)	1.353e-04					
SO4-2	1.286e-04	1.057e-04	-3.891	-3.976	-0.085	14.71
CaSO4	3.270e-06	3.272e-06	-5.485	-5.485	0.000	7.55
MgSO4	2.361e-06	2.362e-06	-5.627	-5.627	0.000	5.88
HSO4-	4.417e-07	4.204e-07	-6.355	-6.376	-0.022	40.37
NaSO4-	3.081e-07	2.935e-07	-6.511	-6.532	-0.021	13.80
BaSO4	2.410e-07	2.411e-07	-6.618	-6.618	0.000	(0)
KSO4-	4.843e-08	4.613e-08	-7.315	-7.336	-0.021	34.15
ZnSO4	3.137e-08	3.138e-08	-7.503	-7.503	0.000	21.52
MnSO4	1.356e-08	1.356e-08	-7.868	-7.868	0.000	22.01
FeSO4	1.034e-08	1.034e-08	-7.986	-7.985	0.000	17.72
CaHSO4+	9.157e-10	8.715e-10	-9.038	-9.060	-0.022	(0)
CdSO4	1.847e-10	1.848e-10	-9.734	-9.733	0.000	77.46
AlSO4+	3.675e-11	3.498e-11	-10.435	-10.456	-0.021	(0)
Zn(SO4)2-2	3.258e-11	2.672e-11	-10.487	-10.573	-0.086	-12.07
PbSO4	2.346e-11	2.347e-11	-10.630	-10.630	0.000	(0)
FeHSO4+	2.856e-12	2.718e-12	-11.544	-11.566	-0.022	(0)
CuSO4	2.051e-12	2.052e-12	-11.688	-11.688	0.000	13.24

Cd(SO4)2-2	2.592e-13	2.126e-13	-12.586	-12.672	-0.086	-104.85
Al(SO4)2-	1.236e-13	1.176e-13	-12.908	-12.929	-0.021	(0)
Pb(SO4)2-2	1.588e-14	1.302e-14	-13.799	-13.885	-0.086	(0)
AlHSO4+2	1.522e-16	1.249e-16	-15.818	-15.904	-0.086	(0)
FeSO4+	1.158e-19	1.103e-19	-18.936	-18.957	-0.021	(0)
Fe(SO4)2-	2.694e-22	2.564e-22	-21.570	-21.591	-0.022	(0)
FeHSO4+2	1.433e-23	1.176e-23	-22.844	-22.930	-0.086	(0)
Zn 1.687e-06						
Zn+2	1.525e-06	1.254e-06	-5.817	-5.902	-0.085	-25.40
ZnHCO3+	1.283e-07	1.221e-07	-6.892	-6.913	-0.022	(0)
ZnSO4	3.137e-08	3.138e-08	-7.503	-7.503	0.000	21.52
ZnCl+	9.212e-10	8.767e-10	-9.036	-9.057	-0.022	-12.72
ZnF+	8.837e-10	8.410e-10	-9.054	-9.075	-0.022	(0)
ZnCO3	2.334e-10	2.335e-10	-9.632	-9.632	0.000	(0)
ZnOH+	3.975e-11	3.783e-11	-10.401	-10.422	-0.022	(0)
Zn(SO4)2-2	3.258e-11	2.672e-11	-10.487	-10.573	-0.086	-12.07
ZnBr+	7.014e-13	6.675e-13	-12.154	-12.176	-0.022	(0)
ZnOHCl	2.564e-13	2.565e-13	-12.591	-12.591	0.000	(0)
ZnCl2	2.270e-13	2.271e-13	-12.644	-12.644	0.000	99.69
Zn(OH)2	9.934e-15	9.939e-15	-14.003	-14.003	0.000	(0)
Zn(CO3)2-2	5.677e-15	4.657e-15	-14.246	-14.332	-0.086	(0)
ZnCl3-	6.638e-17	6.317e-17	-16.178	-16.199	-0.022	17.10
ZnBr2	5.375e-19	5.377e-19	-18.270	-18.269	0.000	(0)
ZnCl4-2	9.568e-21	7.868e-21	-20.019	-20.104	-0.085	145.37
Zn(OH)3-	8.285e-22	7.885e-22	-21.082	-21.103	-0.022	(0)
Zn(OH)4-2	3.822e-30	3.135e-30	-29.418	-29.504	-0.086	(0)

----------Distribution of alkalinity----------

Total alkalinity (eq/kgw) = 7.698e-04

Species	Alkalinity	Molality	Alk/Mol
HCO3-	8.116e-04	8.116e-04	1.00
H+	-4.170e-05	4.170e-05	-1.00
HF	-2.852e-06	2.852e-06	-1.00
CaHCO3+	1.817e-06	1.817e-06	1.00
MgHCO3+	8.827e-07	8.827e-07	1.00
HSO4-	-4.417e-07	4.417e-07	-1.00
NaHCO3	2.371e-07	2.371e-07	1.00
ZnHCO3+	1.283e-07	1.283e-07	1.00
MnHCO3+	5.098e-08	5.098e-08	1.00
FeHCO3+	4.369e-08	4.369e-08	1.00
BaHCO3+	3.681e-08	3.681e-08	1.00
CO3-2	2.267e-09	1.133e-09	2.00
CaHSO4+	-9.157e-10	9.157e-10	-1.00
CaCO3	5.539e-10	2.769e-10	2.00
HF2-	-5.428e-10	5.428e-10	-1.00
H3PO4	-5.400e-10	5.400e-10	-1.00
ZnCO3	4.667e-10	2.334e-10	2.00
OH-	2.928e-10	2.928e-10	1.00
PbHCO3+	2.546e-10	2.546e-10	1.00
H2BO3-	1.818e-10	1.818e-10	1.00
HPO4-2	1.735e-10	1.735e-10	1.00
MgCO3	1.675e-10	8.373e-11	2.00
CdHCO3+	1.545e-10	1.545e-10	1.00
MnCO3	1.044e-10	5.220e-11	2.00
BF2(OH)2-	-4.623e-11	4.623e-11	-1.00
ZnOH+	3.975e-11	3.975e-11	1.00
CuHCO3+	3.836e-11	3.836e-11	1.00
AlOH+2	3.374e-11	3.374e-11	1.00
FeCO3	2.406e-11	1.203e-11	2.00
NaCO3-	2.133e-11	1.067e-11	2.00
CaHPO4	1.379e-11	1.379e-11	1.00
PbCO3	1.279e-11	6.395e-12	2.00
Al(OH)2+	1.275e-11	6.373e-12	2.00
MgHPO4	9.985e-12	9.985e-12	1.00
MgOH+	9.848e-12	9.848e-12	1.00

FeOH+	4.907e-12	4.907e-12	1.00
BaCO3	4.493e-12	2.246e-12	2.00
FeHSO4+	-2.856e-12	2.856e-12	-1.00
CuCO3	9.438e-13	4.719e-13	2.00
CaOH+	7.543e-13	7.543e-13	1.00
MnOH+	5.269e-13	5.269e-13	1.00
FeHPO4	3.053e-13	3.053e-13	1.00
ZnOHCl	2.564e-13	2.564e-13	1.00
PbOH+	2.029e-13	2.029e-13	1.00
BF3OH-	-1.848e-13	9.238e-14	-2.00
NaHPO4-	1.605e-13	1.605e-13	1.00
Al(OH)3	7.355e-14	2.452e-14	3.00
CuOH+	2.484e-14	2.484e-14	1.00
Zn(CO3)2-2	2.271e-14	5.677e-15	4.00
Zn(OH)2	1.987e-14	9.934e-15	2.00
KHPO4-	1.775e-14	1.775e-14	1.00
CdOH+	1.443e-14	1.443e-14	1.00
CdCO3	8.908e-15	4.454e-15	2.00
Al(OH)4-	4.957e-15	1.239e-15	4.00
BaOH+	4.062e-15	4.062e-15	1.00
Cu(OH)2	2.477e-15	1.239e-15	2.00
BF4-	-2.100e-15	7.002e-16	-3.00
CaPO4-	1.761e-15	8.806e-16	2.00
CdOHCl	1.509e-15	1.509e-15	1.00
MgPO4-	1.272e-15	6.362e-16	2.00
AlHSO4+2	-1.522e-16	1.522e-16	-1.00
Pb(CO3)2-2	7.312e-17	1.828e-17	4.00
FeF2+	-2.772e-17	1.386e-17	-2.00
FeOH+2	-1.959e-17	1.959e-17	-1.00
FeF+2	-1.700e-17	8.499e-18	-2.00
PO4-3	5.171e-18	2.586e-18	2.00
Pb(OH)2	3.767e-18	1.883e-18	2.00
Cu(CO3)2-2	2.704e-18	6.761e-19	4.00
Fe(OH)2	2.217e-18	1.108e-18	2.00
FeF3	-1.963e-18	9.814e-19	-2.00
Fe(OH)3	4.774e-19	4.774e-19	1.00
Fe+3	-2.811e-19	1.405e-19	-2.00
FeSO4+	-2.316e-19	1.158e-19	-2.00
Cd(CO3)2-2	6.411e-20	1.603e-20	4.00
Cd(OH)2	3.380e-20	1.690e-20	2.00
FeH2PO4+2	-5.500e-21	2.750e-21	-2.00
Pb2OH+3	2.664e-21	2.664e-21	1.00
Zn(OH)3-	2.486e-21	8.285e-22	3.00
FeCl+2	-1.740e-21	8.698e-22	-2.00
Cu2(OH)2+2	6.728e-22	3.364e-22	2.00
Cd2OH+3	6.221e-22	6.221e-22	1.00
Fe(SO4)2-	-5.388e-22	2.694e-22	-2.00
FeHSO4+2	-4.299e-23	1.433e-23	-3.00
Fe(OH)4-	2.409e-23	1.205e-23	2.00
NaOH	1.530e-23	1.530e-23	1.00
Cu(OH)3-	5.906e-24	1.969e-24	3.00
FeHPO4+	-3.884e-24	3.884e-24	-1.00
Fe(OH)3-	3.296e-24	1.099e-24	3.00
Pb(OH)3-	1.711e-24	5.703e-25	3.00
FeCl2+	-1.589e-24	7.947e-25	-2.00
Mn(OH)3-	5.556e-28	1.852e-28	3.00
Cd(OH)3-	1.500e-28	5.001e-29	3.00
FeCl3	-3.724e-29	1.862e-29	-2.00
Zn(OH)4-2	1.529e-29	3.822e-30	4.00
Pb(OH)4-2	1.521e-31	3.803e-32	4.00
Cu(OH)4-2	4.573e-32	1.143e-32	4.00
Fe2(OH)2+4	-2.935e-32	1.468e-32	-2.00
Pb3(OH)4+2	1.878e-34	4.695e-35	4.00
Cd(OH)4-2	5.189e-38	1.297e-38	4.00
Fe3(OH)4+5	-0.000e+00	0.000e+00	-2.00

Saturation indices

Phase	SI**	log IAP	log K(299 K, 1 atm)	
Al(OH)3(a)	-7.51	3.21	10.72	Al(OH)3
Alunite	-14.18	-15.73	-1.55	KAl3(SO4)2(OH)6
Anglesite	-5.60	-13.38	-7.78	PbSO4
Anhydrite	-3.45	-7.74	-4.29	CaSO4
Aragonite	-4.45	-12.79	-8.34	CaCO3
BaCl2	-14.78	-12.56	2.22	BaCl2
BaCl2:2H2O	-12.78	-12.56	0.22	BaCl2:2H2O
BaCl2:H2O	-13.39	-12.56	0.83	BaCl2:H2O
Barite	0.51	-9.32	-9.83	BaSO4
Calcite	-4.31	-12.79	-8.49	CaCO3
Cd(OH)2	-13.07	0.58	13.65	Cd(OH)2
CdSO4	-12.05	-12.20	-0.14	CdSO4
Cerussite	-5.32	-18.43	-13.12	PbCO3
CO2(g)	0.32	-1.17	-1.48	CO2
Dolomite	-8.74	-25.86	-17.12	CaMg(CO3)2
Fe(OH)3(a)	-10.73	-5.84	4.89	Fe(OH)3
Fluorite	-1.84	-12.42	-10.59	CaF2
Gibbsite	-4.83	3.21	8.04	Al(OH)3
Goethite	-4.79	-5.83	-1.04	FeOOH
Gypsum	-3.16	-7.74	-4.58	CaSO4:2H2O
H2(g)	-9.31	-12.41	-3.10	H2
H2O(g)	-1.47	-0.00	1.47	H2O
Halite	-8.44	-6.87	1.57	NaCl
Hausmannite	-43.53	17.20	60.73	Mn3O4
Hematite	-7.57	-11.67	-4.10	Fe2O3
Hydroxyapatite	-27.23	-30.75	-3.53	Ca5(PO4)3OH
Jarosite-K	-33.57	-42.87	-9.30	KFe3(SO4)2(OH)6
Manganite	-18.07	7.27	25.34	MnOOH
Melanterite	-8.05	-10.25	-2.19	FeSO4:7H2O
O2(g)	-64.27	-67.17	-2.90	O2
Otavite	-5.15	-17.25	-12.10	CdCO3
Pb(OH)2	-8.71	-0.60	8.11	Pb(OH)2
Pyrochroite	-12.55	2.65	15.20	Mn(OH)2
Pyrolusite	-29.29	11.90	41.19	MnO2:H2O
Rhodochrosite	-4.05	-15.18	-11.13	MnCO3
Siderite	-4.40	-15.30	-10.90	FeCO3
Smithsonite	-4.92	-14.93	-10.01	ZnCO3
Sylvite	-8.73	-7.83	0.91	KCl
Vivianite	-18.37	-54.37	-36.00	Fe3(PO4)2:8H2O
Witherite	-5.81	-14.37	-8.56	BaCO3
Zn(OH)2(e)	-8.60	2.90	11.50	Zn(OH)2

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
For ideal gases, phi = 1.

Initial solution 20.

-----------------------------Solution composition-------------------------------

Elements	Molality	Moles
Al	4.743e-06	4.743e-06
Alkalinity	1.310e-03	1.310e-03
B	1.221e-05	1.221e-05
Ba	8.739e-06	8.739e-06
Br	5.632e-06	5.632e-06
Ca	3.618e-04	3.618e-04
Cd	9.076e-09	9.076e-09
Cl	2.539e-04	2.539e-04
Cu	7.035e-08	7.035e-08
F	5.791e-05	5.791e-05
Fe	3.085e-06	3.085e-06
K	7.162e-05	7.162e-05
Mg	1.534e-04	1.534e-04
Mn	1.675e-06	1.675e-06
N(5)	2.942e-04	2.942e-04

Na	6.656e-04	6.656e-04
P	1.808e-06	1.808e-06
Pb	5.068e-09	5.068e-09
S(6)	1.260e-04	1.260e-04
Zn	1.519e-06	1.519e-06

----------Description of solution----------

pH	= 6.100
pe	= 0.280
Specific Conductance (µS/cm, 24°C)	= 201
Density (g/cm³)	= 0.99737
Volume (L)	= 1.00289
Activity of water	= 1.000
Ionic strength (mol/kgw)	= 2.592e-03
Mass of water (kg)	= 1.000e+00
Total carbon (mol/kg)	= 3.533e-03
Total CO2 (mol/kg)	= 3.533e-03
Temperature (°C)	= 24.26
Electrical balance (eq)	= -3.636e-04
Percent error, 100*(Cat-|An|)/(Cat+|An|)	= -9.28
Iterations	= 13 (212 overall)
Total H	= 1.110138e+02
Total O	= 5.551602e+01

----------Distribution of species----------

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma	mole V cm³/mol
H+	8.366e-07	7.943e-07	-6.077	-6.100	-0.023	0.00
OH-	1.274e-08	1.204e-08	-7.895	-7.919	-0.025	-4.12
H2O	5.551e+01	9.999e-01	1.744	-0.000	0.000	18.07
Al	4.743e-06					
AlF2+	2.950e-06	2.793e-06	-5.530	-5.554	-0.024	(0)
AlF3	1.548e-06	1.549e-06	-5.810	-5.810	0.000	(0)
AlF+2	1.579e-07	1.269e-07	-6.802	-6.897	-0.095	(0)
Al(OH)2+	3.363e-08	3.184e-08	-7.473	-7.497	-0.024	(0)
AlF4-	2.875e-08	2.719e-08	-7.541	-7.566	-0.024	(0)
Al(OH)4-	1.388e-08	1.313e-08	-7.857	-7.882	-0.024	(0)
Al(OH)3	5.588e-09	5.591e-09	-8.253	-8.253	0.000	(0)
AlOH+2	4.287e-09	3.443e-09	-8.368	-8.463	-0.095	-27.67
Al+3	4.610e-10	2.890e-10	-9.336	-9.539	-0.203	-42.11
AlSO4+	9.045e-11	8.557e-11	-10.044	-10.068	-0.024	(0)
Al(SO4)2-	2.695e-13	2.549e-13	-12.569	-12.594	-0.024	(0)
AlHSO4+2	7.488e-18	5.988e-18	-17.126	-17.223	-0.097	(0)
B	1.221e-05					
H3BO3	1.220e-05	1.221e-05	-4.914	-4.913	0.000	39.17
H2BO3-	9.228e-09	8.727e-09	-8.035	-8.059	-0.024	(0)
BF(OH)3-	2.249e-10	2.127e-10	-9.648	-9.672	-0.024	(0)
BF2(OH)2-	8.451e-13	7.991e-13	-12.073	-12.097	-0.024	(0)
BF3OH-	3.290e-17	3.111e-17	-16.483	-16.507	-0.024	(0)
BF4-	4.700e-21	4.445e-21	-20.328	-20.352	-0.024	(0)
Ba	8.739e-06					
Ba+2	8.336e-06	6.670e-06	-5.079	-5.176	-0.097	-12.72
BaSO4	3.158e-07	3.160e-07	-6.501	-6.500	0.000	(0)
BaHCO3+	8.148e-08	7.705e-08	-7.089	-7.113	-0.024	(0)
BaCl+	5.247e-09	4.962e-09	-8.280	-8.304	-0.024	(0)
BaNO3+	2.468e-10	2.334e-10	-9.608	-9.632	-0.024	(0)
BaCO3	2.434e-10	2.435e-10	-9.614	-9.613	0.000	-10.71
BaOH+	3.006e-13	2.845e-13	-12.522	-12.546	-0.024	(0)
Br	5.632e-06					
Br-	5.632e-06	5.321e-06	-5.249	-5.274	-0.025	24.54
CdBr+	5.633e-12	5.327e-12	-11.249	-11.274	-0.024	(0)
ZnBr+	1.551e-12	1.467e-12	-11.809	-11.834	-0.024	(0)
PbBr+	4.574e-13	4.325e-13	-12.340	-12.364	-0.024	(0)
CdBr2	1.516e-16	1.517e-16	-15.819	-15.819	0.000	(0)
ZnBr2	3.105e-18	3.107e-18	-17.508	-17.508	0.000	(0)

PbBr2	1.089e-18	1.090e-18	-17.963	-17.963	0.000	(0)
C(4)	3.533e-03					
CO2	2.222e-03	2.224e-03	-2.653	-2.653	0.000	34.40
HCO3-	1.303e-03	1.234e-03	-2.885	-2.909	-0.024	24.65
CaHCO3+	4.648e-06	4.402e-06	-5.333	-5.356	-0.024	9.66
MgHCO3+	1.819e-06	1.720e-06	-5.740	-5.764	-0.024	5.47
NaHCO3	4.373e-07	4.376e-07	-6.359	-6.359	0.000	1.80
FeHCO3+	2.888e-07	2.731e-07	-6.539	-6.564	-0.024	(0)
ZnHCO3+	1.721e-07	1.627e-07	-6.764	-6.789	-0.024	(0)
MnHCO3+	1.408e-07	1.332e-07	-6.852	-6.875	-0.024	(0)
CO3-2	8.931e-08	7.174e-08	-7.049	-7.144	-0.095	-5.26
(CO2)2	8.852e-08	8.857e-08	-7.053	-7.053	0.000	68.79
BaHCO3+	8.148e-08	7.705e-08	-7.089	-7.113	-0.024	(0)
CaCO3	3.358e-08	3.360e-08	-7.474	-7.474	0.000	-14.60
ZnCO3	1.499e-08	1.500e-08	-7.824	-7.824	0.000	(0)
MgCO3	8.089e-09	8.093e-09	-8.092	-8.092	0.000	-17.09
MnCO3	6.901e-09	6.905e-09	-8.161	-8.161	0.000	(0)
FeCO3	3.808e-09	3.810e-09	-8.419	-8.419	0.000	(0)
PbCO3	1.741e-09	1.742e-09	-8.759	-8.759	0.000	(0)
PbHCO3+	1.448e-09	1.369e-09	-8.839	-8.864	-0.024	(0)
NaCO3-	8.548e-10	8.083e-10	-9.068	-9.092	-0.024	-1.07
CdHCO3+	2.783e-10	2.631e-10	-9.556	-9.580	-0.024	(0)
BaCO3	2.434e-10	2.435e-10	-9.614	-9.613	0.000	-10.71
CuHCO3+	1.547e-10	1.463e-10	-9.810	-9.835	-0.024	(0)
CuCO3	9.113e-11	9.118e-11	-10.040	-10.040	0.000	(0)
Zn(CO3)2-2	2.877e-11	2.301e-11	-10.541	-10.638	-0.097	(0)
Pb(CO3)2-2	3.926e-13	3.139e-13	-12.406	-12.503	-0.097	(0)
CdCO3	3.842e-13	3.844e-13	-12.415	-12.415	0.000	(0)
Cu(CO3)2-2	1.030e-14	8.235e-15	-13.987	-14.084	-0.097	(0)
Cd(CO3)2-2	1.091e-16	8.720e-17	-15.962	-16.059	-0.097	(0)
Ca	3.618e-04					
Ca+2	3.524e-04	2.830e-04	-3.453	-3.548	-0.095	-18.08
CaSO4	4.728e-06	4.731e-06	-5.325	-5.325	0.000	7.47
CaHCO3+	4.648e-06	4.402e-06	-5.333	-5.356	-0.024	9.66
CaCO3	3.358e-08	3.360e-08	-7.474	-7.474	0.000	-14.60
CaHPO4	1.815e-08	1.816e-08	-7.741	-7.741	0.000	(0)
CaH2PO4+	1.150e-08	1.088e-08	-7.939	-7.963	-0.024	(0)
CaOH+	6.251e-11	5.911e-11	-10.204	-10.228	-0.024	(0)
CaPO4-	5.634e-11	5.334e-11	-10.249	-10.273	-0.024	(0)
CaHSO4+	2.585e-11	2.444e-11	-10.588	-10.612	-0.024	(0)
Cd	9.076e-09					
Cd+2	8.436e-09	6.745e-09	-8.074	-8.171	-0.097	-18.72
CdHCO3+	2.783e-10	2.631e-10	-9.556	-9.580	-0.024	(0)
CdSO4	1.830e-10	1.831e-10	-9.738	-9.737	0.000	78.42
CdCl+	1.625e-10	1.537e-10	-9.789	-9.813	-0.024	5.67
CdBr+	5.633e-12	5.327e-12	-11.249	-11.274	-0.024	(0)
CdNO3+	5.090e-12	4.813e-12	-11.293	-11.318	-0.024	17.57
CdF+	3.960e-12	3.745e-12	-11.402	-11.427	-0.024	(0)
CdOH+	7.069e-13	6.685e-13	-12.151	-12.175	-0.024	(0)
CdCO3	3.842e-13	3.844e-13	-12.415	-12.415	0.000	(0)
Cd(SO4)2-2	2.384e-13	1.907e-13	-12.623	-12.720	-0.097	-106.06
CdCl2	1.527e-13	1.528e-13	-12.816	-12.816	0.000	23.14
CdOHCl	7.861e-14	7.865e-14	-13.105	-13.104	0.000	(0)
CdF2	4.145e-16	4.148e-16	-15.382	-15.382	0.000	(0)
CdBr2	1.516e-16	1.517e-16	-15.819	-15.819	0.000	(0)
Cd(CO3)2-2	1.091e-16	8.720e-17	-15.962	-16.059	-0.097	(0)
Cd(OH)2	4.772e-17	4.774e-17	-16.321	-16.321	0.000	(0)
CdCl3-	2.411e-17	2.280e-17	-16.618	-16.642	-0.024	69.87
Cd2OH+3	3.687e-20	2.229e-20	-19.433	-19.652	-0.219	(0)
Cd(OH)3-	7.131e-24	6.743e-24	-23.147	-23.171	-0.024	(0)
Cd(OH)4-2	9.462e-32	7.566e-32	-31.024	-31.121	-0.097	(0)
Cl	2.539e-04					
Cl-	2.530e-04	2.392e-04	-3.597	-3.621	-0.024	18.07
NaCl	8.938e-07	8.943e-07	-6.049	-6.049	0.000	(0)
BaCl+	5.247e-09	4.962e-09	-8.280	-8.304	-0.024	(0)
MnCl+	1.247e-09	1.181e-09	-8.904	-8.928	-0.024	-3.26
CuCl2-	1.241e-09	1.173e-09	-8.906	-8.931	-0.024	(0)
FeCl+	7.729e-10	7.309e-10	-9.112	-9.136	-0.024	(0)

ZnCl+	6.904e-10	6.528e-10	-9.161	-9.185	-0.024	-14.63
CdCl+	1.625e-10	1.537e-10	-9.789	-9.813	-0.024	5.67
PbCl+	1.381e-11	1.306e-11	-10.860	-10.884	-0.024	7.94
ZnOHCl	1.044e-11	1.045e-11	-10.981	-10.981	0.000	(0)
CuCl3-2	5.527e-13	4.433e-13	-12.258	-12.353	-0.096	(0)
ZnCl2	1.629e-13	1.630e-13	-12.788	-12.788	0.000	103.49
CuCl+	1.554e-13	1.469e-13	-12.809	-12.833	-0.024	0.84
CdCl2	1.527e-13	1.528e-13	-12.816	-12.816	0.000	23.14
MnCl2	1.232e-13	1.232e-13	-12.909	-12.909	0.000	86.80
CdOHCl	7.861e-14	7.865e-14	-13.105	-13.104	0.000	(0)
PbCl2	5.017e-15	5.020e-15	-14.300	-14.299	0.000	34.91
ZnCl3-	4.605e-17	4.355e-17	-16.337	-16.361	-0.024	16.92
CdCl3-	2.411e-17	2.280e-17	-16.618	-16.642	-0.024	69.87
CuCl2	1.871e-17	1.872e-17	-16.728	-16.728	0.000	30.15
MnCl3-	8.578e-18	8.118e-18	-17.067	-17.091	-0.024	43.40
PbCl3-	1.004e-18	9.492e-19	-17.998	-18.023	-0.024	65.88
ZnCl4-2	6.469e-21	5.189e-21	-20.189	-20.285	-0.096	145.14
FeCl+2	3.402e-21	2.729e-21	-20.468	-20.564	-0.096	(0)
PbCl4-2	1.351e-22	1.080e-22	-21.869	-21.966	-0.097	101.30
CuCl3-	1.658e-23	1.568e-23	-22.780	-22.805	-0.024	(0)
FeCl2+	3.154e-24	2.985e-24	-23.501	-23.525	-0.024	(0)
FeCl3	7.134e-29	7.138e-29	-28.147	-28.146	0.000	(0)
CuCl4-2	2.303e-29	1.847e-29	-28.638	-28.734	-0.096	(0)
Cu(1)	6.980e-08					
Cu+	6.856e-08	6.474e-08	-7.164	-7.189	-0.025	(0)
CuCl2-	1.241e-09	1.173e-09	-8.906	-8.931	-0.024	(0)
CuCl3-2	5.527e-13	4.433e-13	-12.258	-12.353	-0.096	(0)
Cu(2)	5.558e-10					
Cu+2	2.941e-10	2.367e-10	-9.532	-9.626	-0.094	-26.54
CuHCO3+	1.547e-10	1.463e-10	-9.810	-9.835	-0.024	(0)
CuCO3	9.113e-11	9.118e-11	-10.040	-10.040	0.000	(0)
Cu(OH)2	7.831e-12	7.836e-12	-11.106	-11.106	0.000	(0)
CuSO4	4.542e-12	4.545e-12	-11.343	-11.342	0.000	13.00
CuOH+	3.151e-12	2.979e-12	-11.502	-11.526	-0.024	(0)
CuF+	1.995e-13	1.886e-13	-12.700	-12.724	-0.024	(0)
CuCl+	1.554e-13	1.469e-13	-12.809	-12.833	-0.024	0.84
Cu(CO3)2-2	1.030e-14	8.235e-15	-13.987	-14.084	-0.097	(0)
CuCl2	1.871e-17	1.872e-17	-16.728	-16.728	0.000	30.15
Cu2(OH)2+2	4.513e-18	3.608e-18	-17.346	-17.443	-0.097	(0)
Cu(OH)3-	6.285e-19	5.943e-19	-18.202	-18.226	-0.024	(0)
CuCl3-	1.658e-23	1.568e-23	-22.780	-22.805	-0.024	(0)
Cu(OH)4-2	1.867e-25	1.493e-25	-24.729	-24.826	-0.097	(0)
CuCl4-2	2.303e-29	1.847e-29	-28.638	-28.734	-0.096	(0)
F	5.791e-05					
F-	4.666e-05	4.410e-05	-4.331	-4.356	-0.025	-1.31
AlF2+	2.950e-06	2.793e-06	-5.530	-5.554	-0.024	(0)
AlF3	1.548e-06	1.549e-06	-5.810	-5.810	0.000	(0)
MgF+	3.634e-07	3.437e-07	-6.440	-6.464	-0.024	-10.56
AlF+2	1.579e-07	1.269e-07	-6.802	-6.897	-0.095	(0)
HF	5.181e-08	5.184e-08	-7.286	-7.285	0.000	12.47
AlF4-	2.875e-08	2.719e-08	-7.541	-7.566	-0.024	(0)
NaF	1.593e-08	1.594e-08	-7.798	-7.798	0.000	7.23
FeF+	1.032e-09	9.762e-10	-8.986	-9.010	-0.024	(0)
ZnF+	6.838e-10	6.467e-10	-9.165	-9.189	-0.024	(0)
MnF+	3.906e-10	3.696e-10	-9.408	-9.432	-0.024	(0)
BF(OH)3-	2.249e-10	2.127e-10	-9.648	-9.672	-0.024	(0)
HF2-	9.221e-12	8.720e-12	-11.035	-11.059	-0.024	22.05
CdF+	3.960e-12	3.745e-12	-11.402	-11.427	-0.024	(0)
PbF+	1.159e-12	1.096e-12	-11.936	-11.960	-0.024	(0)
BF2(OH)2-	8.451e-13	7.991e-13	-12.073	-12.097	-0.024	(0)
CuF+	1.995e-13	1.886e-13	-12.700	-12.724	-0.024	(0)
PbF2	9.858e-16	9.864e-16	-15.006	-15.006	0.000	(0)
CdF2	4.145e-16	4.148e-16	-15.382	-15.382	0.000	(0)
FeF2+	4.914e-17	4.651e-17	-16.309	-16.332	-0.024	(0)
FeF+2	3.332e-17	2.673e-17	-16.477	-16.573	-0.096	(0)
BF3OH-	3.290e-17	3.111e-17	-16.483	-16.507	-0.024	(0)
FeF3	3.240e-18	3.242e-18	-17.489	-17.489	0.000	(0)
PbF3-	3.332e-19	3.151e-19	-18.477	-18.502	-0.024	(0)

BF4-	4.700e-21	4.445e-21	-20.328	-20.352	-0.024	(0)
PbF4-2	8.317e-24	6.651e-24	-23.080	-23.177	-0.097	(0)
Fe(2)	3.085e-06					
Fe+2	2.751e-06	2.214e-06	-5.561	-5.655	-0.094	-22.12
FeHCO3+	2.888e-07	2.731e-07	-6.539	-6.564	-0.024	(0)
FeSO4	3.670e-08	3.672e-08	-7.435	-7.435	0.000	19.75
FeCO3	3.808e-09	3.810e-09	-8.419	-8.419	0.000	(0)
FeH2PO4+	1.787e-09	1.692e-09	-8.748	-8.772	-0.024	(0)
FeHPO4	1.046e-09	1.046e-09	-8.981	-8.980	0.000	(0)
FeF+	1.032e-09	9.762e-10	-8.986	-9.010	-0.024	(0)
FeOH+	8.810e-10	8.337e-10	-9.055	-9.079	-0.024	(0)
FeCl+	7.729e-10	7.309e-10	-9.112	-9.136	-0.024	(0)
FeHSO4+	2.022e-13	1.912e-13	-12.694	-12.718	-0.024	(0)
Fe(OH)2	8.370e-15	8.375e-15	-14.077	-14.077	0.000	(0)
Fe(OH)3-	4.109e-19	3.888e-19	-18.386	-18.410	-0.024	(0)
Fe(3)	1.484e-12					
Fe(OH)2+	1.288e-12	1.220e-12	-11.890	-11.914	-0.024	(0)
Fe(OH)3	1.914e-13	1.915e-13	-12.718	-12.718	0.000	(0)
FeOH+2	3.752e-15	3.009e-15	-14.426	-14.522	-0.096	(0)
Fe(OH)4-	2.254e-16	2.134e-16	-15.647	-15.671	-0.024	(0)
FeF2+	4.914e-17	4.651e-17	-16.309	-16.332	-0.024	(0)
FeF+2	3.332e-17	2.673e-17	-16.477	-16.573	-0.096	(0)
FeF3	3.240e-18	3.242e-18	-17.489	-17.489	0.000	(0)
Fe+3	6.171e-19	3.868e-19	-18.210	-18.413	-0.203	(0)
FeSO4+	4.168e-19	3.944e-19	-18.380	-18.404	-0.024	(0)
FeH2PO4+2	1.976e-19	1.588e-19	-18.704	-18.799	-0.095	(0)
FeHPO4+	1.275e-20	1.206e-20	-19.895	-19.919	-0.024	(0)
FeCl+2	3.402e-21	2.729e-21	-20.468	-20.564	-0.096	(0)
Fe(SO4)2-	8.603e-22	8.135e-22	-21.065	-21.090	-0.024	(0)
FeCl2+	3.154e-24	2.985e-24	-23.501	-23.525	-0.024	(0)
FeHSO4+2	1.050e-24	8.393e-25	-23.979	-24.076	-0.097	(0)
Fe2(OH)2+4	6.149e-28	2.514e-28	-27.211	-27.600	-0.389	(0)
FeCl3	7.134e-29	7.138e-29	-28.147	-28.146	0.000	(0)
Fe3(OH)4+5	2.775e-37	6.859e-38	-36.557	-37.164	-0.607	(0)
H(0)	2.477e-16					
H2	1.239e-16	1.239e-16	-15.907	-15.907	0.000	28.61
K	7.162e-05					
K+	7.157e-05	6.765e-05	-4.145	-4.170	-0.024	9.00
KSO4-	4.686e-08	4.436e-08	-7.329	-7.353	-0.024	34.10
KHPO4-	1.654e-11	1.566e-11	-10.782	-10.805	-0.024	38.18
Mg	1.534e-04					
Mg+2	1.486e-04	1.196e-04	-3.828	-3.922	-0.094	-21.73
MgSO4	2.598e-06	2.600e-06	-5.585	-5.585	0.000	5.81
MgHCO3+	1.819e-06	1.720e-06	-5.740	-5.764	-0.024	5.47
MgF+	3.634e-07	3.437e-07	-6.440	-6.464	-0.024	-10.56
MgHPO4	1.037e-08	1.038e-08	-7.984	-7.984	0.000	(0)
MgCO3	8.089e-09	8.093e-09	-8.092	-8.092	0.000	-17.09
MgH2PO4+	6.187e-09	5.857e-09	-8.209	-8.232	-0.024	(0)
MgOH+	5.394e-10	5.111e-10	-9.268	-9.291	-0.023	(0)
MgPO4-	3.212e-11	3.041e-11	-10.493	-10.517	-0.024	(0)
Mn(2)	1.675e-06					
Mn+2	1.505e-06	1.212e-06	-5.822	-5.917	-0.094	-20.60
MnHCO3+	1.408e-07	1.332e-07	-6.852	-6.875	-0.024	(0)
MnSO4	2.007e-08	2.008e-08	-7.697	-7.697	0.000	22.87
MnCO3	6.901e-09	6.905e-09	-8.161	-8.161	0.000	(0)
MnCl+	1.247e-09	1.181e-09	-8.904	-8.928	-0.024	-3.26
MnF+	3.906e-10	3.696e-10	-9.408	-9.432	-0.024	(0)
MnOH+	3.900e-11	3.690e-11	-10.409	-10.433	-0.024	(0)
Mn(NO3)2	3.730e-13	3.732e-13	-12.428	-12.428	0.000	41.24
MnCl2	1.232e-13	1.232e-13	-12.909	-12.909	0.000	86.80
MnCl3-	8.578e-18	8.118e-18	-17.067	-17.091	-0.024	43.40
Mn(OH)3-	4.048e-23	3.831e-23	-22.393	-22.417	-0.024	(0)
Mn(3)	1.021e-31					
Mn+3	1.021e-31	6.402e-32	-30.991	-31.194	-0.203	(0)
N(5)	2.942e-04					
NO3-	2.942e-04	2.779e-04	-3.531	-3.556	-0.025	29.44
BaNO3+	2.468e-10	2.334e-10	-9.608	-9.632	-0.024	(0)
PbNO3+	6.074e-12	5.744e-12	-11.217	-11.241	-0.024	(0)

CdNO3+	5.090e-12	4.813e-12	-11.293	-11.318	-0.024	17.57
Mn(NO3)2	3.730e-13	3.732e-13	-12.428	-12.428	0.000	41.24
Na	6.656e-04					
Na+	6.639e-04	6.281e-04	-3.178	-3.202	-0.024	-1.49
NaCl	8.938e-07	8.943e-07	-6.049	-6.049	0.000	(0)
NaHCO3	4.373e-07	4.376e-07	-6.359	-6.359	0.000	1.80
NaSO4-	3.129e-07	2.962e-07	-6.505	-6.528	-0.024	13.92
NaF	1.593e-08	1.594e-08	-7.798	-7.798	0.000	7.23
NaCO3-	8.548e-10	8.083e-10	-9.068	-9.092	-0.024	-1.07
NaHPO4-	1.536e-10	1.454e-10	-9.814	-9.837	-0.024	33.64
NaOH	7.558e-22	7.563e-22	-21.122	-21.121	0.000	(0)
O(0)	0.000e+00					
O2	0.000e+00	0.000e+00	-60.806	-60.806	0.000	30.34
P	1.808e-06					
H2PO4-	1.611e-06	1.525e-06	-5.793	-5.817	-0.024	33.24
HPO4-2	1.480e-07	1.187e-07	-6.830	-6.926	-0.096	6.81
CaHPO4	1.815e-08	1.816e-08	-7.741	-7.741	0.000	(0)
CaH2PO4+	1.150e-08	1.088e-08	-7.939	-7.963	-0.024	(0)
MgHPO4	1.037e-08	1.038e-08	-7.984	-7.984	0.000	(0)
MgH2PO4+	6.187e-09	5.857e-09	-8.209	-8.232	-0.024	(0)
FeH2PO4+	1.787e-09	1.692e-09	-8.748	-8.772	-0.024	(0)
FeHPO4	1.046e-09	1.046e-09	-8.981	-8.980	0.000	(0)
H3PO4	1.767e-10	1.768e-10	-9.753	-9.753	0.000	47.37
NaHPO4-	1.536e-10	1.454e-10	-9.814	-9.837	-0.024	33.64
CaPO4-	5.634e-11	5.334e-11	-10.249	-10.273	-0.024	(0)
MgPO4-	3.212e-11	3.041e-11	-10.493	-10.517	-0.024	(0)
KHPO4-	1.654e-11	1.566e-11	-10.782	-10.805	-0.024	38.18
PO4-3	1.098e-13	6.637e-14	-12.959	-13.178	-0.219	-23.01
FeH2PO4+2	1.976e-19	1.588e-19	-18.704	-18.799	-0.095	(0)
FeHPO4+	1.275e-20	1.206e-20	-19.895	-19.919	-0.024	(0)
Pb	5.068e-09					
Pb+2	1.747e-09	1.397e-09	-8.758	-8.855	-0.097	-15.47
PbCO3	1.741e-09	1.742e-09	-8.759	-8.759	0.000	(0)
PbHCO3+	1.448e-09	1.369e-09	-8.839	-8.864	-0.024	(0)
PbSO4	7.424e-11	7.428e-11	-10.129	-10.129	0.000	(0)
PbOH+	3.627e-11	3.429e-11	-10.441	-10.465	-0.024	(0)
PbCl+	1.381e-11	1.306e-11	-10.860	-10.884	-0.024	7.94
PbNO3+	6.074e-12	5.744e-12	-11.217	-11.241	-0.024	(0)
PbF+	1.159e-12	1.096e-12	-11.936	-11.960	-0.024	(0)
PbBr+	4.574e-13	4.325e-13	-12.340	-12.364	-0.024	(0)
Pb(CO3)2-2	3.926e-13	3.139e-13	-12.406	-12.503	-0.097	(0)
Pb(SO4)2-2	4.609e-14	3.685e-14	-13.336	-13.434	-0.097	(0)
Pb(OH)2	1.678e-14	1.679e-14	-13.775	-13.775	0.000	(0)
PbCl2	5.017e-15	5.020e-15	-14.300	-14.299	0.000	34.91
PbF2	9.858e-16	9.864e-16	-15.006	-15.006	0.000	(0)
Pb2OH+3	1.774e-18	1.073e-18	-17.751	-17.970	-0.219	(0)
PbBr2	1.089e-18	1.090e-18	-17.963	-17.963	0.000	(0)
PbCl3-	1.004e-18	9.492e-19	-17.998	-18.023	-0.024	65.88
PbF3-	3.332e-19	3.151e-19	-18.477	-18.502	-0.024	(0)
Pb(OH)3-	2.567e-19	2.427e-19	-18.591	-18.615	-0.024	(0)
PbCl4-2	1.351e-22	1.080e-22	-21.869	-21.966	-0.097	101.30
PbF4-2	8.317e-24	6.651e-24	-23.080	-23.177	-0.097	(0)
Pb(OH)4-2	8.754e-25	7.000e-25	-24.058	-24.155	-0.097	(0)
Pb3(OH)4+2	1.010e-26	8.078e-27	-25.996	-26.093	-0.097	(0)
S(6)	1.260e-04					
SO4-2	1.179e-04	9.454e-05	-3.929	-4.024	-0.096	14.49
CaSO4	4.728e-06	4.731e-06	-5.325	-5.325	0.000	7.47
MgSO4	2.598e-06	2.600e-06	-5.585	-5.585	0.000	5.81
BaSO4	3.158e-07	3.160e-07	-6.501	-6.500	0.000	(0)
NaSO4-	3.129e-07	2.962e-07	-6.505	-6.528	-0.024	13.92
KSO4-	4.686e-08	4.436e-08	-7.329	-7.353	-0.024	34.10
FeSO4	3.670e-08	3.672e-08	-7.435	-7.435	0.000	19.75
ZnSO4	2.308e-08	2.309e-08	-7.637	-7.637	0.000	21.83
MnSO4	2.007e-08	2.008e-08	-7.697	-7.697	0.000	22.87
HSO4-	7.598e-09	7.185e-09	-8.119	-8.144	-0.024	40.24
CdSO4	1.830e-10	1.831e-10	-9.738	-9.737	0.000	78.42
AlSO4+	9.045e-11	8.557e-11	-10.044	-10.068	-0.024	(0)
PbSO4	7.424e-11	7.428e-11	-10.129	-10.129	0.000	(0)

CaHSO4+	2.585e-11	2.444e-11	-10.588	-10.612	-0.024	(0)
Zn(SO4)2-2	2.232e-11	1.785e-11	-10.651	-10.748	-0.097	-13.68
CuSO4	4.542e-12	4.545e-12	-11.343	-11.342	0.000	13.00
Al(SO4)2-	2.695e-13	2.549e-13	-12.569	-12.594	-0.024	(0)
Cd(SO4)2-2	2.384e-13	1.907e-13	-12.623	-12.720	-0.097	-106.06
FeHSO4+	2.022e-13	1.912e-13	-12.694	-12.718	-0.024	(0)
Pb(SO4)2-2	4.609e-14	3.685e-14	-13.336	-13.434	-0.097	(0)
AlHSO4+2	7.488e-18	5.988e-18	-17.126	-17.223	-0.097	(0)
FeSO4+	4.168e-19	3.944e-19	-18.380	-18.404	-0.024	(0)
Fe(SO4)2-	8.603e-22	8.135e-22	-21.065	-21.090	-0.024	(0)
FeHSO4+2	1.050e-24	8.393e-25	-23.979	-24.076	-0.097	(0)
Zn	1.519e-06					
Zn+2	1.306e-06	1.048e-06	-5.884	-5.980	-0.096	-25.25
ZnHCO3+	1.721e-07	1.627e-07	-6.764	-6.789	-0.024	(0)
ZnSO4	2.308e-08	2.309e-08	-7.637	-7.637	0.000	21.83
ZnCO3	1.499e-08	1.500e-08	-7.824	-7.824	0.000	(0)
ZnOH+	1.446e-09	1.367e-09	-8.840	-8.864	-0.024	(0)
ZnCl+	6.904e-10	6.528e-10	-9.161	-9.185	-0.024	-14.63
ZnF+	6.838e-10	6.467e-10	-9.165	-9.189	-0.024	(0)
Zn(CO3)2-2	2.877e-11	2.301e-11	-10.541	-10.638	-0.097	(0)
Zn(SO4)2-2	2.232e-11	1.785e-11	-10.651	-10.748	-0.097	-13.68
Zn(OH)2	2.089e-11	2.090e-11	-10.680	-10.680	0.000	(0)
ZnOHCl	1.044e-11	1.045e-11	-10.981	-10.981	0.000	(0)
ZnBr+	1.551e-12	1.467e-12	-11.809	-11.834	-0.024	(0)
ZnCl2	1.629e-13	1.630e-13	-12.788	-12.788	0.000	103.49
Zn(OH)3-	8.800e-17	8.321e-17	-16.056	-16.080	-0.024	(0)
ZnCl3-	4.605e-17	4.355e-17	-16.337	-16.361	-0.024	16.92
ZnBr2	3.105e-18	3.107e-18	-17.508	-17.508	0.000	(0)
ZnCl4-2	6.469e-21	5.189e-21	-20.189	-20.285	-0.096	145.14
Zn(OH)4-2	2.076e-23	1.660e-23	-22.683	-22.780	-0.097	(0)

----------Distribution of alkalinity----------

Total alkalinity (eq/kgw) = 1.310e-03

Species	Alkalinity	Molality	Alk/Mol
HCO3-	1.303e-03	1.303e-03	1.00
CaHCO3+	4.648e-06	4.648e-06	1.00
MgHCO3+	1.819e-06	1.819e-06	1.00
H+	-8.366e-07	8.366e-07	-1.00
NaHCO3	4.373e-07	4.373e-07	1.00
FeHCO3+	2.888e-07	2.888e-07	1.00
CO3-2	1.786e-07	8.931e-08	2.00
ZnHCO3+	1.721e-07	1.721e-07	1.00
HPO4-2	1.480e-07	1.480e-07	1.00
MnHCO3+	1.408e-07	1.408e-07	1.00
BaHCO3+	8.148e-08	8.148e-08	1.00
Al(OH)2+	6.726e-08	3.363e-08	2.00
CaCO3	6.717e-08	3.358e-08	2.00
Al(OH)4-	5.554e-08	1.388e-08	4.00
HF	-5.181e-08	5.181e-08	-1.00
ZnCO3	2.998e-08	1.499e-08	2.00
CaHPO4	1.815e-08	1.815e-08	1.00
Al(OH)3	1.676e-08	5.588e-09	3.00
MgCO3	1.618e-08	8.089e-09	2.00
MnCO3	1.380e-08	6.901e-09	2.00
OH-	1.274e-08	1.274e-08	1.00
MgHPO4	1.037e-08	1.037e-08	1.00
H2BO3-	9.228e-09	9.228e-09	1.00
FeCO3	7.615e-09	3.808e-09	2.00
HSO4-	-7.598e-09	7.598e-09	-1.00
AlOH+2	4.287e-09	4.287e-09	1.00
PbCO3	3.482e-09	1.741e-09	2.00
NaCO3-	1.710e-09	8.548e-10	2.00
PbHCO3+	1.448e-09	1.448e-09	1.00
ZnOH+	1.446e-09	1.446e-09	1.00
FeHPO4	1.046e-09	1.046e-09	1.00

FeOH+	8.810e-10	8.810e-10	1.00
MgOH+	5.394e-10	5.394e-10	1.00
BaCO3	4.868e-10	2.434e-10	2.00
CdHCO3+	2.783e-10	2.783e-10	1.00
CuCO3	1.823e-10	9.113e-11	2.00
H3PO4	-1.767e-10	1.767e-10	-1.00
CuHCO3+	1.547e-10	1.547e-10	1.00
NaHPO4-	1.536e-10	1.536e-10	1.00
Zn(CO3)2-2	1.151e-10	2.877e-11	4.00
CaPO4-	1.127e-10	5.634e-11	2.00
MgPO4-	6.424e-11	3.212e-11	2.00
CaOH+	6.251e-11	6.251e-11	1.00
Zn(OH)2	4.178e-11	2.089e-11	2.00
MnOH+	3.900e-11	3.900e-11	1.00
PbOH+	3.627e-11	3.627e-11	1.00
CaHSO4+	-2.585e-11	2.585e-11	-1.00
KHPO4-	1.654e-11	1.654e-11	1.00
Cu(OH)2	1.566e-11	7.831e-12	2.00
ZnOHCl	1.044e-11	1.044e-11	1.00
HF2-	-9.221e-12	9.221e-12	-1.00
CuOH+	3.151e-12	3.151e-12	1.00
Pb(CO3)2-2	1.570e-12	3.926e-13	4.00
BF2(OH)2-	-8.451e-13	8.451e-13	-1.00
CdCO3	7.683e-13	3.842e-13	2.00
CdOH+	7.069e-13	7.069e-13	1.00
BaOH+	3.006e-13	3.006e-13	1.00
PO4-3	2.197e-13	1.098e-13	2.00
FeHSO4+	-2.022e-13	2.022e-13	-1.00
Fe(OH)3	1.914e-13	1.914e-13	1.00
CdOHCl	7.861e-14	7.861e-14	1.00
Cu(CO3)2-2	4.120e-14	1.030e-14	4.00
Pb(OH)2	3.357e-14	1.678e-14	2.00
Fe(OH)2	1.674e-14	8.370e-15	2.00
FeOH+2	-3.752e-15	3.752e-15	-1.00
Fe(OH)4-	4.508e-16	2.254e-16	2.00
Cd(CO3)2-2	4.362e-16	1.091e-16	4.00
Zn(OH)3-	2.640e-16	8.800e-17	3.00
FeF2+	-9.829e-17	4.914e-17	-2.00
Cd(OH)2	9.543e-17	4.772e-17	2.00
FeF+2	-6.664e-17	3.332e-17	-2.00
BF3OH-	-6.581e-17	3.290e-17	-2.00
Cu2(OH)2+2	9.025e-18	4.513e-18	2.00
AlHSO4+2	-7.488e-18	7.488e-18	-1.00
FeF3	-6.481e-18	3.240e-18	-2.00
Cu(OH)3-	1.886e-18	6.285e-19	3.00
Pb2OH+3	1.774e-18	1.774e-18	1.00
Fe+3	-1.234e-18	6.171e-19	-2.00
Fe(OH)3-	1.233e-18	4.109e-19	3.00
FeSO4+	-8.336e-19	4.168e-19	-2.00
Pb(OH)3-	7.701e-19	2.567e-19	3.00
FeH2PO4+2	-3.953e-19	1.976e-19	-2.00
Cd2OH+3	3.687e-20	3.687e-20	1.00
BF4-	-1.410e-20	4.700e-21	-3.00
FeHPO4+	-1.275e-20	1.275e-20	-1.00
FeCl+2	-6.804e-21	3.402e-21	-2.00
Fe(SO4)2-	-1.721e-21	8.603e-22	-2.00
NaOH	7.558e-22	7.558e-22	1.00
Mn(OH)3-	1.214e-22	4.048e-23	3.00
Zn(OH)4-2	8.305e-23	2.076e-23	4.00
Cd(OH)3-	2.139e-23	7.131e-24	3.00
FeCl2+	-6.307e-24	3.154e-24	-2.00
Pb(OH)4-2	3.502e-24	8.754e-25	4.00
FeHSO4+2	-3.149e-24	1.050e-24	-3.00
Cu(OH)4-2	7.468e-25	1.867e-25	4.00
Pb3(OH)4+2	4.041e-26	1.010e-26	4.00
Fe2(OH)2+4	-1.230e-27	6.149e-28	-2.00
FeCl3	-1.427e-28	7.134e-29	-2.00
Cd(OH)4-2	3.785e-31	9.462e-32	4.00

Fe3(OH)4+5	-5.550e-37	2.775e-37	-2.00

----------Saturation indices----------

Phase	SI**	log IAP	log K(297 K, 1 atm)	
Al(OH)3(a)	-2.09	8.76	10.85	Al(OH)3
Alunite	-2.93	-4.24	-1.31	KAl3(SO4)2(OH)6
Anglesite	-5.09	-12.88	-7.79	PbSO4
Anhydrite	-3.30	-7.57	-4.27	CaSO4
Aragonite	-2.36	-10.69	-8.33	CaCO3
BaCl2	-14.65	-12.42	2.23	BaCl2
BaCl2:2H2O	-12.62	-12.42	0.20	BaCl2:2H2O
BaCl2:H2O	-13.24	-12.42	0.82	BaCl2:H2O
Barite	0.65	-9.20	-9.85	BaSO4
Calcite	-2.22	-10.69	-8.48	CaCO3
Cd(OH)2	-9.62	4.03	13.65	Cd(OH)2
CdSO4	-12.12	-12.20	-0.07	CdSO4
Cerussite	-2.86	-16.00	-13.14	PbCO3
CO2(g)	-1.19	-2.65	-1.46	CO2
Dolomite	-4.69	-21.76	-17.07	CaMg(CO3)2
Fe(OH)3(a)	-5.00	-0.11	4.89	Fe(OH)3
Fluorite	-1.65	-12.26	-10.61	CaF2
Gibbsite	0.61	8.76	8.15	Al(OH)3
Goethite	0.86	-0.11	-0.97	FeOOH
Gypsum	-2.99	-7.57	-4.58	CaSO4:2H2O
H2(g)	-12.81	-15.91	-3.10	H2
H2O(g)	-1.52	-0.00	1.52	H2O
Halite	-8.39	-6.82	1.57	NaCl
Hausmannite	-29.60	31.61	61.21	Mn3O4
Hematite	3.73	-0.23	-3.95	Fe2O3
Hydroxyapatite	-10.76	-14.12	-3.36	Ca5(PO4)3OH
Jarosite-K	-21.70	-30.86	-9.15	KFe3(SO4)2(OH)6
Manganite	-12.68	12.66	25.34	MnOOH
Melanterite	-7.46	-9.68	-2.22	FeSO4:7H2O
O2(g)	-57.92	-60.81	-2.89	O2
Otavite	-3.22	-15.32	-12.10	CdCO3
Pb(OH)2	-4.83	3.35	8.18	Pb(OH)2
Pyrochroite	-8.92	6.28	15.20	Mn(OH)2
Pyrolusite	-22.46	19.04	41.50	MnO2:H2O
Rhodochrosite	-1.93	-13.06	-11.13	MnCO3
Siderite	-1.91	-12.80	-10.89	FeCO3
Smithsonite	-3.13	-13.12	-9.99	ZnCO3
Sylvite	-8.69	-7.79	0.90	KCl
Vivianite	-7.32	-43.32	-36.00	Fe3(PO4)2:8H2O
Witherite	-3.76	-12.32	-8.56	BaCO3
Zn(OH)2(e)	-5.28	6.22	11.50	Zn(OH)2

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
For ideal gases, phi = 1.

Initial solution 21.

----------Solution composition----------

Elements	Molality	Moles
Al	8.203e-07	8.203e-07
Alkalinity	1.638e-03	1.638e-03
B	1.147e-05	1.147e-05
Ba	1.304e-05	1.304e-05
Br	5.007e-06	5.007e-06
Ca	3.493e-04	3.493e-04
Cd	5.428e-09	5.428e-09
Cl	1.128e-04	1.128e-04
Cu	3.226e-08	3.226e-08
F	5.370e-05	5.370e-05
Fe	1.413e-07	1.413e-07

K	5.116e-05	5.116e-05
Mg	1.645e-04	1.645e-04
Mn	7.519e-08	7.519e-08
N(5)	3.542e-04	3.542e-04
Na	7.831e-04	7.831e-04
P	9.687e-08	9.687e-08
Pb	3.138e-09	3.138e-09
S(6)	2.082e-05	2.082e-05
Zn	1.927e-06	1.927e-06

----------Description of solution----------

pH	= 6.400
pe	= 0.313
Specific Conductance (µS/cm, 25°C)	= 204
Density (g/cm³)	= 0.99709
Volume (L)	= 1.00315
Activity of water	= 1.000
Ionic strength (mol/kgw)	= 2.574e-03
Mass of water (kg)	= 1.000e+00
Total carbon (mol/kg)	= 3.011e-03
Total CO2 (mol/kg)	= 3.011e-03
Temperature (°C)	= 25.37
Electrical balance (eq)	= -3.107e-04
Percent error, 100*(Cat-|An|)/(Cat+|An|)	= -7.63
Iterations	= 11 (223 overall)
Total H	= 1.110141e+02
Total O	= 5.551506e+01

----------Distribution of species----------

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma	mole V cm³/mol
H+	4.193e-07	3.981e-07	-6.377	-6.400	-0.023	0.00
OH-	2.766e-08	2.615e-08	-7.558	-7.583	-0.024	-4.07
H2O	5.551e+01	9.999e-01	1.744	-0.000	0.000	18.07
Al	8.203e-07					
AlF2+	4.607e-07	4.362e-07	-6.337	-6.360	-0.024	(0)
AlF3	2.669e-07	2.671e-07	-6.574	-6.573	0.000	(0)
Al(OH)4-	3.643e-08	3.447e-08	-7.439	-7.463	-0.024	(0)
AlF+2	2.223e-08	1.787e-08	-7.653	-7.748	-0.095	(0)
Al(OH)2+	2.012e-08	1.905e-08	-7.696	-7.720	-0.024	(0)
Al(OH)3	7.239e-09	7.244e-09	-8.140	-8.140	0.000	(0)
AlF4-	5.464e-09	5.169e-09	-8.262	-8.287	-0.024	(0)
AlOH+2	1.166e-09	9.370e-10	-8.933	-9.028	-0.095	-27.71
Al+3	5.846e-11	3.667e-11	-10.233	-10.436	-0.203	-42.18
AlSO4+	1.919e-12	1.816e-12	-11.717	-11.741	-0.024	(0)
Al(SO4)2-	9.475e-16	8.964e-16	-15.023	-15.048	-0.024	(0)
AlHSO4+2	8.040e-20	6.431e-20	-19.095	-19.192	-0.097	(0)
B	1.147e-05					
H3BO3	1.145e-05	1.146e-05	-4.941	-4.941	0.000	39.26
H2BO3-	1.764e-08	1.668e-08	-7.754	-7.778	-0.024	(0)
BF(OH)3-	2.355e-10	2.227e-10	-9.628	-9.652	-0.024	(0)
BF2(OH)2-	4.882e-13	4.617e-13	-12.311	-12.336	-0.024	(0)
BF3OH-	1.029e-17	9.733e-18	-16.988	-17.012	-0.024	(0)
BF4-	8.112e-22	7.671e-22	-21.091	-21.115	-0.024	(0)
Ba	1.304e-05					
Ba+2	1.279e-05	1.024e-05	-4.893	-4.990	-0.097	-12.66
BaHCO3+	1.618e-07	1.530e-07	-6.791	-6.815	-0.024	(0)
BaSO4	7.990e-08	7.995e-08	-7.097	-7.097	0.000	(0)
BaCl+	3.637e-09	3.440e-09	-8.439	-8.463	-0.024	(0)
BaCO3	9.740e-10	9.746e-10	-9.011	-9.011	0.000	-10.70
BaNO3+	4.559e-10	4.312e-10	-9.341	-9.365	-0.024	(0)
BaOH+	9.204e-13	8.711e-13	-12.036	-12.060	-0.024	(0)
Br	5.007e-06					
Br-	5.007e-06	4.730e-06	-5.300	-5.325	-0.025	24.59
CdBr+	3.038e-12	2.873e-12	-11.517	-11.542	-0.024	(0)

ZnBr+	1.695e-12	1.603e-12	-11.771	-11.795	-0.024	(0)
PbBr+	1.604e-13	1.517e-13	-12.795	-12.819	-0.024	(0)
CdBr2	7.306e-17	7.310e-17	-16.136	-16.136	0.000	(0)
ZnBr2	3.016e-18	3.018e-18	-17.521	-17.520	0.000	(0)
PbBr2	3.334e-19	3.336e-19	-18.477	-18.477	0.000	(0)
C(4)	3.011e-03					
HCO3-	1.628e-03	1.542e-03	-2.788	-2.812	-0.024	24.73
CO2	1.373e-03	1.374e-03	-2.862	-2.862	0.000	34.45
CaHCO3+	5.748e-06	5.445e-06	-5.240	-5.264	-0.024	9.70
MgHCO3+	2.477e-06	2.343e-06	-5.606	-5.630	-0.024	5.50
NaHCO3	6.396e-07	6.400e-07	-6.194	-6.194	0.000	1.80
ZnHCO3+	2.643e-07	2.500e-07	-6.578	-6.602	-0.024	(0)
CO3-2	2.277e-07	1.829e-07	-6.643	-6.738	-0.095	-5.17
BaHCO3+	1.618e-07	1.530e-07	-6.791	-6.815	-0.024	(0)
CaCO3	8.519e-08	8.524e-08	-7.070	-7.069	0.000	-14.60
ZnCO3	4.699e-08	4.702e-08	-7.328	-7.328	0.000	(0)
(CO2)2	3.504e-08	3.506e-08	-7.455	-7.455	0.000	68.90
MgCO3	2.275e-08	2.277e-08	-7.643	-7.643	0.000	-17.09
FeHCO3+	1.629e-08	1.541e-08	-7.788	-7.812	-0.024	(0)
MnHCO3+	7.766e-09	7.350e-09	-8.110	-8.134	-0.024	(0)
NaCO3-	2.715e-09	2.568e-09	-8.566	-8.590	-0.024	-0.97
PbCO3	1.720e-09	1.721e-09	-8.764	-8.764	0.000	(0)
BaCO3	9.740e-10	9.746e-10	-9.011	-9.011	0.000	-10.70
MnCO3	7.770e-10	7.774e-10	-9.110	-9.109	0.000	(0)
PbHCO3+	7.010e-10	6.629e-10	-9.154	-9.179	-0.024	(0)
FeCO3	4.383e-10	4.386e-10	-9.358	-9.358	0.000	(0)
Zn(CO3)2-2	2.299e-10	1.839e-10	-9.638	-9.735	-0.097	(0)
CdHCO3+	2.120e-10	2.005e-10	-9.674	-9.698	-0.024	(0)
CuCO3	1.150e-10	1.151e-10	-9.939	-9.939	0.000	(0)
CuHCO3+	9.571e-11	9.051e-11	-10.019	-10.043	-0.024	(0)
Pb(CO3)2-2	9.888e-13	7.909e-13	-12.005	-12.102	-0.097	(0)
CdCO3	5.974e-13	5.977e-13	-12.224	-12.224	0.000	(0)
Cu(CO3)2-2	3.314e-14	2.651e-14	-13.480	-13.577	-0.097	(0)
Cd(CO3)2-2	4.323e-16	3.458e-16	-15.364	-15.461	-0.097	(0)
Ca	3.493e-04					
Ca+2	3.427e-04	2.753e-04	-3.465	-3.560	-0.095	-18.07
CaHCO3+	5.748e-06	5.445e-06	-5.240	-5.264	-0.024	9.70
CaSO4	7.647e-07	7.651e-07	-6.117	-6.116	0.000	7.51
CaCO3	8.519e-08	8.524e-08	-7.070	-7.069	0.000	-14.60
CaHPO4	1.765e-09	1.767e-09	-8.753	-8.753	0.000	(0)
CaH2PO4+	5.573e-10	5.276e-10	-9.254	-9.278	-0.024	(0)
CaOH+	1.213e-10	1.148e-10	-9.916	-9.940	-0.024	(0)
CaPO4-	1.117e-11	1.057e-11	-10.952	-10.976	-0.024	(0)
CaHSO4+	2.128e-12	2.013e-12	-11.672	-11.696	-0.024	(0)
Cd	5.428e-09					
Cd+2	5.142e-09	4.113e-09	-8.289	-8.386	-0.097	-18.67
CdHCO3+	2.120e-10	2.005e-10	-9.674	-9.698	-0.024	(0)
CdCl+	4.418e-11	4.178e-11	-10.355	-10.379	-0.024	5.95
CdSO4	1.852e-11	1.853e-11	-10.732	-10.732	0.000	77.87
CdNO3+	3.616e-12	3.420e-12	-11.442	-11.466	-0.024	17.53
CdBr+	3.038e-12	2.873e-12	-11.517	-11.542	-0.024	(0)
CdF+	2.662e-12	2.517e-12	-11.575	-11.599	-0.024	(0)
CdOH+	9.338e-13	8.831e-13	-12.030	-12.054	-0.024	(0)
CdCO3	5.974e-13	5.977e-13	-12.224	-12.224	0.000	(0)
CdOHCl	4.366e-14	4.369e-14	-13.360	-13.360	0.000	(0)
CdCl2	1.852e-14	1.853e-14	-13.732	-13.732	0.000	23.14
Cd(SO4)2-2	3.950e-15	3.159e-15	-14.403	-14.500	-0.097	-105.35
Cd(CO3)2-2	4.323e-16	3.458e-16	-15.364	-15.461	-0.097	(0)
CdF2	3.073e-16	3.074e-16	-15.512	-15.512	0.000	(0)
Cd(OH)2	1.158e-16	1.159e-16	-15.936	-15.936	0.000	(0)
CdBr2	7.306e-17	7.310e-17	-16.136	-16.136	0.000	(0)
CdCl3-	1.320e-18	1.249e-18	-17.879	-17.904	-0.024	69.07
Cd2OH+3	2.927e-20	1.771e-20	-19.534	-19.752	-0.218	(0)
Cd(OH)3-	3.454e-23	3.266e-23	-22.462	-22.486	-0.024	(0)
Cd(OH)4-2	9.141e-31	7.312e-31	-30.039	-30.136	-0.097	(0)
Cl	1.128e-04					
Cl-	1.124e-04	1.062e-04	-3.949	-3.974	-0.024	18.10
NaCl	4.712e-07	4.715e-07	-6.327	-6.327	0.000	(0)

BaCl+	3.637e-09	3.440e-09	-8.439	-8.463	-0.024	(0)
ZnCl+	3.958e-10	3.743e-10	-9.402	-9.427	-0.024	-13.53
CuCl2-	1.132e-10	1.070e-10	-9.946	-9.971	-0.024	(0)
CdCl+	4.418e-11	4.178e-11	-10.355	-10.379	-0.024	5.95
MnCl+	2.446e-11	2.315e-11	-10.612	-10.635	-0.024	-2.99
FeCl+	1.550e-11	1.466e-11	-10.810	-10.834	-0.024	(0)
ZnOHCl	1.137e-11	1.138e-11	-10.944	-10.944	0.000	(0)
PbCl+	2.443e-12	2.311e-12	-11.612	-11.636	-0.024	7.98
CdOHCl	4.366e-14	4.369e-14	-13.360	-13.360	0.000	(0)
ZnCl2	4.168e-14	4.170e-14	-13.380	-13.380	0.000	101.31
CuCl+	3.607e-14	3.411e-14	-13.443	-13.467	-0.024	0.55
CuCl3-2	2.248e-14	1.804e-14	-13.648	-13.744	-0.096	(0)
CdCl2	1.852e-14	1.853e-14	-13.732	-13.732	0.000	23.14
MnCl2	1.073e-15	1.074e-15	-14.969	-14.969	0.000	85.44
PbCl2	3.861e-16	3.864e-16	-15.413	-15.413	0.000	35.00
ZnCl3-	5.268e-18	4.982e-18	-17.278	-17.303	-0.024	17.02
CuCl2	1.953e-18	1.954e-18	-17.709	-17.709	0.000	31.44
CdCl3-	1.320e-18	1.249e-18	-17.879	-17.904	-0.024	69.07
PbCl3-	3.455e-20	3.268e-20	-19.462	-19.486	-0.024	66.01
MnCl3-	3.319e-20	3.141e-20	-19.479	-19.503	-0.024	43.36
ZnCl4-2	3.315e-22	2.660e-22	-21.479	-21.575	-0.096	145.29
FeCl+2	8.100e-23	6.499e-23	-22.092	-22.187	-0.096	(0)
PbCl4-2	2.083e-24	1.666e-24	-23.681	-23.778	-0.097	101.48
CuCl3-	7.839e-25	7.413e-25	-24.106	-24.130	-0.024	(0)
FeCl2+	3.221e-26	3.048e-26	-25.492	-25.516	-0.024	(0)
CuCl4-2	4.961e-31	3.981e-31	-30.304	-30.400	-0.096	(0)
FeCl3	3.236e-31	3.238e-31	-30.490	-30.490	0.000	(0)
Cu(1)	3.189e-08					
Cu+	3.178e-08	3.001e-08	-7.498	-7.523	-0.025	(0)
CuCl2-	1.132e-10	1.070e-10	-9.946	-9.971	-0.024	(0)
CuCl3-2	2.248e-14	1.804e-14	-13.648	-13.744	-0.096	(0)
Cu(2)	3.753e-10					
Cu+2	1.455e-10	1.172e-10	-9.837	-9.931	-0.094	-26.55
CuCO3	1.150e-10	1.151e-10	-9.939	-9.939	0.000	(0)
CuHCO3+	9.571e-11	9.051e-11	-10.019	-10.043	-0.024	(0)
Cu(OH)2	1.543e-11	1.544e-11	-10.812	-10.811	0.000	(0)
CuOH+	3.112e-12	2.942e-12	-11.507	-11.531	-0.024	(0)
CuSO4	3.735e-13	3.737e-13	-12.428	-12.427	0.000	13.14
CuF+	1.100e-13	1.040e-13	-12.959	-12.983	-0.024	(0)
CuCl+	3.607e-14	3.411e-14	-13.443	-13.467	-0.024	0.55
Cu(CO3)2-2	3.314e-14	2.651e-14	-13.480	-13.577	-0.097	(0)
Cu2(OH)2+2	4.913e-18	3.930e-18	-17.309	-17.406	-0.097	(0)
Cu(OH)3-	2.471e-18	2.337e-18	-17.607	-17.631	-0.024	(0)
CuCl2	1.953e-18	1.954e-18	-17.709	-17.709	0.000	31.44
Cu(OH)4-2	1.464e-24	1.171e-24	-23.834	-23.931	-0.097	(0)
CuCl3-	7.839e-25	7.413e-25	-24.106	-24.130	-0.024	(0)
CuCl4-2	4.961e-31	3.981e-31	-30.304	-30.400	-0.096	(0)
F	5.370e-05					
F-	5.144e-05	4.862e-05	-4.289	-4.313	-0.024	-1.29
AlF2+	4.607e-07	4.362e-07	-6.337	-6.360	-0.024	(0)
MgF+	4.432e-07	4.193e-07	-6.353	-6.377	-0.024	-10.56
AlF3	2.669e-07	2.671e-07	-6.574	-6.573	0.000	(0)
HF	2.920e-08	2.922e-08	-7.535	-7.534	0.000	12.52
AlF+2	2.223e-08	1.787e-08	-7.653	-7.748	-0.095	(0)
NaF	2.068e-08	2.070e-08	-7.684	-7.684	0.000	7.28
AlF4-	5.464e-09	5.169e-09	-8.262	-8.287	-0.024	(0)
ZnF+	9.397e-10	8.886e-10	-9.027	-9.051	-0.024	(0)
BF(OH)3-	2.355e-10	2.227e-10	-9.628	-9.652	-0.024	(0)
FeF+	5.138e-11	4.859e-11	-10.289	-10.313	-0.024	(0)
MnF+	1.901e-11	1.799e-11	-10.721	-10.745	-0.024	(0)
HF2-	5.781e-12	5.467e-12	-11.238	-11.262	-0.024	22.10
CdF+	2.662e-12	2.517e-12	-11.575	-11.599	-0.024	(0)
PbF+	4.949e-13	4.680e-13	-12.305	-12.330	-0.024	(0)
BF2(OH)2-	4.882e-13	4.617e-13	-12.311	-12.336	-0.024	(0)
CuF+	1.100e-13	1.040e-13	-12.959	-12.983	-0.024	(0)
PbF2	4.643e-16	4.646e-16	-15.333	-15.333	0.000	(0)
CdF2	3.073e-16	3.074e-16	-15.512	-15.512	0.000	(0)
BF3OH-	1.029e-17	9.733e-18	-16.988	-17.012	-0.024	(0)

FeF2+	3.187e-18	3.016e-18	-17.497	-17.521	-0.024	(0)
FeF+2	1.934e-18	1.552e-18	-17.714	-17.809	-0.096	(0)
FeF3	2.326e-19	2.327e-19	-18.633	-18.633	0.000	(0)
PbF3-	1.730e-19	1.636e-19	-18.762	-18.786	-0.024	(0)
BF4-	8.112e-22	7.671e-22	-21.091	-21.115	-0.024	(0)
PbF4-2	4.761e-24	3.808e-24	-23.322	-23.419	-0.097	(0)
Fe(2)	1.413e-07					
Fe+2	1.241e-07	9.994e-08	-6.906	-7.000	-0.094	-22.05
FeHCO3+	1.629e-08	1.541e-08	-7.788	-7.812	-0.024	(0)
FeCO3	4.383e-10	4.386e-10	-9.358	-9.358	0.000	(0)
FeSO4	2.787e-10	2.789e-10	-9.555	-9.555	0.000	18.58
FeOH+	8.621e-11	8.160e-11	-10.064	-10.088	-0.024	(0)
FeF+	5.138e-11	4.859e-11	-10.289	-10.313	-0.024	(0)
FeCl+	1.550e-11	1.466e-11	-10.810	-10.834	-0.024	(0)
FeHPO4	4.621e-12	4.624e-12	-11.335	-11.335	0.000	(0)
FeH2PO4+	3.935e-12	3.725e-12	-11.405	-11.429	-0.024	(0)
Fe(OH)2	1.800e-15	1.801e-15	-14.745	-14.744	0.000	(0)
FeHSO4+	7.726e-16	7.307e-16	-15.112	-15.136	-0.024	(0)
Fe(OH)3-	1.783e-19	1.687e-19	-18.749	-18.773	-0.024	(0)
Fe(3)	3.882e-13					
Fe(OH)2+	2.956e-13	2.799e-13	-12.529	-12.553	-0.024	(0)
Fe(OH)3	9.198e-14	9.203e-14	-13.036	-13.036	0.000	(0)
FeOH+2	4.135e-16	3.318e-16	-15.383	-15.479	-0.096	(0)
Fe(OH)4-	2.260e-16	2.140e-16	-15.646	-15.670	-0.024	(0)
FeF2+	3.187e-18	3.016e-18	-17.497	-17.521	-0.024	(0)
FeF+2	1.934e-18	1.552e-18	-17.714	-17.809	-0.096	(0)
FeF3	2.326e-19	2.327e-19	-18.633	-18.633	0.000	(0)
Fe+3	3.193e-20	2.002e-20	-19.496	-19.698	-0.203	(0)
FeSO4+	3.645e-21	3.450e-21	-20.438	-20.462	-0.024	(0)
FeH2PO4+2	4.988e-22	4.008e-22	-21.302	-21.397	-0.095	(0)
FeCl+2	8.100e-23	6.499e-23	-22.092	-22.187	-0.096	(0)
FeHPO4+	6.698e-23	6.340e-23	-22.174	-22.198	-0.024	(0)
Fe(SO4)2-	1.246e-24	1.178e-24	-23.905	-23.929	-0.024	(0)
FeCl2+	3.221e-26	3.048e-26	-25.492	-25.516	-0.024	(0)
FeHSO4+2	4.597e-27	3.677e-27	-26.337	-26.434	-0.097	(0)
Fe2(OH)2+4	7.131e-30	2.919e-30	-29.147	-29.535	-0.388	(0)
FeCl3	3.236e-31	3.238e-31	-30.490	-30.490	0.000	(0)
Fe3(OH)4+5	6.661e-40	1.650e-40	-39.176	-39.783	-0.606	(0)
H(0)	5.287e-17					
H2	2.643e-17	2.645e-17	-16.578	-16.578	0.000	28.61
K	5.116e-05					
K+	5.115e-05	4.835e-05	-4.291	-4.316	-0.024	9.04
KSO4-	5.629e-09	5.329e-09	-8.250	-8.273	-0.024	34.13
KHPO4-	1.157e-12	1.096e-12	-11.937	-11.960	-0.024	38.11
Mg	1.645e-04					
Mg+2	1.611e-04	1.297e-04	-3.793	-3.887	-0.094	-21.77
MgHCO3+	2.477e-06	2.343e-06	-5.606	-5.630	-0.024	5.50
MgSO4	4.780e-07	4.783e-07	-6.321	-6.320	0.000	5.85
MgF+	4.432e-07	4.193e-07	-6.353	-6.377	-0.024	-10.56
MgCO3	2.275e-08	2.277e-08	-7.643	-7.643	0.000	-17.09
MgOH+	1.290e-09	1.223e-09	-8.889	-8.913	-0.023	(0)
MgHPO4	1.124e-09	1.125e-09	-8.949	-8.949	0.000	(0)
MgH2PO4+	3.342e-10	3.165e-10	-9.476	-9.500	-0.024	(0)
MgPO4-	7.094e-12	6.717e-12	-11.149	-11.173	-0.024	(0)
Mn(2)	7.519e-08					
Mn+2	6.645e-08	5.350e-08	-7.178	-7.272	-0.094	-20.59
MnHCO3+	7.766e-09	7.350e-09	-8.110	-8.134	-0.024	(0)
MnCO3	7.770e-10	7.774e-10	-9.110	-9.109	0.000	(0)
MnSO4	1.492e-10	1.493e-10	-9.826	-9.826	0.000	22.38
MnCl+	2.446e-11	2.315e-11	-10.612	-10.635	-0.024	-2.99
MnF+	1.901e-11	1.799e-11	-10.721	-10.745	-0.024	(0)
MnOH+	3.761e-12	3.559e-12	-11.425	-11.449	-0.024	(0)
Mn(NO3)2	2.381e-14	2.383e-14	-13.623	-13.623	0.000	40.94
MnCl2	1.073e-15	1.074e-15	-14.969	-14.969	0.000	85.44
MnCl3-	3.319e-20	3.141e-20	-19.479	-19.503	-0.024	43.36
Mn(OH)3-	1.419e-23	1.343e-23	-22.848	-22.872	-0.024	(0)
Mn(3)	5.720e-33					
Mn+3	5.720e-33	3.587e-33	-32.243	-32.445	-0.203	(0)

N(5)	3.542e-04					
NO3-	3.542e-04	3.346e-04	-3.451	-3.475	-0.025	29.54
BaNO3+	4.559e-10	4.312e-10	-9.341	-9.365	-0.024	(0)
CdNO3+	3.616e-12	3.420e-12	-11.442	-11.466	-0.024	17.53
PbNO3+	2.833e-12	2.679e-12	-11.548	-11.572	-0.024	(0)
Mn(NO3)2	2.381e-14	2.383e-14	-13.623	-13.623	0.000	40.94
Na	7.831e-04					
Na+	7.819e-04	7.398e-04	-3.107	-3.131	-0.024	-1.43
NaHCO3	6.396e-07	6.400e-07	-6.194	-6.194	0.000	1.80
NaCl	4.712e-07	4.715e-07	-6.327	-6.327	0.000	(0)
NaSO4-	6.118e-08	5.792e-08	-7.213	-7.237	-0.024	13.89
NaF	2.068e-08	2.070e-08	-7.684	-7.684	0.000	7.28
NaCO3-	2.715e-09	2.568e-09	-8.566	-8.590	-0.024	-0.97
NaHPO4-	1.771e-11	1.677e-11	-10.752	-10.776	-0.024	33.61
NaOH	1.933e-21	1.934e-21	-20.714	-20.713	0.000	(0)
O(0)	0.000e+00					
O2	0.000e+00	0.000e+00	-59.106	-59.106	0.000	30.43
P	9.687e-08					
H2PO4-	7.855e-08	7.437e-08	-7.105	-7.129	-0.024	33.22
HPO4-2	1.448e-08	1.162e-08	-7.839	-7.935	-0.096	6.77
CaHPO4	1.765e-09	1.767e-09	-8.753	-8.753	0.000	(0)
MgHPO4	1.124e-09	1.125e-09	-8.949	-8.949	0.000	(0)
CaH2PO4+	5.573e-10	5.276e-10	-9.254	-9.278	-0.024	(0)
MgH2PO4+	3.342e-10	3.165e-10	-9.476	-9.500	-0.024	(0)
NaHPO4-	1.771e-11	1.677e-11	-10.752	-10.776	-0.024	33.61
CaPO4-	1.117e-11	1.057e-11	-10.952	-10.976	-0.024	(0)
MgPO4-	7.094e-12	6.717e-12	-11.149	-11.173	-0.024	(0)
FeHPO4	4.621e-12	4.624e-12	-11.335	-11.335	0.000	(0)
H3PO4	4.376e-12	4.378e-12	-11.359	-11.359	0.000	47.43
FeH2PO4+	3.935e-12	3.725e-12	-11.405	-11.429	-0.024	(0)
KHPO4-	1.157e-12	1.096e-12	-11.937	-11.960	-0.024	38.11
PO4-3	2.193e-14	1.326e-14	-13.659	-13.877	-0.218	-23.11
FeH2PO4+2	4.988e-22	4.008e-22	-21.302	-21.397	-0.095	(0)
FeHPO4+	6.698e-23	6.340e-23	-22.174	-22.198	-0.024	(0)
Pb	3.138e-09					
PbCO3	1.720e-09	1.721e-09	-8.764	-8.764	0.000	(0)
PbHCO3+	7.010e-10	6.629e-10	-9.154	-9.179	-0.024	(0)
Pb+2	6.768e-10	5.414e-10	-9.170	-9.267	-0.097	-15.48
PbOH+	2.804e-11	2.651e-11	-10.552	-10.577	-0.024	(0)
PbSO4	4.742e-12	4.745e-12	-11.324	-11.324	0.000	(0)
PbNO3+	2.833e-12	2.679e-12	-11.548	-11.572	-0.024	(0)
PbCl+	2.443e-12	2.311e-12	-11.612	-11.636	-0.024	7.98
Pb(CO3)2-2	9.888e-13	7.909e-13	-12.005	-12.102	-0.097	(0)
PbF+	4.949e-13	4.680e-13	-12.305	-12.330	-0.024	(0)
PbBr+	1.604e-13	1.517e-13	-12.795	-12.819	-0.024	(0)
Pb(OH)2	2.589e-14	2.591e-14	-13.587	-13.587	0.000	(0)
Pb(SO4)2-2	4.852e-16	3.881e-16	-15.314	-15.411	-0.097	(0)
PbF2	4.643e-16	4.646e-16	-15.333	-15.333	0.000	(0)
PbCl2	3.861e-16	3.864e-16	-15.413	-15.413	0.000	35.00
Pb(OH)3-	7.900e-19	7.471e-19	-18.102	-18.127	-0.024	(0)
Pb2OH+3	5.311e-19	3.213e-19	-18.275	-18.493	-0.218	(0)
PbBr2	3.334e-19	3.336e-19	-18.477	-18.477	0.000	(0)
PbF3-	1.730e-19	1.636e-19	-18.762	-18.786	-0.024	(0)
PbCl3-	3.455e-20	3.268e-20	-19.462	-19.486	-0.024	66.01
Pb(OH)4-2	5.374e-24	4.299e-24	-23.270	-23.367	-0.097	(0)
PbF4-2	4.761e-24	3.808e-24	-23.322	-23.419	-0.097	(0)
PbCl4-2	2.083e-24	1.666e-24	-23.681	-23.778	-0.097	101.48
Pb3(OH)4+2	1.100e-26	8.798e-27	-25.959	-26.056	-0.097	(0)
S(6)	2.082e-05					
SO4-2	1.943e-05	1.559e-05	-4.712	-4.807	-0.096	14.63
CaSO4	7.647e-07	7.651e-07	-6.117	-6.116	0.000	7.51
MgSO4	4.780e-07	4.783e-07	-6.321	-6.320	0.000	5.85
BaSO4	7.990e-08	7.995e-08	-7.097	-7.097	0.000	(0)
NaSO4-	6.118e-08	5.792e-08	-7.213	-7.237	-0.024	13.89
KSO4-	5.629e-09	5.329e-09	-8.250	-8.273	-0.024	34.13
ZnSO4	4.716e-09	4.719e-09	-8.326	-8.326	0.000	21.66
HSO4-	6.430e-10	6.081e-10	-9.192	-9.216	-0.024	40.32
FeSO4	2.787e-10	2.789e-10	-9.555	-9.555	0.000	18.58

MnSO4	1.492e-10	1.493e-10	-9.826	-9.826	0.000	22.38
CdSO4	1.852e-11	1.853e-11	-10.732	-10.732	0.000	77.87
PbSO4	4.742e-12	4.745e-12	-11.324	-11.324	0.000	(0)
CaHSO4+	2.128e-12	2.013e-12	-11.672	-11.696	-0.024	(0)
AlSO4+	1.919e-12	1.816e-12	-11.717	-11.741	-0.024	(0)
Zn(SO4)2-2	7.453e-13	5.961e-13	-12.128	-12.225	-0.097	-12.74
CuSO4	3.735e-13	3.737e-13	-12.428	-12.427	0.000	13.14
Cd(SO4)2-2	3.950e-15	3.159e-15	-14.403	-14.500	-0.097	-105.35
Al(SO4)2-	9.475e-16	8.964e-16	-15.023	-15.048	-0.024	(0)
FeHSO4+	7.726e-16	7.307e-16	-15.112	-15.136	-0.024	(0)
Pb(SO4)2-2	4.852e-16	3.881e-16	-15.314	-15.411	-0.097	(0)
AlHSO4+2	8.040e-20	6.431e-20	-19.095	-19.192	-0.097	(0)
FeSO4+	3.645e-21	3.450e-21	-20.438	-20.462	-0.024	(0)
Fe(SO4)2-	1.246e-24	1.178e-24	-23.905	-23.929	-0.024	(0)
FeHSO4+2	4.597e-27	3.677e-27	-26.337	-26.434	-0.097	(0)
Zn	1.927e-06					
Zn+2	1.605e-06	1.288e-06	-5.794	-5.890	-0.096	-25.32
ZnHCO3+	2.643e-07	2.500e-07	-6.578	-6.602	-0.024	(0)
ZnCO3	4.699e-08	4.702e-08	-7.328	-7.328	0.000	(0)
ZnSO4	4.716e-09	4.719e-09	-8.326	-8.326	0.000	21.66
ZnOH+	3.857e-09	3.648e-09	-8.414	-8.438	-0.024	(0)
ZnF+	9.397e-10	8.886e-10	-9.027	-9.051	-0.024	(0)
ZnCl+	3.958e-10	3.743e-10	-9.402	-9.427	-0.024	-13.53
Zn(CO3)2-2	2.299e-10	1.839e-10	-9.638	-9.735	-0.097	(0)
Zn(OH)2	1.022e-10	1.023e-10	-9.990	-9.990	0.000	(0)
ZnOHCl	1.137e-11	1.138e-11	-10.944	-10.944	0.000	(0)
ZnBr+	1.695e-12	1.603e-12	-11.771	-11.795	-0.024	(0)
Zn(SO4)2-2	7.453e-13	5.961e-13	-12.128	-12.225	-0.097	-12.74
ZnCl2	4.168e-14	4.170e-14	-13.380	-13.380	0.000	101.31
Zn(OH)3-	8.591e-16	8.125e-16	-15.066	-15.090	-0.024	(0)
ZnCl3-	5.268e-18	4.982e-18	-17.278	-17.303	-0.024	17.02
ZnBr2	3.016e-18	3.018e-18	-17.521	-17.520	0.000	(0)
Zn(OH)4-2	4.043e-22	3.234e-22	-21.393	-21.490	-0.097	(0)
ZnCl4-2	3.315e-22	2.660e-22	-21.479	-21.575	-0.096	145.29

----------Distribution of alkalinity----------

Total alkalinity (eq/kgw) = 1.638e-03

Species	Alkalinity	Molality	Alk/Mol
HCO3-	1.628e-03	1.628e-03	1.00
CaHCO3+	5.748e-06	5.748e-06	1.00
MgHCO3+	2.477e-06	2.477e-06	1.00
NaHCO3	6.396e-07	6.396e-07	1.00
CO3-2	4.554e-07	2.277e-07	2.00
H+	-4.193e-07	4.193e-07	-1.00
ZnHCO3+	2.643e-07	2.643e-07	1.00
CaCO3	1.704e-07	8.519e-08	2.00
BaHCO3+	1.618e-07	1.618e-07	1.00
Al(OH)4-	1.457e-07	3.643e-08	4.00
ZnCO3	9.398e-08	4.699e-08	2.00
MgCO3	4.550e-08	2.275e-08	2.00
Al(OH)2+	4.024e-08	2.012e-08	2.00
HF	-2.920e-08	2.920e-08	-1.00
OH-	2.766e-08	2.766e-08	1.00
Al(OH)3	2.172e-08	7.239e-09	3.00
H2BO3-	1.764e-08	1.764e-08	1.00
FeHCO3+	1.629e-08	1.629e-08	1.00
HPO4-2	1.448e-08	1.448e-08	1.00
MnHCO3+	7.766e-09	7.766e-09	1.00
NaCO3-	5.430e-09	2.715e-09	2.00
ZnOH+	3.857e-09	3.857e-09	1.00
PbCO3	3.440e-09	1.720e-09	2.00
BaCO3	1.948e-09	9.740e-10	2.00
CaHPO4	1.765e-09	1.765e-09	1.00
MnCO3	1.554e-09	7.770e-10	2.00
MgOH+	1.290e-09	1.290e-09	1.00

AlOH+2	1.166e-09	1.166e-09	1.00
MgHPO4	1.124e-09	1.124e-09	1.00
Zn(CO3)2-2	9.196e-10	2.299e-10	4.00
FeCO3	8.766e-10	4.383e-10	2.00
PbHCO3+	7.010e-10	7.010e-10	1.00
HSO4-	-6.430e-10	6.430e-10	-1.00
CuCO3	2.301e-10	1.150e-10	2.00
CdHCO3+	2.120e-10	2.120e-10	1.00
Zn(OH)2	2.045e-10	1.022e-10	2.00
CaOH+	1.213e-10	1.213e-10	1.00
CuHCO3+	9.571e-11	9.571e-11	1.00
FeOH+	8.621e-11	8.621e-11	1.00
Cu(OH)2	3.086e-11	1.543e-11	2.00
PbOH+	2.804e-11	2.804e-11	1.00
CaPO4-	2.233e-11	1.117e-11	2.00
NaHPO4-	1.771e-11	1.771e-11	1.00
MgPO4-	1.419e-11	7.094e-12	2.00
ZnOHCl	1.137e-11	1.137e-11	1.00
HF2-	-5.781e-12	5.781e-12	-1.00
FeHPO4	4.621e-12	4.621e-12	1.00
H3PO4	-4.376e-12	4.376e-12	-1.00
Pb(CO3)2-2	3.955e-12	9.888e-13	4.00
MnOH+	3.761e-12	3.761e-12	1.00
CuOH+	3.112e-12	3.112e-12	1.00
CaHSO4+	-2.128e-12	2.128e-12	-1.00
CdCO3	1.195e-12	5.974e-13	2.00
KHPO4-	1.157e-12	1.157e-12	1.00
CdOH+	9.338e-13	9.338e-13	1.00
BaOH+	9.204e-13	9.204e-13	1.00
BF2(OH)2-	-4.882e-13	4.882e-13	-1.00
Cu(CO3)2-2	1.326e-13	3.314e-14	4.00
Fe(OH)3	9.198e-14	9.198e-14	1.00
Pb(OH)2	5.178e-14	2.589e-14	2.00
PO4-3	4.385e-14	2.193e-14	2.00
CdOHCl	4.366e-14	4.366e-14	1.00
Fe(OH)2	3.601e-15	1.800e-15	2.00
Zn(OH)3-	2.577e-15	8.591e-16	3.00
Cd(CO3)2-2	1.729e-15	4.323e-16	4.00
FeHSO4+	-7.726e-16	7.726e-16	-1.00
Fe(OH)4-	4.520e-16	2.260e-16	2.00
FeOH+2	-4.135e-16	4.135e-16	-1.00
Cd(OH)2	2.317e-16	1.158e-16	2.00
BF3OH-	-2.058e-17	1.029e-17	-2.00
Cu2(OH)2+2	9.827e-18	4.913e-18	2.00
Cu(OH)3-	7.413e-18	2.471e-18	3.00
FeF2+	-6.374e-18	3.187e-18	-2.00
FeF+2	-3.867e-18	1.934e-18	-2.00
Pb(OH)3-	2.370e-18	7.900e-19	3.00
Fe(OH)3-	5.348e-19	1.783e-19	3.00
Pb2OH+3	5.311e-19	5.311e-19	1.00
FeF3	-4.652e-19	2.326e-19	-2.00
AlHSO4+2	-8.040e-20	8.040e-20	-1.00
Fe+3	-6.385e-20	3.193e-20	-2.00
Cd2OH+3	2.927e-20	2.927e-20	1.00
FeSO4+	-7.290e-21	3.645e-21	-2.00
BF4-	-2.433e-21	8.112e-22	-3.00
NaOH	1.933e-21	1.933e-21	1.00
Zn(OH)4-2	1.617e-21	4.043e-22	4.00
FeH2PO4+2	-9.976e-22	4.988e-22	-2.00
FeCl+2	-1.620e-22	8.100e-23	-2.00
Cd(OH)3-	1.036e-22	3.454e-23	3.00
FeHPO4+	-6.698e-23	6.698e-23	-1.00
Mn(OH)3-	4.258e-23	1.419e-23	3.00
Pb(OH)4-2	2.150e-23	5.374e-24	4.00
Cu(OH)4-2	5.857e-24	1.464e-24	4.00
Fe(SO4)2-	-2.491e-24	1.246e-24	-2.00
FeCl2+	-6.441e-26	3.221e-26	-2.00
Pb3(OH)4+2	4.400e-26	1.100e-26	4.00

FeHSO4+2	-1.379e-26	4.597e-27	-3.00
Fe2(OH)2+4	-1.426e-29	7.131e-30	-2.00
Cd(OH)4-2	3.656e-30	9.141e-31	4.00
FeCl3	-6.473e-31	3.236e-31	-2.00
Fe3(OH)4+5	-1.332e-39	6.661e-40	-2.00

----------Saturation indices----------

Phase	SI**	log IAP	log K(298 K, 1 atm)	
Al(OH)3(a)	-2.01	8.76	10.78	Al(OH)3
Alunite	-5.39	-6.84	-1.45	KAl3(SO4)2(OH)6
Anglesite	-6.29	-14.07	-7.79	PbSO4
Anhydrite	-4.09	-8.37	-4.28	CaSO4
Aragonite	-1.96	-10.30	-8.34	CaCO3
BaCl2	-15.16	-12.94	2.23	BaCl2
BaCl2:2H2O	-13.15	-12.94	0.21	BaCl2:2H2O
BaCl2:H2O	-13.76	-12.94	0.83	BaCl2:H2O
Barite	0.04	-9.80	-9.84	BaSO4
Calcite	-1.82	-10.30	-8.48	CaCO3
Cd(OH)2	-9.24	4.41	13.65	Cd(OH)2
CdSO4	-13.08	-13.19	-0.11	CdSO4
Cerussite	-2.88	-16.00	-13.13	PbCO3
CO2(g)	-1.39	-2.86	-1.47	CO2
Dolomite	-3.82	-20.92	-17.10	CaMg(CO3)2
Fe(OH)3(a)	-5.39	-0.50	4.89	Fe(OH)3
Fluorite	-1.59	-12.19	-10.60	CaF2
Gibbsite	0.67	8.76	8.09	Al(OH)3
Goethite	0.51	-0.50	-1.01	FeOOH
Gypsum	-3.79	-8.37	-4.58	CaSO4:2H2O
H2(g)	-13.48	-16.58	-3.10	H2
H2O(g)	-1.49	-0.00	1.49	H2O
Halite	-8.67	-7.10	1.57	NaCl
Hausmannite	-30.93	30.01	60.94	Mn3O4
Hematite	3.04	-1.00	-4.04	Fe2O3
Hydroxyapatite	-12.55	-16.01	-3.45	Ca5(PO4)3OH
Jarosite-K	-25.39	-34.63	-9.24	KFe3(SO4)2(OH)6
Manganite	-13.10	12.24	25.34	MnOOH
Melanterite	-9.60	-11.81	-2.20	FeSO4:7H2O
O2(g)	-56.21	-59.11	-2.90	O2
Otavite	-3.02	-15.12	-12.10	CdCO3
Pb(OH)2	-4.60	3.53	8.14	Pb(OH)2
Pyrochroite	-9.67	5.53	15.20	Mn(OH)2
Pyrolusite	-22.37	18.95	41.32	MnO2:H2O
Rhodochrosite	-2.88	-14.01	-11.13	MnCO3
Siderite	-2.85	-13.74	-10.89	FeCO3
Smithsonite	-2.62	-12.63	-10.00	ZnCO3
Sylvite	-9.19	-8.29	0.90	KCl
Vivianite	-12.76	-48.76	-36.00	Fe3(PO4)2:8H2O
Witherite	-3.17	-11.73	-8.56	BaCO3
Zn(OH)2(e)	-4.59	6.91	11.50	Zn(OH)2

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
For ideal gases, phi = 1.

Initial solution 22.

----------Solution composition----------

Elements	Molality	Moles
Al	2.302e-07	2.302e-07
Alkalinity	4.915e-03	4.915e-03
B	7.325e-06	7.325e-06
Ba	5.463e-06	5.463e-06
Br	5.509e-06	5.509e-06
Ca	9.060e-04	9.060e-04
Cd	8.099e-09	8.099e-09

Cl	4.515e-04	4.515e-04
Cu	3.054e-08	3.054e-08
F	6.424e-05	6.424e-05
Fe	1.349e-06	1.349e-06
K	1.177e-04	1.177e-04
Mg	3.053e-04	3.053e-04
Mn	2.488e-06	2.488e-06
N(5)	2.293e-04	2.293e-04
Na	2.524e-03	2.524e-03
P	3.682e-06	3.682e-06
Pb	6.567e-09	6.567e-09
S(6)	3.749e-05	3.749e-05
Zn	1.035e-07	1.035e-07

----------Description of solution----------

pH	= 6.900
pe	= 0.437
Specific Conductance (µS/cm, 25°C)	= 498
Density (g/cm³)	= 0.99743
Volume (L)	= 1.00308
Activity of water	= 1.000
Ionic strength (mol/kgw)	= 6.536e-03
Mass of water (kg)	= 1.000e+00
Total carbon (mol/kg)	= 6.172e-03
Total CO2 (mol/kg)	= 6.172e-03
Temperature (°C)	= 24.83
Electrical balance (eq)	= -6.608e-04
Percent error, 100*(Cat-|An|)/(Cat+|An|)	= -6.19
Iterations	= 10 (233 overall)
Total H	= 1.110174e+02
Total O	= 5.552434e+01

----------Distribution of species----------

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma	mole V cm³/mol
H+	1.359e-07	1.259e-07	-6.867	-6.900	-0.033	0.00
OH-	8.655e-08	7.935e-08	-7.063	-7.100	-0.038	-4.06
H2O	5.551e+01	9.998e-01	1.744	-0.000	0.000	18.07
Al	2.302e-07					
Al(OH)4-	1.565e-07	1.438e-07	-6.806	-6.842	-0.037	(0)
AlF2+	3.172e-08	2.920e-08	-7.499	-7.535	-0.036	(0)
AlF3	2.124e-08	2.128e-08	-7.673	-7.672	0.001	(0)
Al(OH)3	9.612e-09	9.627e-09	-8.017	-8.017	0.001	(0)
Al(OH)2+	9.051e-09	8.330e-09	-8.043	-8.079	-0.036	(0)
AlF+2	1.404e-09	1.007e-09	-8.853	-8.997	-0.144	(0)
AlF4-	5.338e-10	4.904e-10	-9.273	-9.309	-0.037	(0)
AlOH+2	1.893e-10	1.358e-10	-9.723	-9.867	-0.144	-27.60
Al+3	3.469e-12	1.741e-12	-11.460	-11.759	-0.299	-41.97
AlSO4+	1.425e-13	1.309e-13	-12.846	-12.883	-0.037	(0)
Al(SO4)2-	1.073e-16	9.857e-17	-15.969	-16.006	-0.037	(0)
AlHSO4+2	2.054e-21	1.459e-21	-20.687	-20.836	-0.149	(0)
B	7.325e-06					
H3BO3	7.288e-06	7.299e-06	-5.137	-5.137	0.001	39.22
H2BO3-	3.623e-08	3.326e-08	-7.441	-7.478	-0.037	(0)
BF(OH)3-	1.829e-10	1.679e-10	-9.738	-9.775	-0.037	(0)
BF2(OH)2-	1.429e-13	1.312e-13	-12.845	-12.882	-0.037	(0)
BF3OH-	1.146e-18	1.052e-18	-17.941	-17.978	-0.037	(0)
BF4-	3.405e-23	3.126e-23	-22.468	-22.505	-0.037	(0)
Ba	5.463e-06					
Ba+2	5.238e-06	3.725e-06	-5.281	-5.429	-0.148	-12.60
BaHCO3+	1.725e-07	1.584e-07	-6.763	-6.800	-0.037	(0)
BaSO4	4.442e-08	4.448e-08	-7.352	-7.352	0.001	(0)
BaCl+	5.206e-09	4.779e-09	-8.284	-8.321	-0.037	(0)
BaCO3	3.171e-09	3.176e-09	-8.499	-8.498	0.001	-10.70
BaNO3+	1.072e-10	9.845e-11	-9.970	-10.007	-0.037	(0)

BaOH+	1.090e-12	1.002e-12	-11.963	-11.999	-0.036	(0)
Br	5.509e-06					
Br-	5.509e-06	5.045e-06	-5.259	-5.297	-0.038	24.60
CdBr+	4.079e-12	3.745e-12	-11.389	-11.427	-0.037	(0)
ZnBr+	6.298e-14	5.782e-14	-13.201	-13.238	-0.037	(0)
PbBr+	6.164e-14	5.659e-14	-13.210	-13.247	-0.037	(0)
CdBr2	1.012e-16	1.014e-16	-15.995	-15.994	0.001	(0)
PbBr2	1.337e-19	1.339e-19	-18.874	-18.873	0.001	(0)
ZnBr2	1.160e-19	1.161e-19	-18.936	-18.935	0.001	(0)
C(4)	6.172e-03					
HCO3-	4.847e-03	4.461e-03	-2.315	-2.351	-0.036	24.73
CO2	1.264e-03	1.266e-03	-2.898	-2.898	0.001	34.42
CaHCO3+	3.813e-05	3.513e-05	-4.419	-4.454	-0.036	9.70
MgHCO3+	1.190e-05	1.093e-05	-4.924	-4.962	-0.037	5.51
NaHCO3	5.788e-06	5.797e-06	-5.237	-5.237	0.001	1.80
CO3-2	2.308e-06	1.656e-06	-5.637	-5.781	-0.144	-5.10
CaCO3	1.713e-06	1.716e-06	-5.766	-5.765	0.001	-14.60
MnHCO3+	5.494e-07	5.053e-07	-6.260	-6.296	-0.036	(0)
FeHCO3+	3.404e-07	3.125e-07	-6.468	-6.505	-0.037	(0)
MgCO3	3.297e-07	3.302e-07	-6.482	-6.481	0.001	-17.09
BaHCO3+	1.725e-07	1.584e-07	-6.763	-6.800	-0.037	(0)
MnCO3	1.669e-07	1.672e-07	-6.777	-6.777	0.001	(0)
NaCO3-	7.688e-08	7.058e-08	-7.114	-7.151	-0.037	-0.97
(CO2)2	2.919e-08	2.923e-08	-7.535	-7.534	0.001	68.85
FeCO3	2.779e-08	2.783e-08	-7.556	-7.556	0.001	(0)
ZnHCO3+	2.665e-08	2.447e-08	-7.574	-7.611	-0.037	(0)
ZnCO3	1.438e-08	1.440e-08	-7.842	-7.842	0.001	(0)
PbCO3	5.489e-09	5.497e-09	-8.261	-8.260	0.001	(0)
BaCO3	3.171e-09	3.176e-09	-8.499	-8.498	0.001	-10.70
CuCO3	1.156e-09	1.158e-09	-8.937	-8.936	0.001	(0)
CdHCO3+	7.704e-10	7.073e-10	-9.113	-9.150	-0.037	(0)
PbHCO3+	7.373e-10	6.768e-10	-9.132	-9.170	-0.037	(0)
Zn(CO3)2-2	7.176e-10	5.097e-10	-9.144	-9.293	-0.149	(0)
CuHCO3+	3.170e-10	2.911e-10	-9.499	-9.536	-0.037	(0)
Pb(CO3)2-2	3.219e-11	2.287e-11	-10.492	-10.641	-0.149	(0)
CdCO3	6.586e-12	6.596e-12	-11.181	-11.181	0.001	(0)
Cu(CO3)2-2	3.398e-12	2.414e-12	-11.469	-11.617	-0.149	(0)
Cd(CO3)2-2	4.863e-14	3.454e-14	-13.313	-13.462	-0.149	(0)
Ca	9.060e-04					
Ca+2	8.632e-04	6.189e-04	-3.064	-3.208	-0.144	-17.99
CaHCO3+	3.813e-05	3.513e-05	-4.419	-4.454	-0.036	9.70
CaSO4	2.616e-06	2.620e-06	-5.582	-5.582	0.001	7.49
CaCO3	1.713e-06	1.716e-06	-5.766	-5.765	0.001	-14.60
CaHPO4	2.986e-07	2.991e-07	-6.525	-6.524	0.001	(0)
CaH2PO4+	3.078e-08	2.833e-08	-7.512	-7.548	-0.036	(0)
CaPO4-	6.088e-09	5.603e-09	-8.216	-8.252	-0.036	(0)
CaOH+	8.886e-10	8.158e-10	-9.051	-9.088	-0.037	(0)
CaHSO4+	2.355e-12	2.162e-12	-11.628	-11.665	-0.037	(0)
Cd	8.099e-09					
Cd+2	7.059e-09	5.014e-09	-8.151	-8.300	-0.149	-18.60
CdHCO3+	7.704e-10	7.073e-10	-9.113	-9.150	-0.037	(0)
CdCl+	2.132e-10	1.957e-10	-9.671	-9.708	-0.037	5.87
CdSO4	3.437e-11	3.442e-11	-10.464	-10.463	0.001	78.13
CdCO3	6.586e-12	6.596e-12	-11.181	-11.181	0.001	(0)
CdBr+	4.079e-12	3.745e-12	-11.389	-11.427	-0.037	(0)
CdF+	3.981e-12	3.655e-12	-11.400	-11.437	-0.037	(0)
CdOH+	3.563e-12	3.271e-12	-11.448	-11.485	-0.037	(0)
CdNO3+	2.895e-12	2.658e-12	-11.538	-11.575	-0.037	17.57
CdOHCl	6.387e-13	6.397e-13	-12.195	-12.194	0.001	(0)
CdCl2	3.330e-13	3.335e-13	-12.478	-12.477	0.001	23.14
Cd(CO3)2-2	4.863e-14	3.454e-14	-13.313	-13.462	-0.149	(0)
Cd(SO4)2-2	1.268e-14	9.004e-15	-13.897	-14.046	-0.149	-105.61
Cd(OH)2	1.411e-15	1.413e-15	-14.851	-14.850	0.001	(0)
CdF2	5.307e-16	5.315e-16	-15.275	-15.274	0.001	(0)
CdBr2	1.012e-16	1.014e-16	-15.995	-15.994	0.001	(0)
CdCl3-	9.349e-17	8.582e-17	-16.029	-16.066	-0.037	69.49
Cd2OH+3	1.738e-19	8.049e-20	-18.760	-19.094	-0.334	(0)
Cd(OH)3-	1.371e-21	1.259e-21	-20.863	-20.900	-0.037	(0)

Cd(OH)4-2	1.254e-28	8.910e-29	-27.902	-28.050	-0.149	(0)
Cl	4.515e-04					
Cl-	4.458e-04	4.090e-04	-3.351	-3.388	-0.037	18.12
NaCl	5.635e-06	5.643e-06	-5.249	-5.248	0.001	(0)
BaCl+	5.206e-09	4.779e-09	-8.284	-8.321	-0.037	(0)
MnCl+	2.303e-09	2.117e-09	-8.638	-8.674	-0.036	-3.09
CuCl2-	1.438e-09	1.320e-09	-8.842	-8.880	-0.037	(0)
FeCl+	4.308e-10	3.955e-10	-9.366	-9.403	-0.037	(0)
CdCl+	2.132e-10	1.957e-10	-9.671	-9.708	-0.037	5.87
ZnCl+	5.187e-11	4.760e-11	-10.285	-10.322	-0.037	-14.05
ZnOHCl	4.679e-12	4.686e-12	-11.330	-11.329	0.001	(0)
PbCl+	3.373e-12	3.097e-12	-11.472	-11.509	-0.037	7.98
CuCl3-2	1.195e-12	8.547e-13	-11.923	-12.068	-0.146	(0)
CdOHCl	6.387e-13	6.397e-13	-12.195	-12.194	0.001	(0)
MnCl2	3.774e-13	3.780e-13	-12.423	-12.423	0.001	86.10
CdCl2	3.330e-13	3.335e-13	-12.478	-12.477	0.001	23.14
CuCl+	1.548e-13	1.421e-13	-12.810	-12.847	-0.037	0.72
ZnCl2	2.034e-14	2.037e-14	-13.692	-13.691	0.001	102.36
PbCl2	2.011e-15	2.014e-15	-14.697	-14.696	0.001	34.96
CdCl3-	9.349e-17	8.582e-17	-16.029	-16.066	-0.037	69.49
MnCl3-	4.630e-17	4.258e-17	-16.334	-16.371	-0.036	43.41
CuCl2	3.111e-17	3.115e-17	-16.507	-16.506	0.001	30.82
ZnCl3-	1.017e-17	9.338e-18	-16.992	-17.030	-0.037	16.97
PbCl3-	7.118e-19	6.535e-19	-18.148	-18.185	-0.037	65.98
FeCl+2	3.114e-21	2.227e-21	-20.507	-20.652	-0.146	(0)
ZnCl4-2	2.672e-21	1.911e-21	-20.573	-20.719	-0.146	145.34
PbCl4-2	1.798e-22	1.277e-22	-21.745	-21.894	-0.149	101.51
CuCl3-	4.911e-23	4.507e-23	-22.309	-22.346	-0.037	(0)
FeCl2+	4.448e-24	4.090e-24	-23.352	-23.388	-0.036	(0)
FeCl3	1.670e-28	1.673e-28	-27.777	-27.777	0.001	(0)
CuCl4-2	1.287e-28	9.202e-29	-27.891	-28.036	-0.146	(0)
Cu(1)	2.870e-08					
Cu+	2.726e-08	2.494e-08	-7.564	-7.603	-0.039	(0)
CuCl2-	1.438e-09	1.320e-09	-8.842	-8.880	-0.037	(0)
CuCl3-2	1.195e-12	8.547e-13	-11.923	-12.068	-0.146	(0)
Cu(2)	1.841e-09					
CuCO3	1.156e-09	1.158e-09	-8.937	-8.936	0.001	(0)
CuHCO3+	3.170e-10	2.911e-10	-9.499	-9.536	-0.037	(0)
Cu+2	1.806e-10	1.302e-10	-9.743	-9.885	-0.142	-26.45
Cu(OH)2	1.713e-10	1.716e-10	-9.766	-9.766	0.001	(0)
CuOH+	1.127e-11	1.034e-11	-10.948	-10.986	-0.037	(0)
Cu(CO3)2-2	3.398e-12	2.414e-12	-11.469	-11.617	-0.149	(0)
CuSO4	6.317e-13	6.327e-13	-12.199	-12.199	0.001	13.07
CuCl+	1.548e-13	1.421e-13	-12.810	-12.847	-0.037	0.72
CuF+	1.492e-13	1.370e-13	-12.826	-12.863	-0.037	(0)
Cu(OH)3-	8.943e-17	8.210e-17	-16.049	-16.086	-0.037	(0)
Cu2(OH)2+2	6.475e-17	4.600e-17	-16.189	-16.337	-0.149	(0)
CuCl2	3.111e-17	3.115e-17	-16.507	-16.506	0.001	30.82
Cu(OH)4-2	1.832e-22	1.301e-22	-21.737	-21.886	-0.149	(0)
CuCl3-	4.911e-23	4.507e-23	-22.309	-22.346	-0.037	(0)
CuCl4-2	1.287e-28	9.202e-29	-27.891	-28.036	-0.146	(0)
F	6.424e-05					
F-	6.315e-05	5.790e-05	-4.200	-4.237	-0.038	-1.27
MgF+	8.696e-07	7.989e-07	-6.061	-6.098	-0.037	-10.53
NaF	7.680e-08	7.692e-08	-7.115	-7.114	0.001	7.26
AlF2+	3.172e-08	2.920e-08	-7.499	-7.535	-0.036	(0)
AlF3	2.124e-08	2.128e-08	-7.673	-7.672	0.001	(0)
HF	1.088e-08	1.090e-08	-7.963	-7.963	0.001	12.49
AlF+2	1.404e-09	1.007e-09	-8.853	-8.997	-0.144	(0)
MnF+	5.536e-10	5.091e-10	-9.257	-9.293	-0.036	(0)
AlF4-	5.338e-10	4.904e-10	-9.273	-9.309	-0.037	(0)
FeF+	4.418e-10	4.056e-10	-9.355	-9.392	-0.037	(0)
BF(OH)3-	1.829e-10	1.679e-10	-9.738	-9.775	-0.037	(0)
ZnF+	3.873e-11	3.556e-11	-10.412	-10.449	-0.037	(0)
CdF+	3.981e-12	3.655e-12	-11.400	-11.437	-0.037	(0)
HF2-	2.634e-12	2.418e-12	-11.579	-11.617	-0.037	22.10
PbF+	2.142e-13	1.967e-13	-12.669	-12.706	-0.037	(0)
CuF+	1.492e-13	1.370e-13	-12.826	-12.863	-0.037	(0)

BF2(OH)2-	1.429e-13	1.312e-13	-12.845	-12.882	-0.037	(0)
CdF2	5.307e-16	5.315e-16	-15.275	-15.274	0.001	(0)
PbF2	2.321e-16	2.325e-16	-15.634	-15.634	0.001	(0)
FeF2+	4.150e-17	3.817e-17	-16.382	-16.418	-0.036	(0)
FeF+2	2.320e-17	1.659e-17	-16.635	-16.780	-0.146	(0)
FeF3	3.495e-18	3.500e-18	-17.457	-17.456	0.001	(0)
BF3OH-	1.146e-18	1.052e-18	-17.941	-17.978	-0.037	(0)
PbF3-	1.062e-19	9.752e-20	-18.974	-19.011	-0.037	(0)
BF4-	3.405e-23	3.126e-23	-22.468	-22.505	-0.037	(0)
PbF4-2	3.804e-24	2.702e-24	-23.420	-23.568	-0.149	(0)
Fe(2)	1.349e-06					
Fe+2	9.719e-07	7.005e-07	-6.012	-6.155	-0.142	-21.99
FeHCO3+	3.404e-07	3.125e-07	-6.468	-6.505	-0.037	(0)
FeCO3	2.779e-08	2.783e-08	-7.556	-7.556	0.001	(0)
FeSO4	2.955e-09	2.959e-09	-8.529	-8.529	0.001	19.15
FeHPO4	2.462e-09	2.466e-09	-8.609	-8.608	0.001	(0)
FeOH+	1.889e-09	1.737e-09	-8.724	-8.760	-0.036	(0)
FeH2PO4+	6.846e-10	6.300e-10	-9.165	-9.201	-0.036	(0)
FeF+	4.418e-10	4.056e-10	-9.355	-9.392	-0.037	(0)
FeCl+	4.308e-10	3.955e-10	-9.366	-9.403	-0.037	(0)
Fe(OH)2	1.155e-13	1.157e-13	-12.937	-12.937	0.001	(0)
FeHSO4+	2.666e-15	2.447e-15	-14.574	-14.611	-0.037	(0)
Fe(OH)3-	3.706e-17	3.408e-17	-16.431	-16.467	-0.036	(0)
Fe(3)	5.072e-11					
Fe(OH)2+	2.613e-11	2.405e-11	-10.583	-10.619	-0.036	(0)
Fe(OH)3	2.438e-11	2.442e-11	-10.613	-10.612	0.001	(0)
Fe(OH)4-	1.909e-13	1.757e-13	-12.719	-12.755	-0.036	(0)
FeOH+2	1.287e-14	9.203e-15	-13.891	-14.036	-0.146	(0)
FeF2+	4.150e-17	3.817e-17	-16.382	-16.418	-0.036	(0)
FeF+2	2.320e-17	1.659e-17	-16.635	-16.780	-0.146	(0)
FeF3	3.495e-18	3.500e-18	-17.457	-17.456	0.001	(0)
Fe+3	3.612e-19	1.813e-19	-18.442	-18.742	-0.299	(0)
FeH2PO4+2	1.220e-19	8.756e-20	-18.913	-19.058	-0.144	(0)
FeSO4+	5.132e-20	4.719e-20	-19.290	-19.326	-0.036	(0)
FeHPO4+	4.665e-20	4.290e-20	-19.331	-19.368	-0.036	(0)
FeCl+2	3.114e-21	2.227e-21	-20.507	-20.652	-0.146	(0)
Fe(SO4)2-	2.678e-23	2.459e-23	-22.572	-22.609	-0.037	(0)
FeCl2+	4.448e-24	4.090e-24	-23.352	-23.388	-0.036	(0)
FeHSO4+2	2.240e-26	1.591e-26	-25.650	-25.798	-0.149	(0)
Fe2(OH)2+4	9.018e-27	2.296e-27	-26.045	-26.639	-0.594	(0)
FeCl3	1.670e-28	1.673e-28	-27.777	-27.777	0.001	(0)
Fe3(OH)4+5	9.937e-35	1.172e-35	-34.003	-34.931	-0.928	(0)
H(0)	3.000e-18					
H2	1.500e-18	1.502e-18	-17.824	-17.823	0.001	28.61
K	1.177e-04					
K+	1.177e-04	1.079e-04	-3.929	-3.967	-0.038	9.05
KSO4-	1.957e-08	1.801e-08	-7.708	-7.744	-0.036	34.15
KHPO4-	2.021e-10	1.860e-10	-9.694	-9.730	-0.036	38.18
Mg	3.053e-04					
Mg+2	2.909e-04	2.095e-04	-3.536	-3.679	-0.143	-21.66
MgHCO3+	1.190e-05	1.093e-05	-4.924	-4.962	-0.037	5.51
MgSO4	1.163e-06	1.165e-06	-5.934	-5.934	0.001	5.83
MgF+	8.696e-07	7.989e-07	-6.061	-6.098	-0.037	-10.53
MgCO3	3.297e-07	3.302e-07	-6.482	-6.481	0.001	-17.09
MgHPO4	1.367e-07	1.369e-07	-6.864	-6.864	0.001	(0)
MgH2PO4+	1.327e-08	1.221e-08	-7.877	-7.913	-0.036	(0)
MgOH+	6.450e-09	5.949e-09	-8.190	-8.226	-0.035	(0)
MgPO4-	2.780e-09	2.558e-09	-8.556	-8.592	-0.036	(0)
Mn(2)	2.488e-06					
Mn+2	1.763e-06	1.271e-06	-5.754	-5.896	-0.142	-20.10
MnHCO3+	5.494e-07	5.053e-07	-6.260	-6.296	-0.036	(0)
MnCO3	1.669e-07	1.672e-07	-6.777	-6.777	0.001	(0)
MnSO4	5.360e-09	5.368e-09	-8.271	-8.270	0.001	22.62
MnCl+	2.303e-09	2.117e-09	-8.638	-8.674	-0.036	-3.09
MnF+	5.536e-10	5.091e-10	-9.257	-9.293	-0.036	(0)
MnOH+	2.782e-10	2.559e-10	-9.556	-9.592	-0.036	(0)
MnCl2	3.774e-13	3.780e-13	-12.423	-12.423	0.001	86.10
Mn(NO3)2	2.228e-13	2.232e-13	-12.652	-12.651	0.001	41.08

MnCl3-	4.630e-17	4.258e-17	-16.334	-16.371	-0.036	43.41
Mn(OH)3-	1.097e-20	1.009e-20	-19.960	-19.996	-0.036	(0)
Mn(3)	2.088e-31					
Mn+3	2.088e-31	1.048e-31	-30.680	-30.980	-0.299	(0)
N(5)	2.293e-04					
NO3-	2.293e-04	2.100e-04	-3.640	-3.678	-0.038	29.52
BaNO3+	1.072e-10	9.845e-11	-9.970	-10.007	-0.037	(0)
CdNO3+	2.895e-12	2.658e-12	-11.538	-11.575	-0.037	17.57
PbNO3+	6.462e-13	5.933e-13	-12.190	-12.227	-0.037	(0)
Mn(NO3)2	2.228e-13	2.232e-13	-12.652	-12.651	0.001	41.08
Na	2.524e-03					
Na+	2.512e-03	2.309e-03	-2.600	-2.637	-0.037	-1.42
NaHCO3	5.788e-06	5.797e-06	-5.237	-5.237	0.001	1.80
NaCl	5.635e-06	5.643e-06	-5.249	-5.248	0.001	(0)
NaSO4-	2.993e-07	2.754e-07	-6.524	-6.560	-0.036	14.16
NaCO3-	7.688e-08	7.058e-08	-7.114	-7.151	-0.037	-0.97
NaF	7.680e-08	7.692e-08	-7.115	-7.114	0.001	7.26
NaHPO4-	4.324e-09	3.980e-09	-8.364	-8.400	-0.036	33.93
NaOH	1.829e-20	1.832e-20	-19.738	-19.737	0.001	(0)
O(0)	0.000e+00					
O2	0.000e+00	0.000e+00	-56.789	-56.789	0.001	30.39
P	3.682e-06					
H2PO4-	1.950e-06	1.794e-06	-5.710	-5.746	-0.036	33.26
HPO4-2	1.236e-06	8.842e-07	-5.908	-6.053	-0.146	6.90
CaHPO4	2.986e-07	2.991e-07	-6.525	-6.524	0.001	(0)
MgHPO4	1.367e-07	1.369e-07	-6.864	-6.864	0.001	(0)
CaH2PO4+	3.078e-08	2.833e-08	-7.512	-7.548	-0.036	(0)
MgH2PO4+	1.327e-08	1.221e-08	-7.877	-7.913	-0.036	(0)
CaPO4-	6.088e-09	5.603e-09	-8.216	-8.252	-0.036	(0)
NaHPO4-	4.324e-09	3.980e-09	-8.364	-8.400	-0.036	33.93
MgPO4-	2.780e-09	2.558e-09	-8.556	-8.592	-0.036	(0)
FeHPO4	2.462e-09	2.466e-09	-8.609	-8.608	0.001	(0)
FeH2PO4+	6.846e-10	6.300e-10	-9.165	-9.201	-0.036	(0)
KHPO4-	2.021e-10	1.860e-10	-9.694	-9.730	-0.036	38.18
H3PO4	3.314e-11	3.319e-11	-10.480	-10.479	0.001	47.40
PO4-3	6.830e-12	3.155e-12	-11.166	-11.501	-0.335	-22.81
FeH2PO4+2	1.220e-19	8.756e-20	-18.913	-19.058	-0.144	(0)
FeHPO4+	4.665e-20	4.290e-20	-19.331	-19.368	-0.036	(0)
Pb	6.567e-09					
PbCO3	5.489e-09	5.497e-09	-8.261	-8.260	0.001	(0)
PbHCO3+	7.373e-10	6.768e-10	-9.132	-9.170	-0.037	(0)
Pb+2	2.689e-10	1.910e-10	-9.570	-9.719	-0.149	-15.38
PbOH+	3.222e-11	2.958e-11	-10.492	-10.529	-0.037	(0)
Pb(CO3)2-2	3.219e-11	2.287e-11	-10.492	-10.641	-0.149	(0)
PbCl+	3.373e-12	3.097e-12	-11.472	-11.509	-0.037	7.98
PbSO4	2.556e-12	2.560e-12	-11.592	-11.592	0.001	(0)
PbNO3+	6.462e-13	5.933e-13	-12.190	-12.227	-0.037	(0)
PbF+	2.142e-13	1.967e-13	-12.669	-12.706	-0.037	(0)
Pb(OH)2	9.126e-14	9.140e-14	-13.040	-13.039	0.001	(0)
PbBr+	6.164e-14	5.659e-14	-13.210	-13.247	-0.037	(0)
PbCl2	2.011e-15	2.014e-15	-14.697	-14.696	0.001	34.96
Pb(SO4)2-2	4.507e-16	3.201e-16	-15.346	-15.495	-0.149	(0)
PbF2	2.321e-16	2.325e-16	-15.634	-15.634	0.001	(0)
Pb(OH)3-	9.078e-18	8.334e-18	-17.042	-17.079	-0.037	(0)
PbCl3-	7.118e-19	6.535e-19	-18.148	-18.185	-0.037	65.98
Pb2OH+3	2.731e-19	1.265e-19	-18.564	-18.898	-0.334	(0)
PbBr2	1.337e-19	1.339e-19	-18.874	-18.873	0.001	(0)
PbF3-	1.062e-19	9.752e-20	-18.974	-19.011	-0.037	(0)
Pb(OH)4-2	2.135e-22	1.516e-22	-21.671	-21.819	-0.149	(0)
PbCl4-2	1.798e-22	1.277e-22	-21.745	-21.894	-0.149	101.51
PbF4-2	3.804e-24	2.702e-24	-23.420	-23.568	-0.149	(0)
Pb3(OH)4+2	5.016e-26	3.563e-26	-25.300	-25.448	-0.149	(0)
S(6)	3.749e-05					
SO4-2	3.334e-05	2.383e-05	-4.477	-4.623	-0.146	14.68
CaSO4	2.616e-06	2.620e-06	-5.582	-5.582	0.001	7.49
MgSO4	1.163e-06	1.165e-06	-5.934	-5.934	0.001	5.83
NaSO4-	2.993e-07	2.754e-07	-6.524	-6.560	-0.036	14.16
BaSO4	4.442e-08	4.448e-08	-7.352	-7.352	0.001	(0)

KSO4-	1.957e-08	1.801e-08	-7.708	-7.744	-0.036	34.15
MnSO4	5.360e-09	5.368e-09	-8.271	-8.270	0.001	22.62
FeSO4	2.955e-09	2.959e-09	-8.529	-8.529	0.001	19.15
HSO4-	3.165e-10	2.906e-10	-9.500	-9.537	-0.037	40.31
ZnSO4	2.427e-10	2.431e-10	-9.615	-9.614	0.001	21.74
CdSO4	3.437e-11	3.442e-11	-10.464	-10.463	0.001	78.13
PbSO4	2.556e-12	2.560e-12	-11.592	-11.592	0.001	(0)
CaHSO4+	2.355e-12	2.162e-12	-11.628	-11.665	-0.037	(0)
CuSO4	6.317e-13	6.327e-13	-12.199	-12.199	0.001	13.07
AlSO4+	1.425e-13	1.309e-13	-12.846	-12.883	-0.037	(0)
Zn(SO4)2-2	6.638e-14	4.715e-14	-13.178	-13.327	-0.149	-13.05
Cd(SO4)2-2	1.268e-14	9.004e-15	-13.897	-14.046	-0.149	-105.61
FeHSO4+	2.666e-15	2.447e-15	-14.574	-14.611	-0.037	(0)
Pb(SO4)2-2	4.507e-16	3.201e-16	-15.346	-15.495	-0.149	(0)
Al(SO4)2-	1.073e-16	9.857e-17	-15.969	-16.006	-0.037	(0)
FeSO4+	5.132e-20	4.719e-20	-19.290	-19.326	-0.036	(0)
AlHSO4+2	2.054e-21	1.459e-21	-20.687	-20.836	-0.149	(0)
Fe(SO4)2-	2.678e-23	2.459e-23	-22.572	-22.609	-0.037	(0)
FeHSO4+2	2.240e-26	1.591e-26	-25.650	-25.798	-0.149	(0)
Zn	1.035e-07					
Zn+2	6.092e-08	4.357e-08	-7.215	-7.361	-0.146	-25.19
ZnHCO3+	2.665e-08	2.447e-08	-7.574	-7.611	-0.037	(0)
ZnCO3	1.438e-08	1.440e-08	-7.842	-7.842	0.001	(0)
Zn(CO3)2-2	7.176e-10	5.097e-10	-9.144	-9.293	-0.149	(0)
ZnOH+	4.080e-10	3.746e-10	-9.389	-9.426	-0.037	(0)
ZnSO4	2.427e-10	2.431e-10	-9.615	-9.614	0.001	21.74
ZnCl+	5.187e-11	4.760e-11	-10.285	-10.322	-0.037	-14.05
ZnF+	3.873e-11	3.556e-11	-10.412	-10.449	-0.037	(0)
Zn(OH)2	3.455e-11	3.460e-11	-10.462	-10.461	0.001	(0)
ZnOHCl	4.679e-12	4.686e-12	-11.330	-11.329	0.001	(0)
Zn(SO4)2-2	6.638e-14	4.715e-14	-13.178	-13.327	-0.149	-13.05
ZnBr+	6.298e-14	5.782e-14	-13.201	-13.238	-0.037	(0)
ZnCl2	2.034e-14	2.037e-14	-13.692	-13.691	0.001	102.36
Zn(OH)3-	9.465e-16	8.689e-16	-15.024	-15.061	-0.037	(0)
ZnCl3-	1.017e-17	9.338e-18	-16.992	-17.030	-0.037	16.97
ZnBr2	1.160e-19	1.161e-19	-18.936	-18.935	0.001	(0)
ZnCl4-2	2.672e-21	1.911e-21	-20.573	-20.719	-0.146	145.34
Zn(OH)4-2	1.540e-21	1.094e-21	-20.813	-20.961	-0.149	(0)

----------Distribution of alkalinity----------

Total alkalinity (eq/kgw) = 4.915e-03

Species	Alkalinity	Molality	Alk/Mol
HCO3-	4.847e-03	4.847e-03	1.00
CaHCO3+	3.813e-05	3.813e-05	1.00
MgHCO3+	1.190e-05	1.190e-05	1.00
NaHCO3	5.788e-06	5.788e-06	1.00
CO3-2	4.616e-06	2.308e-06	2.00
CaCO3	3.427e-06	1.713e-06	2.00
HPO4-2	1.236e-06	1.236e-06	1.00
MgCO3	6.594e-07	3.297e-07	2.00
Al(OH)4-	6.259e-07	1.565e-07	4.00
MnHCO3+	5.494e-07	5.494e-07	1.00
FeHCO3+	3.404e-07	3.404e-07	1.00
MnCO3	3.339e-07	1.669e-07	2.00
CaHPO4	2.986e-07	2.986e-07	1.00
BaHCO3+	1.725e-07	1.725e-07	1.00
NaCO3-	1.538e-07	7.688e-08	2.00
MgHPO4	1.367e-07	1.367e-07	1.00
H+	-1.359e-07	1.359e-07	-1.00
OH-	8.655e-08	8.655e-08	1.00
FeCO3	5.557e-08	2.779e-08	2.00
H2BO3-	3.623e-08	3.623e-08	1.00
Al(OH)3	2.884e-08	9.612e-09	3.00
ZnCO3	2.875e-08	1.438e-08	2.00
ZnHCO3+	2.665e-08	2.665e-08	1.00

Al(OH)2+	1.810e-08	9.051e-09	2.00
CaPO4-	1.218e-08	6.088e-09	2.00
PbCO3	1.098e-08	5.489e-09	2.00
HF	-1.088e-08	1.088e-08	-1.00
MgOH+	6.450e-09	6.450e-09	1.00
BaCO3	6.342e-09	3.171e-09	2.00
MgPO4-	5.559e-09	2.780e-09	2.00
NaHPO4-	4.324e-09	4.324e-09	1.00
Zn(CO3)2-2	2.870e-09	7.176e-10	4.00
FeHPO4	2.462e-09	2.462e-09	1.00
CuCO3	2.312e-09	1.156e-09	2.00
FeOH+	1.889e-09	1.889e-09	1.00
CaOH+	8.886e-10	8.886e-10	1.00
CdHCO3+	7.704e-10	7.704e-10	1.00
PbHCO3+	7.373e-10	7.373e-10	1.00
ZnOH+	4.080e-10	4.080e-10	1.00
Cu(OH)2	3.426e-10	1.713e-10	2.00
CuHCO3+	3.170e-10	3.170e-10	1.00
HSO4-	-3.165e-10	3.165e-10	-1.00
MnOH+	2.782e-10	2.782e-10	1.00
KHPO4-	2.021e-10	2.021e-10	1.00
AlOH+2	1.893e-10	1.893e-10	1.00
Pb(CO3)2-2	1.288e-10	3.219e-11	4.00
Zn(OH)2	6.909e-11	3.455e-11	2.00
H3PO4	-3.314e-11	3.314e-11	-1.00
PbOH+	3.222e-11	3.222e-11	1.00
Fe(OH)3	2.438e-11	2.438e-11	1.00
PO4-3	1.366e-11	6.830e-12	2.00
Cu(CO3)2-2	1.359e-11	3.398e-12	4.00
CdCO3	1.317e-11	6.586e-12	2.00
CuOH+	1.127e-11	1.127e-11	1.00
ZnOHCl	4.679e-12	4.679e-12	1.00
CdOH+	3.563e-12	3.563e-12	1.00
HF2-	-2.634e-12	2.634e-12	-1.00
CaHSO4+	-2.355e-12	2.355e-12	-1.00
BaOH+	1.090e-12	1.090e-12	1.00
CdOHCl	6.387e-13	6.387e-13	1.00
Fe(OH)4-	3.818e-13	1.909e-13	2.00
Fe(OH)2	2.310e-13	1.155e-13	2.00
Cd(CO3)2-2	1.945e-13	4.863e-14	4.00
Pb(OH)2	1.825e-13	9.126e-14	2.00
BF2(OH)2-	-1.429e-13	1.429e-13	-1.00
FeOH+2	-1.287e-14	1.287e-14	-1.00
Zn(OH)3-	2.839e-15	9.465e-16	3.00
Cd(OH)2	2.821e-15	1.411e-15	2.00
FeHSO4+	-2.666e-15	2.666e-15	-1.00
Cu(OH)3-	2.683e-16	8.943e-17	3.00
Cu2(OH)2+2	1.295e-16	6.475e-17	2.00
Fe(OH)3-	1.112e-16	3.706e-17	3.00
FeF2+	-8.301e-17	4.150e-17	-2.00
FeF+2	-4.640e-17	2.320e-17	-2.00
Pb(OH)3-	2.723e-17	9.078e-18	3.00
FeF3	-6.990e-18	3.495e-18	-2.00
BF3OH-	-2.292e-18	1.146e-18	-2.00
Fe+3	-7.225e-19	3.612e-19	-2.00
Pb2OH+3	2.731e-19	2.731e-19	1.00
FeH2PO4+2	-2.441e-19	1.220e-19	-2.00
Cd2OH+3	1.738e-19	1.738e-19	1.00
FeSO4+	-1.026e-19	5.132e-20	-2.00
FeHPO4+	-4.665e-20	4.665e-20	-1.00
Mn(OH)3-	3.292e-20	1.097e-20	3.00
NaOH	1.829e-20	1.829e-20	1.00
FeCl+2	-6.227e-21	3.114e-21	-2.00
Zn(OH)4-2	6.159e-21	1.540e-21	4.00
Cd(OH)3-	4.114e-21	1.371e-21	3.00
AlHSO4+2	-2.054e-21	2.054e-21	-1.00
Pb(OH)4-2	8.538e-22	2.135e-22	4.00
Cu(OH)4-2	7.326e-22	1.832e-22	4.00

BF4-	-1.021e-22	3.405e-23	-3.00
Fe(SO4)2-	-5.356e-23	2.678e-23	-2.00
FeCl2+	-8.895e-24	4.448e-24	-2.00
Pb3(OH)4+2	2.007e-25	5.016e-26	4.00
FeHSO4+2	-6.719e-26	2.240e-26	-3.00
Fe2(OH)2+4	-1.804e-26	9.018e-27	-2.00
Cd(OH)4-2	5.017e-28	1.254e-28	4.00
FeCl3	-3.340e-28	1.670e-28	-2.00
Fe3(OH)4+5	-1.987e-34	9.937e-35	-2.00

----------Saturation indices----------

Phase	SI**	log IAP	log K(297 K, 1 atm)	
Al(OH)3(a)	-1.87	8.94	10.81	Al(OH)3
Alunite	-5.71	-7.09	-1.38	KAl3(SO4)2(OH)6
Anglesite	-6.55	-14.34	-7.79	PbSO4
Anhydrite	-3.56	-7.83	-4.28	CaSO4
Aragonite	-0.65	-8.99	-8.33	CaCO3
BaCl2	-14.44	-12.21	2.23	BaCl2
BaCl2:2H2O	-12.41	-12.21	0.21	BaCl2:2H2O
BaCl2:H2O	-13.03	-12.21	0.82	BaCl2:H2O
Barite	-0.21	-10.05	-9.85	BaSO4
Calcite	-0.51	-8.99	-8.48	CaCO3
Cd(OH)2	-8.15	5.50	13.65	Cd(OH)2
CdSO4	-12.83	-12.92	-0.09	CdSO4
Cerussite	-2.37	-15.50	-13.13	PbCO3
CO2(g)	-1.43	-2.90	-1.47	CO2
Dolomite	-1.36	-18.45	-17.09	CaMg(CO3)2
Fe(OH)3(a)	-2.93	1.96	4.89	Fe(OH)3
Fluorite	-1.08	-11.68	-10.60	CaF2
Gibbsite	0.82	8.94	8.12	Al(OH)3
Goethite	2.95	1.96	-0.99	FeOOH
Gypsum	-3.25	-7.83	-4.58	CaSO4:2H2O
H2(g)	-14.72	-17.82	-3.10	H2
H2O(g)	-1.51	-0.00	1.51	H2O
Halite	-7.59	-6.02	1.57	NaCl
Hausmannite	-22.69	38.39	61.07	Mn3O4
Hematite	7.91	3.92	-4.00	Fe2O3
Hydroxyapatite	-3.20	-6.60	-3.41	Ca5(PO4)3OH
Jarosite-K	-18.84	-28.04	-9.20	KFe3(SO4)2(OH)6
Manganite	-10.10	15.24	25.34	MnOOH
Melanterite	-8.57	-10.78	-2.21	FeSO4:7H2O
O2(g)	-53.90	-56.79	-2.89	O2
Otavite	-1.98	-14.08	-12.10	CdCO3
Pb(OH)2	-4.07	4.08	8.16	Pb(OH)2
Pyrochroite	-7.30	7.90	15.20	Mn(OH)2
Pyrolusite	-18.83	22.58	41.41	MnO2:H2O
Rhodochrosite	-0.55	-11.68	-11.13	MnCO3
Siderite	-1.05	-11.94	-10.89	FeCO3
Smithsonite	-3.14	-13.14	-10.00	ZnCO3
Sylvite	-8.25	-7.36	0.90	KCl
Vivianite	-5.47	-41.47	-36.00	Fe3(PO4)2:8H2O
Witherite	-2.65	-11.21	-8.56	BaCO3
Zn(OH)2(e)	-5.06	6.44	11.50	Zn(OH)2

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
For ideal gases, phi = 1.

Initial solution 23.

----------Solution composition----------

Elements	Molality	Moles
Al	3.184e-07	3.184e-07
Alkalinity	1.867e-03	1.867e-03
B	1.058e-05	1.058e-05

Ba	1.835e-05	1.835e-05
Br	5.758e-06	5.758e-06
Ca	4.392e-04	4.392e-04
Cd	5.784e-09	5.784e-09
Cl	5.078e-04	5.078e-04
Cu	6.091e-08	6.091e-08
F	5.580e-05	5.580e-05
Fe	8.272e-06	8.272e-06
K	1.023e-04	1.023e-04
Mg	3.777e-04	3.777e-04
Mn	5.484e-07	5.484e-07
N(5)	3.120e-04	3.120e-04
Na	9.267e-04	9.267e-04
P	9.364e-07	9.364e-07
Pb	2.177e-08	2.177e-08
S(6)	4.998e-05	4.998e-05
Zn	1.630e-06	1.630e-06

----------Description of solution----------

pH	= 5.800
pe	= 0.447
Specific Conductance (µS/cm, 27°C)	= 294
Density (g/cm³)	= 0.99664
Volume (L)	= 1.00385
Activity of water	= 1.000
Ionic strength (mol/kgw)	= 3.625e-03
Mass of water (kg)	= 1.000e+00
Total carbon (mol/kg)	= 7.890e-03
Total CO2 (mol/kg)	= 7.890e-03
Temperature (°C)	= 27.33
Electrical balance (eq)	= -1.284e-04
Percent error, 100*(Cat-|An|)/(Cat+|An|)	= -2.33
Iterations	= 11 (244 overall)
Total H	= 1.110143e+02
Total O	= 5.552504e+01

----------Distribution of species----------

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma	mole V cm³/mol
H+	1.683e-06	1.585e-06	-5.774	-5.800	-0.026	0.00
OH-	8.133e-09	7.611e-09	-8.090	-8.119	-0.029	-4.00
H2O	5.551e+01	9.998e-01	1.744	-0.000	0.000	18.08
Al	3.184e-07					
AlF2+	1.917e-07	1.798e-07	-6.717	-6.745	-0.028	(0)
AlF3	1.142e-07	1.143e-07	-6.942	-6.942	0.000	(0)
AlF+2	9.091e-09	7.034e-09	-8.041	-8.153	-0.111	(0)
AlF4-	2.449e-09	2.295e-09	-8.611	-8.639	-0.028	(0)
Al(OH)2+	6.462e-10	6.061e-10	-9.190	-9.217	-0.028	(0)
AlOH+2	1.296e-10	1.003e-10	-9.887	-9.999	-0.111	-27.75
Al(OH)4-	8.748e-11	8.196e-11	-10.058	-10.086	-0.028	(0)
Al(OH)3	6.662e-11	6.668e-11	-10.176	-10.176	0.000	(0)
Al+3	2.368e-11	1.377e-11	-10.626	-10.861	-0.236	-42.26
AlSO4+	1.662e-12	1.557e-12	-11.779	-11.808	-0.028	(0)
Al(SO4)2-	1.843e-15	1.727e-15	-14.734	-14.763	-0.028	(0)
AlHSO4+2	2.907e-19	2.235e-19	-18.537	-18.651	-0.114	(0)
B	1.058e-05					
H3BO3	1.058e-05	1.059e-05	-4.976	-4.975	0.000	39.40
H2BO3-	4.283e-09	4.010e-09	-8.368	-8.397	-0.029	(0)
BF(OH)3-	2.324e-10	2.176e-10	-9.634	-9.662	-0.029	(0)
BF2(OH)2-	1.983e-12	1.857e-12	-11.703	-11.731	-0.029	(0)
BF3OH-	1.665e-16	1.559e-16	-15.779	-15.807	-0.029	(0)
BF4-	5.401e-20	5.058e-20	-19.268	-19.296	-0.029	(0)
Ba	1.835e-05					
Ba+2	1.783e-05	1.372e-05	-4.749	-4.863	-0.114	-12.53
BaHCO3+	2.625e-07	2.458e-07	-6.581	-6.609	-0.029	(0)

BaSO4	2.385e-07	2.387e-07	-6.623	-6.622	0.000	(0)
BaCl+	2.257e-08	2.114e-08	-7.646	-7.675	-0.029	(0)
BaNO3+	5.383e-10	5.041e-10	-9.269	-9.298	-0.029	(0)
BaCO3	3.992e-10	3.996e-10	-9.399	-9.398	0.000	-10.68
BaOH+	3.129e-13	2.933e-13	-12.505	-12.533	-0.028	(0)
Br	5.758e-06					
Br-	5.758e-06	5.385e-06	-5.240	-5.269	-0.029	24.68
CdBr+	3.427e-12	3.209e-12	-11.465	-11.494	-0.029	(0)
PbBr+	2.032e-12	1.902e-12	-11.692	-11.721	-0.029	(0)
ZnBr+	1.590e-12	1.489e-12	-11.799	-11.827	-0.029	(0)
CdBr2	9.371e-17	9.379e-17	-16.028	-16.028	0.000	(0)
PbBr2	4.610e-18	4.614e-18	-17.336	-17.336	0.000	(0)
ZnBr2	3.190e-18	3.193e-18	-17.496	-17.496	0.000	(0)
C(4)	7.890e-03					
CO2	6.020e-03	6.025e-03	-2.220	-2.220	0.000	34.55
HCO3-	1.852e-03	1.737e-03	-2.732	-2.760	-0.028	24.88
CaHCO3+	8.103e-06	7.605e-06	-5.091	-5.119	-0.028	9.78
MgHCO3+	6.259e-06	5.861e-06	-5.203	-5.232	-0.029	5.56
FeHCO3+	1.034e-06	9.681e-07	-5.986	-6.014	-0.029	(0)
NaHCO3	8.333e-07	8.340e-07	-6.079	-6.079	0.000	1.80
(CO2)2	7.182e-07	7.188e-07	-6.144	-6.143	0.000	69.09
BaHCO3+	2.625e-07	2.458e-07	-6.581	-6.609	-0.029	(0)
ZnHCO3+	2.455e-07	2.299e-07	-6.610	-6.638	-0.029	(0)
CO3-2	6.953e-08	5.379e-08	-7.158	-7.269	-0.111	-5.01
MnHCO3+	6.172e-08	5.786e-08	-7.210	-7.238	-0.028	(0)
CaCO3	3.145e-08	3.147e-08	-7.502	-7.502	0.000	-14.59
MgCO3	1.516e-08	1.517e-08	-7.819	-7.819	0.000	-17.09
ZnCO3	1.128e-08	1.129e-08	-7.948	-7.947	0.000	(0)
PbHCO3+	8.513e-09	7.972e-09	-8.070	-8.098	-0.029	(0)
FeCO3	7.186e-09	7.192e-09	-8.144	-8.143	0.000	(0)
PbCO3	5.397e-09	5.401e-09	-8.268	-8.267	0.000	(0)
MnCO3	1.596e-09	1.597e-09	-8.797	-8.797	0.000	(0)
NaCO3-	1.040e-09	9.737e-10	-8.983	-9.012	-0.029	-0.79
BaCO3	3.992e-10	3.996e-10	-9.399	-9.398	0.000	-10.68
CuHCO3+	2.551e-10	2.389e-10	-9.593	-9.622	-0.029	(0)
CdHCO3+	2.389e-10	2.237e-10	-9.622	-9.650	-0.029	(0)
CuCO3	7.922e-11	7.929e-11	-10.101	-10.101	0.000	(0)
Zn(CO3)2-2	1.688e-11	1.298e-11	-10.773	-10.887	-0.114	(0)
Pb(CO3)2-2	9.492e-13	7.299e-13	-12.023	-12.137	-0.114	(0)
CdCO3	1.739e-13	1.740e-13	-12.760	-12.759	0.000	(0)
Cu(CO3)2-2	6.983e-15	5.370e-15	-14.156	-14.270	-0.114	(0)
Cd(CO3)2-2	3.849e-17	2.960e-17	-16.415	-16.529	-0.114	(0)
Ca	4.392e-04					
Ca+2	4.290e-04	3.317e-04	-3.368	-3.479	-0.112	-18.03
CaHCO3+	8.103e-06	7.605e-06	-5.091	-5.119	-0.028	9.78
CaSO4	2.082e-06	2.083e-06	-5.682	-5.681	0.000	7.58
CaCO3	3.145e-08	3.147e-08	-7.502	-7.502	0.000	-14.59
CaH2PO4+	7.652e-09	7.177e-09	-8.116	-8.144	-0.028	(0)
CaHPO4	6.090e-09	6.095e-09	-8.215	-8.215	0.000	(0)
CaOH+	3.709e-11	3.473e-11	-10.431	-10.459	-0.029	(0)
CaHSO4+	2.398e-11	2.245e-11	-10.620	-10.649	-0.029	(0)
CaPO4-	1.013e-11	9.504e-12	-10.994	-11.022	-0.028	(0)
Cd	5.784e-09					
Cd+2	5.296e-09	4.072e-09	-8.276	-8.390	-0.114	-18.56
CdHCO3+	2.389e-10	2.237e-10	-9.622	-9.650	-0.029	(0)
CdCl+	1.979e-10	1.854e-10	-9.703	-9.732	-0.029	6.45
CdSO4	4.131e-11	4.134e-11	-10.384	-10.384	0.000	76.94
CdBr+	3.427e-12	3.209e-12	-11.465	-11.494	-0.029	(0)
CdNO3+	2.978e-12	2.789e-12	-11.526	-11.555	-0.029	17.47
CdF+	2.759e-12	2.583e-12	-11.559	-11.588	-0.029	(0)
CdCl2	3.683e-13	3.686e-13	-12.434	-12.433	0.000	23.14
CdOH+	2.709e-13	2.536e-13	-12.567	-12.596	-0.029	(0)
CdCO3	1.739e-13	1.740e-13	-12.760	-12.759	0.000	(0)
CdOHCl	5.070e-14	5.074e-14	-13.295	-13.295	0.000	(0)
Cd(SO4)2-2	2.017e-14	1.551e-14	-13.695	-13.809	-0.114	-104.14
CdF2	3.267e-16	3.270e-16	-15.486	-15.485	0.000	(0)
CdCl3-	1.216e-16	1.139e-16	-15.915	-15.944	-0.029	67.74
CdBr2	9.371e-17	9.379e-17	-16.028	-16.028	0.000	(0)

Cd(CO3)2-2	3.849e-17	2.960e-17	-16.415	-16.529	-0.114	(0)
Cd(OH)2	7.233e-18	7.239e-18	-17.141	-17.140	0.000	(0)
Cd2OH+3	8.877e-21	4.915e-21	-20.052	-20.308	-0.257	(0)
Cd(OH)3-	5.472e-25	5.124e-25	-24.262	-24.290	-0.029	(0)
Cd(OH)4-2	3.746e-33	2.881e-33	-32.426	-32.540	-0.114	(0)
Cl	5.078e-04					
Cl-	5.053e-04	4.730e-04	-3.296	-3.325	-0.029	18.16
NaCl	2.487e-06	2.489e-06	-5.604	-5.604	0.000	(0)
BaCl+	2.257e-08	2.114e-08	-7.646	-7.675	-0.029	(0)
CuCl2-	3.951e-09	3.699e-09	-8.403	-8.432	-0.029	(0)
FeCl+	3.886e-09	3.639e-09	-8.411	-8.439	-0.029	(0)
ZnCl+	1.583e-09	1.482e-09	-8.801	-8.829	-0.029	-11.68
MnCl+	7.681e-10	7.201e-10	-9.115	-9.143	-0.028	-2.53
CdCl+	1.979e-10	1.854e-10	-9.703	-9.732	-0.029	6.45
PbCl+	1.230e-10	1.152e-10	-9.910	-9.938	-0.029	8.06
ZnOHCl	1.038e-11	1.039e-11	-10.984	-10.983	0.000	(0)
CuCl3-2	3.623e-12	2.798e-12	-11.441	-11.553	-0.112	(0)
ZnCl2	7.403e-13	7.409e-13	-12.131	-12.130	0.000	97.62
CuCl+	4.179e-13	3.913e-13	-12.379	-12.408	-0.029	0.08
CdCl2	3.683e-13	3.686e-13	-12.434	-12.433	0.000	23.14
MnCl2	1.485e-13	1.487e-13	-12.828	-12.828	0.000	83.13
PbCl2	8.264e-14	8.271e-14	-13.083	-13.082	0.000	35.15
CdOHCl	5.070e-14	5.074e-14	-13.295	-13.295	0.000	(0)
ZnCl3-	4.258e-16	3.987e-16	-15.371	-15.399	-0.029	17.20
CdCl3-	1.216e-16	1.139e-16	-15.915	-15.944	-0.029	67.74
CuCl2	1.018e-16	1.019e-16	-15.992	-15.992	0.000	33.62
PbCl3-	3.366e-17	3.152e-17	-16.473	-16.501	-0.029	66.25
MnCl3-	2.066e-17	1.937e-17	-16.685	-16.713	-0.028	43.29
ZnCl4-2	1.246e-19	9.625e-20	-18.904	-19.017	-0.112	145.57
FeCl+2	3.365e-20	2.599e-20	-19.473	-19.585	-0.112	(0)
PbCl4-2	9.446e-21	7.264e-21	-20.025	-20.139	-0.114	101.81
CuCl3-	1.903e-22	1.781e-22	-21.721	-21.749	-0.029	(0)
FeCl2+	5.443e-23	5.103e-23	-22.264	-22.292	-0.028	(0)
FeCl3	2.411e-27	2.413e-27	-26.618	-26.617	0.000	(0)
CuCl4-2	5.768e-28	4.455e-28	-27.239	-27.351	-0.112	(0)
Cu(1)	6.022e-08					
Cu+	5.626e-08	5.258e-08	-7.250	-7.279	-0.029	(0)
CuCl2-	3.951e-09	3.699e-09	-8.403	-8.432	-0.029	(0)
CuCl3-2	3.623e-12	2.798e-12	-11.441	-11.553	-0.112	(0)
Cu(2)	6.949e-10					
Cu+2	3.537e-10	2.744e-10	-9.451	-9.562	-0.110	-26.54
CuHCO3+	2.551e-10	2.389e-10	-9.593	-9.622	-0.029	(0)
CuCO3	7.922e-11	7.929e-11	-10.101	-10.101	0.000	(0)
Cu(OH)2	2.280e-12	2.282e-12	-11.642	-11.642	0.000	(0)
CuSO4	1.974e-12	1.976e-12	-11.705	-11.704	0.000	13.37
CuOH+	1.849e-12	1.731e-12	-11.733	-11.762	-0.029	(0)
CuCl+	4.179e-13	3.913e-13	-12.379	-12.408	-0.029	0.08
CuF+	2.745e-13	2.570e-13	-12.561	-12.590	-0.029	(0)
Cu(CO3)2-2	6.983e-15	5.370e-15	-14.156	-14.270	-0.114	(0)
CuCl2	1.018e-16	1.019e-16	-15.992	-15.992	0.000	33.62
Cu2(OH)2+2	2.146e-18	1.650e-18	-17.668	-17.782	-0.114	(0)
Cu(OH)3-	9.263e-20	8.674e-20	-19.033	-19.062	-0.029	(0)
CuCl3-	1.903e-22	1.781e-22	-21.721	-21.749	-0.029	(0)
Cu(OH)4-2	1.420e-26	1.092e-26	-25.848	-25.962	-0.114	(0)
CuCl4-2	5.768e-28	4.455e-28	-27.239	-27.351	-0.112	(0)
F	5.580e-05					
F-	5.385e-05	5.039e-05	-4.269	-4.298	-0.029	-1.27
MgF+	1.057e-06	9.902e-07	-5.976	-6.004	-0.028	-10.56
AlF2+	1.917e-07	1.798e-07	-6.717	-6.745	-0.028	(0)
HF	1.248e-07	1.249e-07	-6.904	-6.903	0.000	12.60
AlF3	1.142e-07	1.143e-07	-6.942	-6.942	0.000	(0)
NaF	2.506e-08	2.508e-08	-7.601	-7.601	0.000	7.35
AlF+2	9.091e-09	7.034e-09	-8.041	-8.153	-0.111	(0)
FeF+	2.999e-09	2.808e-09	-8.523	-8.552	-0.029	(0)
AlF4-	2.449e-09	2.295e-09	-8.611	-8.639	-0.028	(0)
ZnF+	8.228e-10	7.705e-10	-9.085	-9.113	-0.029	(0)
BF(OH)3-	2.324e-10	2.176e-10	-9.634	-9.662	-0.029	(0)
MnF+	1.390e-10	1.303e-10	-9.857	-9.885	-0.028	(0)

HF2-	2.625e-11	2.458e-11	-10.581	-10.609	-0.029	22.19
PbF+	5.529e-12	5.177e-12	-11.257	-11.286	-0.029	(0)
CdF+	2.759e-12	2.583e-12	-11.559	-11.588	-0.029	(0)
BF2(OH)2-	1.983e-12	1.857e-12	-11.703	-11.731	-0.029	(0)
CuF+	2.745e-13	2.570e-13	-12.561	-12.590	-0.029	(0)
PbF2	5.322e-15	5.327e-15	-14.274	-14.274	0.000	(0)
CdF2	3.267e-16	3.270e-16	-15.486	-15.485	0.000	(0)
FeF2+	3.077e-16	2.885e-16	-15.512	-15.540	-0.028	(0)
FeF+2	1.812e-16	1.399e-16	-15.742	-15.854	-0.112	(0)
BF3OH-	1.665e-16	1.559e-16	-15.779	-15.807	-0.029	(0)
FeF3	2.320e-17	2.322e-17	-16.635	-16.634	0.000	(0)
PbF3-	2.076e-18	1.944e-18	-17.683	-17.711	-0.029	(0)
BF4-	5.401e-20	5.058e-20	-19.268	-19.296	-0.029	(0)
PbF4-2	6.098e-23	4.690e-23	-22.215	-22.329	-0.114	(0)
Fe(2)	8.272e-06					
Fe+2	7.184e-06	5.573e-06	-5.144	-5.254	-0.110	-21.91
FeHCO3+	1.034e-06	9.681e-07	-5.986	-6.014	-0.029	(0)
FeSO4	3.585e-08	3.588e-08	-7.445	-7.445	0.000	16.61
FeCO3	7.186e-09	7.192e-09	-8.144	-8.143	0.000	(0)
FeCl+	3.886e-09	3.639e-09	-8.411	-8.439	-0.029	(0)
FeF+	2.999e-09	2.808e-09	-8.523	-8.552	-0.029	(0)
FeH2PO4+	2.409e-09	2.259e-09	-8.618	-8.646	-0.028	(0)
FeOH+	1.410e-09	1.322e-09	-8.851	-8.879	-0.028	(0)
FeHPO4	7.115e-10	7.121e-10	-9.148	-9.147	0.000	(0)
FeHSO4+	4.028e-13	3.772e-13	-12.395	-12.423	-0.029	(0)
Fe(OH)2	8.669e-15	8.676e-15	-14.062	-14.062	0.000	(0)
Fe(OH)3-	2.219e-19	2.080e-19	-18.654	-18.682	-0.028	(0)
Fe(3)	2.091e-12					
Fe(OH)2+	1.919e-12	1.800e-12	-11.717	-11.745	-0.028	(0)
Fe(OH)3	1.616e-13	1.618e-13	-12.791	-12.791	0.000	(0)
FeOH+2	1.022e-14	7.892e-15	-13.991	-14.103	-0.112	(0)
FeF2+	3.077e-16	2.885e-16	-15.512	-15.540	-0.028	(0)
FeF+2	1.812e-16	1.399e-16	-15.742	-15.854	-0.112	(0)
Fe(OH)4-	1.089e-16	1.021e-16	-15.963	-15.991	-0.028	(0)
FeF3	2.320e-17	2.322e-17	-16.635	-16.634	0.000	(0)
Fe+3	2.908e-18	1.691e-18	-17.536	-17.772	-0.236	(0)
FeSO4+	7.225e-19	6.773e-19	-18.141	-18.169	-0.028	(0)
FeH2PO4+2	4.757e-19	3.681e-19	-18.323	-18.434	-0.111	(0)
FeCl+2	3.365e-20	2.599e-20	-19.473	-19.585	-0.112	(0)
FeHPO4+	1.680e-20	1.575e-20	-19.775	-19.803	-0.028	(0)
Fe(SO4)2-	5.541e-22	5.189e-22	-21.256	-21.285	-0.029	(0)
FeCl2+	5.443e-23	5.103e-23	-22.264	-22.292	-0.028	(0)
FeHSO4+2	3.739e-24	2.875e-24	-23.427	-23.541	-0.114	(0)
Fe2(OH)2+4	4.357e-27	1.524e-27	-26.361	-26.817	-0.456	(0)
FeCl3	2.411e-27	2.413e-27	-26.618	-26.617	0.000	(0)
Fe3(OH)4+5	2.390e-36	4.628e-37	-35.622	-36.335	-0.713	(0)
H(0)	4.433e-16					
H2	2.216e-16	2.218e-16	-15.654	-15.654	0.000	28.60
K	1.023e-04					
K+	1.023e-04	9.573e-05	-3.990	-4.019	-0.029	9.11
KSO4-	2.592e-08	2.431e-08	-7.586	-7.614	-0.028	34.19
KHPO4-	6.387e-12	5.991e-12	-11.195	-11.223	-0.028	37.98
Mg	3.777e-04					
Mg+2	3.679e-04	2.852e-04	-3.434	-3.545	-0.110	-21.81
MgHCO3+	6.259e-06	5.861e-06	-5.203	-5.232	-0.029	5.56
MgSO4	2.461e-06	2.463e-06	-5.609	-5.609	0.000	5.92
MgF+	1.057e-06	9.902e-07	-5.976	-6.004	-0.028	-10.56
MgCO3	1.516e-08	1.517e-08	-7.819	-7.819	0.000	-17.09
MgH2PO4+	8.378e-09	7.858e-09	-8.077	-8.105	-0.028	(0)
MgHPO4	7.079e-09	7.085e-09	-8.150	-8.150	0.000	(0)
MgOH+	8.572e-10	8.050e-10	-9.067	-9.094	-0.027	(0)
MgPO4-	1.175e-11	1.102e-11	-10.930	-10.958	-0.028	(0)
Mn(2)	5.484e-07					
Mn+2	4.817e-07	3.737e-07	-6.317	-6.427	-0.110	-20.39
MnHCO3+	6.172e-08	5.786e-08	-7.210	-7.238	-0.028	(0)
MnSO4	2.409e-09	2.411e-09	-8.618	-8.618	0.000	21.55
MnCO3	1.596e-09	1.597e-09	-8.797	-8.797	0.000	(0)
MnCl+	7.681e-10	7.201e-10	-9.115	-9.143	-0.028	-2.53

MnF+	1.390e-10	1.303e-10	-9.857	-9.885	-0.028	(0)
MnOH+	7.805e-12	7.317e-12	-11.108	-11.136	-0.028	(0)
MnCl2	1.485e-13	1.487e-13	-12.828	-12.828	0.000	83.13
Mn(NO3)2	1.259e-13	1.261e-13	-12.900	-12.899	0.000	40.44
MnCl3-	2.066e-17	1.937e-17	-16.685	-16.713	-0.028	43.29
Mn(OH)3-	1.586e-24	1.487e-24	-23.800	-23.828	-0.028	(0)
Mn(3)	7.793e-32					
Mn+3	7.793e-32	4.531e-32	-31.108	-31.344	-0.236	(0)
N(5)	3.120e-04					
NO3-	3.120e-04	2.918e-04	-3.506	-3.535	-0.029	29.73
BaNO3+	5.383e-10	5.041e-10	-9.269	-9.298	-0.029	(0)
PbNO3+	2.663e-11	2.494e-11	-10.575	-10.603	-0.029	(0)
CdNO3+	2.978e-12	2.789e-12	-11.526	-11.555	-0.029	17.47
Mn(NO3)2	1.259e-13	1.261e-13	-12.900	-12.899	0.000	40.44
Na	9.267e-04					
Na+	9.232e-04	8.651e-04	-3.035	-3.063	-0.028	-1.32
NaCl	2.487e-06	2.489e-06	-5.604	-5.604	0.000	(0)
NaHCO3	8.333e-07	8.340e-07	-6.079	-6.079	0.000	1.80
NaSO4-	1.628e-07	1.527e-07	-6.788	-6.816	-0.028	13.90
NaF	2.506e-08	2.508e-08	-7.601	-7.601	0.000	7.35
NaCO3-	1.040e-09	9.737e-10	-8.983	-9.012	-0.029	-0.79
NaHPO4-	5.772e-11	5.413e-11	-10.239	-10.267	-0.028	33.65
NaOH	6.578e-22	6.584e-22	-21.182	-21.182	0.000	(0)
O(0)	0.000e+00					
O2	0.000e+00	0.000e+00	-60.326	-60.326	0.000	30.58
P	9.364e-07					
H2PO4-	8.623e-07	8.087e-07	-6.064	-6.092	-0.028	33.18
HPO4-2	4.156e-08	3.209e-08	-7.381	-7.494	-0.112	6.74
MgH2PO4+	8.378e-09	7.858e-09	-8.077	-8.105	-0.028	(0)
CaH2PO4+	7.652e-09	7.177e-09	-8.116	-8.144	-0.028	(0)
MgHPO4	7.079e-09	7.085e-09	-8.150	-8.150	0.000	(0)
CaHPO4	6.090e-09	6.095e-09	-8.215	-8.215	0.000	(0)
FeH2PO4+	2.409e-09	2.259e-09	-8.618	-8.646	-0.028	(0)
FeHPO4	7.115e-10	7.121e-10	-9.148	-9.147	0.000	(0)
H3PO4	1.938e-10	1.940e-10	-9.713	-9.712	0.000	47.53
NaHPO4-	5.772e-11	5.413e-11	-10.239	-10.267	-0.028	33.65
MgPO4-	1.175e-11	1.102e-11	-10.930	-10.958	-0.028	(0)
CaPO4-	1.013e-11	9.504e-12	-10.994	-11.022	-0.028	(0)
KHPO4-	6.387e-12	5.991e-12	-11.195	-11.223	-0.028	37.98
PO4-3	1.728e-14	9.561e-15	-13.762	-14.020	-0.257	-23.21
FeH2PO4+2	4.757e-19	3.681e-19	-18.323	-18.434	-0.111	(0)
FeHPO4+	1.680e-20	1.575e-20	-19.775	-19.803	-0.028	(0)
Pb	2.177e-08					
PbHCO3+	8.513e-09	7.972e-09	-8.070	-8.098	-0.029	(0)
Pb+2	7.514e-09	5.778e-09	-8.124	-8.238	-0.114	-15.47
PbCO3	5.397e-09	5.401e-09	-8.268	-8.267	0.000	(0)
PbCl+	1.230e-10	1.152e-10	-9.910	-9.938	-0.029	8.06
PbSO4	1.127e-10	1.128e-10	-9.948	-9.948	0.000	(0)
PbOH+	7.590e-11	7.107e-11	-10.120	-10.148	-0.029	(0)
PbNO3+	2.663e-11	2.494e-11	-10.575	-10.603	-0.029	(0)
PbF+	5.529e-12	5.177e-12	-11.257	-11.286	-0.029	(0)
PbBr+	2.032e-12	1.902e-12	-11.692	-11.721	-0.029	(0)
Pb(CO3)2-2	9.492e-13	7.299e-13	-12.023	-12.137	-0.114	(0)
PbCl2	8.264e-14	8.271e-14	-13.083	-13.082	0.000	35.15
Pb(SO4)2-2	2.671e-14	2.054e-14	-13.573	-13.687	-0.114	(0)
Pb(OH)2	1.743e-14	1.744e-14	-13.759	-13.758	0.000	(0)
PbF2	5.322e-15	5.327e-15	-14.274	-14.274	0.000	(0)
PbCl3-	3.366e-17	3.152e-17	-16.473	-16.501	-0.029	66.25
Pb2OH+3	1.660e-17	9.193e-18	-16.780	-17.037	-0.257	(0)
PbBr2	4.610e-18	4.614e-18	-17.336	-17.336	0.000	(0)
PbF3-	2.076e-18	1.944e-18	-17.683	-17.711	-0.029	(0)
Pb(OH)3-	1.349e-19	1.263e-19	-18.870	-18.898	-0.029	(0)
PbCl4-2	9.446e-21	7.264e-21	-20.025	-20.139	-0.114	101.81
PbF4-2	6.098e-23	4.690e-23	-22.215	-22.329	-0.114	(0)
Pb(OH)4-2	2.374e-25	1.826e-25	-24.624	-24.739	-0.114	(0)
Pb3(OH)4+2	7.408e-26	5.697e-26	-25.130	-25.244	-0.114	(0)
S(6)	4.998e-05					
SO4-2	4.495e-05	3.471e-05	-4.347	-4.460	-0.112	14.90

MgSO4	2.461e-06	2.463e-06	-5.609	-5.609	0.000	5.92
CaSO4	2.082e-06	2.083e-06	-5.682	-5.681	0.000	7.58
BaSO4	2.385e-07	2.387e-07	-6.623	-6.622	0.000	(0)
NaSO4-	1.628e-07	1.527e-07	-6.788	-6.816	-0.028	13.90
FeSO4	3.585e-08	3.588e-08	-7.445	-7.445	0.000	16.61
KSO4-	2.592e-08	2.431e-08	-7.586	-7.614	-0.028	34.19
ZnSO4	8.701e-09	8.708e-09	-8.060	-8.060	0.000	21.35
HSO4-	6.012e-09	5.629e-09	-8.221	-8.250	-0.029	40.45
MnSO4	2.409e-09	2.411e-09	-8.618	-8.618	0.000	21.55
PbSO4	1.127e-10	1.128e-10	-9.948	-9.948	0.000	(0)
CdSO4	4.131e-11	4.134e-11	-10.384	-10.384	0.000	76.94
CaHSO4+	2.398e-11	2.245e-11	-10.620	-10.649	-0.029	(0)
Zn(SO4)2-2	3.138e-12	2.413e-12	-11.503	-11.617	-0.114	-11.11
CuSO4	1.974e-12	1.976e-12	-11.705	-11.704	0.000	13.37
AlSO4+	1.662e-12	1.557e-12	-11.779	-11.808	-0.028	(0)
FeHSO4+	4.028e-13	3.772e-13	-12.395	-12.423	-0.029	(0)
Pb(SO4)2-2	2.671e-14	2.054e-14	-13.573	-13.687	-0.114	(0)
Cd(SO4)2-2	2.017e-14	1.551e-14	-13.695	-13.809	-0.114	-104.14
Al(SO4)2-	1.843e-15	1.727e-15	-14.734	-14.763	-0.028	(0)
FeSO4+	7.225e-19	6.773e-19	-18.141	-18.169	-0.028	(0)
AlHSO4+2	2.907e-19	2.235e-19	-18.537	-18.651	-0.114	(0)
Fe(SO4)2-	5.541e-22	5.189e-22	-21.256	-21.285	-0.029	(0)
FeHSO4+2	3.739e-24	2.875e-24	-23.427	-23.541	-0.114	(0)
Zn	1.630e-06					
Zn+2	1.362e-06	1.051e-06	-5.866	-5.978	-0.112	-25.42
ZnHCO3+	2.455e-07	2.299e-07	-6.610	-6.638	-0.029	(0)
ZnCO3	1.128e-08	1.129e-08	-7.948	-7.947	0.000	(0)
ZnSO4	8.701e-09	8.708e-09	-8.060	-8.060	0.000	21.35
ZnCl+	1.583e-09	1.482e-09	-8.801	-8.829	-0.029	-11.68
ZnOH+	9.256e-10	8.667e-10	-9.034	-9.062	-0.029	(0)
ZnF+	8.228e-10	7.705e-10	-9.085	-9.113	-0.029	(0)
Zn(CO3)2-2	1.688e-11	1.298e-11	-10.773	-10.887	-0.114	(0)
ZnOHCl	1.038e-11	1.039e-11	-10.984	-10.983	0.000	(0)
Zn(OH)2	5.264e-12	5.268e-12	-11.279	-11.278	0.000	(0)
Zn(SO4)2-2	3.138e-12	2.413e-12	-11.503	-11.617	-0.114	-11.11
ZnBr+	1.590e-12	1.489e-12	-11.799	-11.827	-0.029	(0)
ZnCl2	7.403e-13	7.409e-13	-12.131	-12.130	0.000	97.62
ZnCl3-	4.258e-16	3.987e-16	-15.371	-15.399	-0.029	17.20
Zn(OH)3-	1.122e-17	1.051e-17	-16.950	-16.978	-0.029	(0)
ZnBr2	3.190e-18	3.193e-18	-17.496	-17.496	0.000	(0)
ZnCl4-2	1.246e-19	9.625e-20	-18.904	-19.017	-0.112	145.57
Zn(OH)4-2	1.366e-24	1.051e-24	-23.864	-23.979	-0.114	(0)

----------Distribution of alkalinity----------

Total alkalinity (eq/kgw) = 1.867e-03

Species	Alkalinity	Molality	Alk/Mol
HCO3-	1.852e-03	1.852e-03	1.00
CaHCO3+	8.103e-06	8.103e-06	1.00
MgHCO3+	6.259e-06	6.259e-06	1.00
H+	-1.683e-06	1.683e-06	-1.00
FeHCO3+	1.034e-06	1.034e-06	1.00
NaHCO3	8.333e-07	8.333e-07	1.00
BaHCO3+	2.625e-07	2.625e-07	1.00
ZnHCO3+	2.455e-07	2.455e-07	1.00
CO3-2	1.391e-07	6.953e-08	2.00
HF	-1.248e-07	1.248e-07	-1.00
CaCO3	6.290e-08	3.145e-08	2.00
MnHCO3+	6.172e-08	6.172e-08	1.00
HPO4-2	4.156e-08	4.156e-08	1.00
MgCO3	3.032e-08	1.516e-08	2.00
ZnCO3	2.255e-08	1.128e-08	2.00
FeCO3	1.437e-08	7.186e-09	2.00
PbCO3	1.079e-08	5.397e-09	2.00
PbHCO3+	8.513e-09	8.513e-09	1.00
OH-	8.133e-09	8.133e-09	1.00

MgHPO4	7.079e-09	7.079e-09	1.00
CaHPO4	6.090e-09	6.090e-09	1.00
HSO4-	-6.012e-09	6.012e-09	-1.00
H2BO3-	4.283e-09	4.283e-09	1.00
MnCO3	3.191e-09	1.596e-09	2.00
NaCO3-	2.080e-09	1.040e-09	2.00
FeOH+	1.410e-09	1.410e-09	1.00
Al(OH)2+	1.292e-09	6.462e-10	2.00
ZnOH+	9.256e-10	9.256e-10	1.00
MgOH+	8.572e-10	8.572e-10	1.00
BaCO3	7.985e-10	3.992e-10	2.00
FeHPO4	7.115e-10	7.115e-10	1.00
Al(OH)4-	3.499e-10	8.748e-11	4.00
CuHCO3+	2.551e-10	2.551e-10	1.00
CdHCO3+	2.389e-10	2.389e-10	1.00
Al(OH)3	1.999e-10	6.662e-11	3.00
H3PO4	-1.938e-10	1.938e-10	-1.00
CuCO3	1.584e-10	7.922e-11	2.00
AlOH+2	1.296e-10	1.296e-10	1.00
PbOH+	7.590e-11	7.590e-11	1.00
Zn(CO3)2-2	6.752e-11	1.688e-11	4.00
NaHPO4-	5.772e-11	5.772e-11	1.00
CaOH+	3.709e-11	3.709e-11	1.00
HF2-	-2.625e-11	2.625e-11	-1.00
CaHSO4+	-2.398e-11	2.398e-11	-1.00
MgPO4-	2.351e-11	1.175e-11	2.00
CaPO4-	2.027e-11	1.013e-11	2.00
Zn(OH)2	1.053e-11	5.264e-12	2.00
ZnOHCl	1.038e-11	1.038e-11	1.00
MnOH+	7.805e-12	7.805e-12	1.00
KHPO4-	6.387e-12	6.387e-12	1.00
Cu(OH)2	4.560e-12	2.280e-12	2.00
Pb(CO3)2-2	3.797e-12	9.492e-13	4.00
BF2(OH)2-	-1.983e-12	1.983e-12	-1.00
CuOH+	1.849e-12	1.849e-12	1.00
FeHSO4+	-4.028e-13	4.028e-13	-1.00
CdCO3	3.477e-13	1.739e-13	2.00
BaOH+	3.129e-13	3.129e-13	1.00
CdOH+	2.709e-13	2.709e-13	1.00
Fe(OH)3	1.616e-13	1.616e-13	1.00
CdOHCl	5.070e-14	5.070e-14	1.00
Pb(OH)2	3.486e-14	1.743e-14	2.00
PO4-3	3.456e-14	1.728e-14	2.00
Cu(CO3)2-2	2.793e-14	6.983e-15	4.00
Fe(OH)2	1.734e-14	8.669e-15	2.00
FeOH+2	-1.022e-14	1.022e-14	-1.00
FeF2+	-6.154e-16	3.077e-16	-2.00
FeF+2	-3.623e-16	1.812e-16	-2.00
BF3OH-	-3.330e-16	1.665e-16	-2.00
Fe(OH)4-	2.178e-16	1.089e-16	2.00
Cd(CO3)2-2	1.540e-16	3.849e-17	4.00
FeF3	-4.640e-17	2.320e-17	-2.00
Zn(OH)3-	3.367e-17	1.122e-17	3.00
Pb2OH+3	1.660e-17	1.660e-17	1.00
Cd(OH)2	1.447e-17	7.233e-18	2.00
Fe+3	-5.817e-18	2.908e-18	-2.00
Cu2(OH)2+2	4.292e-18	2.146e-18	2.00
FeSO4+	-1.445e-18	7.225e-19	-2.00
FeH2PO4+2	-9.514e-19	4.757e-19	-2.00
Fe(OH)3-	6.657e-19	2.219e-19	3.00
Pb(OH)3-	4.047e-19	1.349e-19	3.00
AlHSO4+2	-2.907e-19	2.907e-19	-1.00
Cu(OH)3-	2.779e-19	9.263e-20	3.00
BF4-	-1.620e-19	5.401e-20	-3.00
FeCl+2	-6.731e-20	3.365e-20	-2.00
FeHPO4+	-1.680e-20	1.680e-20	-1.00
Cd2OH+3	8.877e-21	8.877e-21	1.00
Fe(SO4)2-	-1.108e-21	5.541e-22	-2.00

NaOH	6.578e-22	6.578e-22	1.00
FeCl2+	-1.089e-22	5.443e-23	-2.00
FeHSO4+2	-1.122e-23	3.739e-24	-3.00
Zn(OH)4-2	5.466e-24	1.366e-24	4.00
Mn(OH)3-	4.759e-24	1.586e-24	3.00
Cd(OH)3-	1.642e-24	5.472e-25	3.00
Pb(OH)4-2	9.498e-25	2.374e-25	4.00
Pb3(OH)4+2	2.963e-25	7.408e-26	4.00
Cu(OH)4-2	5.679e-26	1.420e-26	4.00
Fe2(OH)2+4	-8.715e-27	4.357e-27	-2.00
FeCl3	-4.823e-27	2.411e-27	-2.00
Cd(OH)4-2	1.499e-32	3.746e-33	4.00
Fe3(OH)4+5	-4.781e-36	2.390e-36	-2.00

-----Saturation indices-----

Phase	SI**	log IAP	log K(300 K, 1 atm)	
Al(OH)3(a)	-4.11	6.54	10.65	Al(OH)3
Alunite	-9.04	-10.72	-1.69	KAl3(SO4)2(OH)6
Anglesite	-4.92	-12.70	-7.78	PbSO4
Anhydrite	-3.64	-7.94	-4.30	CaSO4
Aragonite	-2.40	-10.75	-8.35	CaCO3
BaCl2	-13.72	-11.51	2.21	BaCl2
BaCl2:2H2O	-11.74	-11.51	0.23	BaCl2:2H2O
BaCl2:H2O	-12.34	-11.51	0.83	BaCl2:H2O
Barite	0.50	-9.32	-9.82	BaSO4
Calcite	-2.26	-10.75	-8.49	CaCO3
Cd(OH)2	-10.44	3.21	13.65	Cd(OH)2
CdSO4	-12.67	-12.85	-0.18	CdSO4
Cerussite	-2.41	-15.51	-13.10	PbCO3
CO2(g)	-0.73	-2.22	-1.50	CO2
Dolomite	-4.42	-21.56	-17.14	CaMg(CO3)2
Fe(OH)3(a)	-5.26	-0.37	4.89	Fe(OH)3
Fluorite	-1.50	-12.07	-10.57	CaF2
Gibbsite	-1.44	6.54	7.98	Al(OH)3
Goethite	0.71	-0.37	-1.08	FeOOH
Gypsum	-3.36	-7.94	-4.58	CaSO4:2H2O
H2(g)	-12.55	-15.65	-3.11	H2
H2O(g)	-1.44	-0.00	1.44	H2O
Halite	-7.96	-6.39	1.57	NaCl
Hausmannite	-32.45	28.01	60.46	Mn3O4
Hematite	3.44	-0.74	-4.18	Fe2O3
Hydroxyapatite	-13.05	-16.68	-3.63	Ca5(PO4)3OH
Jarosite-K	-22.07	-31.45	-9.39	KFe3(SO4)2(OH)6
Manganite	-13.92	11.42	25.34	MnOOH
Melanterite	-7.53	-9.71	-2.18	FeSO4:7H2O
O2(g)	-57.42	-60.33	-2.91	O2
Otavite	-3.56	-15.66	-12.10	CdCO3
Pb(OH)2	-4.71	3.36	8.07	Pb(OH)2
Pyrochroite	-10.03	5.17	15.20	Mn(OH)2
Pyrolusite	-23.34	17.67	41.01	MnO2:H2O
Rhodochrosite	-2.56	-13.70	-11.14	MnCO3
Siderite	-1.62	-12.52	-10.90	FeCO3
Smithsonite	-3.22	-13.25	-10.02	ZnCO3
Sylvite	-8.26	-7.34	0.91	KCl
Vivianite	-7.80	-43.80	-36.00	Fe3(PO4)2:8H2O
Witherite	-3.57	-12.13	-8.56	BaCO3
Zn(OH)2(e)	-5.88	5.62	11.50	Zn(OH)2

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
For ideal gases, phi = 1.

Initial solution 24.

-----Solution composition-----

Elements	Molality	Moles

Al	2.297e-06 2.297e-06
Alkalinity	1.218e-02 1.218e-02
B	5.603e-05 5.603e-05
Ba	1.443e-05 1.443e-05
Br	6.138e-06 6.138e-06
Ca	4.995e-04 4.995e-04
Cd	7.391e-09 7.391e-09
Cl	1.045e-03 1.045e-03
Cu	3.906e-08 3.906e-08
F	3.177e-04 3.177e-04
Fe	5.481e-07 5.481e-07
K	8.447e-05 8.447e-05
Mg	5.574e-04 5.574e-04
Mn	1.018e-07 1.018e-07
N(5)	2.030e-04 2.030e-04
Na	1.041e-02 1.041e-02
P	3.878e-07 3.878e-07
Pb	5.218e-09 5.218e-09
S(6)	3.751e-05 3.751e-05
Zn	2.015e-06 2.015e-06

----------Description of solution----------

pH	= 8.400
pe	= 0.404
Specific Conductance (µS/cm, 27°C)	= 1201
Density (g/cm³)	= 0.99737
Volume (L)	= 1.00371
Activity of water	= 1.000
Ionic strength (mol/kgw)	= 1.395e-02
Mass of water (kg)	= 1.000e+00
Total carbon (mol/kg)	= 1.193e-02
Total CO2 (mol/kg)	= 1.193e-02
Temperature (°C)	= 26.74
Electrical balance (eq)	= -1.174e-03
Percent error, 100*(Cat-|An|)/(Cat+|An|)	= -4.58
Iterations	= 11 (255 overall)
Total H	= 1.110241e+02
Total O	= 5.554286e+01

----------Distribution of species----------

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma	mole V cm³/mol
OH-	3.276e-06	2.899e-06	-5.485	-5.538	-0.053	-3.95
H+	4.413e-09	3.981e-09	-8.355	-8.400	-0.045	0.00
H2O	5.551e+01	9.996e-01	1.744	-0.000	0.000	18.08
Al	2.297e-06					
Al(OH)4-	2.293e-06	2.037e-06	-5.640	-5.691	-0.051	(0)
Al(OH)3	4.186e-09	4.199e-09	-8.378	-8.377	0.001	(0)
Al(OH)2+	1.122e-10	1.000e-10	-9.950	-10.000	-0.050	(0)
AlF3	2.075e-11	2.082e-11	-10.683	-10.682	0.001	(0)
AlF2+	6.753e-12	6.020e-12	-11.170	-11.220	-0.050	(0)
AlF4-	2.559e-12	2.273e-12	-11.592	-11.643	-0.051	(0)
AlOH+2	6.929e-14	4.374e-14	-13.159	-13.359	-0.200	-27.57
AlF+2	6.877e-14	4.341e-14	-13.163	-13.362	-0.200	(0)
Al+3	3.962e-17	1.567e-17	-16.402	-16.805	-0.403	-41.90
AlSO4+	1.208e-18	1.073e-18	-17.918	-17.969	-0.051	(0)
Al(SO4)2-	8.152e-22	7.242e-22	-21.089	-21.140	-0.051	(0)
AlHSO4+2	6.205e-28	3.848e-28	-27.207	-27.415	-0.208	(0)
B	5.603e-05					
H3BO3	4.794e-05	4.809e-05	-4.319	-4.318	0.001	39.36
H2BO3-	8.085e-06	7.174e-06	-5.092	-5.144	-0.052	(0)
BF(OH)3-	6.024e-09	5.346e-09	-8.220	-8.272	-0.052	(0)
BF2(OH)2-	7.033e-13	6.241e-13	-12.153	-12.205	-0.052	(0)
BF3OH-	8.160e-19	7.241e-19	-18.088	-18.140	-0.052	(0)

BF4-	3.622e-24	3.214e-24	-23.441	-23.493	-0.052	(0)
Ba	1.443e-05					
Ba+2	1.287e-05	7.988e-06	-4.891	-5.098	-0.207	-12.38
BaHCO3+	9.256e-07	8.213e-07	-6.034	-6.085	-0.052	(0)
BaCO3	5.273e-07	5.290e-07	-6.278	-6.277	0.001	-10.68
BaSO4	8.450e-08	8.477e-08	-7.073	-7.072	0.001	(0)
BaCl+	2.564e-08	2.275e-08	-7.591	-7.643	-0.052	(0)
BaNO3+	2.031e-10	1.802e-10	-9.692	-9.744	-0.052	(0)
BaOH+	7.636e-11	6.796e-11	-10.117	-10.168	-0.051	(0)
Br	6.138e-06					
Br-	6.138e-06	5.419e-06	-5.212	-5.266	-0.054	24.71
CdBr+	2.907e-12	2.580e-12	-11.536	-11.588	-0.052	(0)
ZnBr+	2.410e-14	2.139e-14	-13.618	-13.670	-0.052	(0)
PbBr+	5.956e-16	5.285e-16	-15.225	-15.277	-0.052	(0)
CdBr2	7.544e-17	7.568e-17	-16.122	-16.121	0.001	(0)
ZnBr2	4.600e-20	4.614e-20	-19.337	-19.336	0.001	(0)
PbBr2	1.298e-21	1.302e-21	-20.887	-20.885	0.001	(0)
C(4)	1.193e-02					
HCO3-	1.139e-02	1.015e-02	-1.943	-1.993	-0.050	24.92
CO3-2	1.961e-04	1.238e-04	-3.708	-3.907	-0.200	-4.82
CO2	8.880e-05	8.908e-05	-4.052	-4.050	0.001	34.52
CaCO3	5.496e-05	5.514e-05	-4.260	-4.259	0.001	-14.59
NaHCO3	5.155e-05	5.172e-05	-4.288	-4.286	0.001	1.80
MgHCO3+	4.060e-05	3.599e-05	-4.392	-4.444	-0.052	5.59
CaHCO3+	3.806e-05	3.399e-05	-4.420	-4.469	-0.049	9.80
MgCO3	3.634e-05	3.646e-05	-4.440	-4.438	0.001	-17.09
NaCO3-	2.593e-05	2.301e-05	-4.586	-4.638	-0.052	-0.74
Zn(CO3)2-2	1.582e-06	9.811e-07	-5.801	-6.008	-0.208	(0)
BaHCO3+	9.256e-07	8.213e-07	-6.034	-6.085	-0.052	(0)
BaCO3	5.273e-07	5.290e-07	-6.278	-6.277	0.001	-10.68
ZnCO3	3.695e-07	3.707e-07	-6.432	-6.431	0.001	(0)
FeCO3	2.103e-07	2.110e-07	-6.677	-6.676	0.001	(0)
FeHCO3+	8.129e-08	7.214e-08	-7.090	-7.142	-0.052	(0)
MnCO3	8.046e-08	8.072e-08	-7.094	-7.093	0.001	(0)
ZnHCO3+	2.162e-08	1.918e-08	-7.665	-7.717	-0.052	(0)
CuCO3	1.057e-08	1.060e-08	-7.976	-7.975	0.001	(0)
MnHCO3+	8.347e-09	7.429e-09	-8.078	-8.129	-0.051	(0)
PbCO3	3.453e-09	3.464e-09	-8.462	-8.460	0.001	(0)
Cu(CO3)2-2	2.664e-09	1.652e-09	-8.574	-8.782	-0.208	(0)
Pb(CO3)2-2	1.737e-09	1.077e-09	-8.760	-8.968	-0.208	(0)
CdHCO3+	1.174e-09	1.042e-09	-8.930	-8.982	-0.052	(0)
CdCO3	3.180e-10	3.191e-10	-9.498	-9.496	0.001	(0)
Cd(CO3)2-2	2.014e-10	1.249e-10	-9.696	-9.903	-0.208	(0)
(CO2)2	1.537e-10	1.542e-10	-9.813	-9.812	0.001	69.04
CuHCO3+	9.145e-11	8.115e-11	-10.039	-10.091	-0.052	(0)
PbHCO3+	1.464e-11	1.299e-11	-10.835	-10.886	-0.052	(0)
Ca	4.995e-04					
Ca+2	4.054e-04	2.558e-04	-3.392	-3.592	-0.200	-17.86
CaCO3	5.496e-05	5.514e-05	-4.260	-4.259	0.001	-14.59
CaHCO3+	3.806e-05	3.399e-05	-4.420	-4.469	-0.049	9.80
CaSO4	9.725e-07	9.756e-07	-6.012	-6.011	0.001	7.56
CaHPO4	2.415e-08	2.423e-08	-7.617	-7.616	0.001	(0)
CaPO4-	1.669e-08	1.487e-08	-7.778	-7.828	-0.050	(0)
CaOH+	1.201e-08	1.066e-08	-7.920	-7.972	-0.052	(0)
CaH2PO4+	8.062e-11	7.186e-11	-10.094	-10.143	-0.050	(0)
CaHSO4+	2.951e-14	2.618e-14	-13.530	-13.582	-0.052	(0)
Cd	7.391e-09					
Cd+2	5.233e-09	3.245e-09	-8.281	-8.489	-0.208	-18.41
CdHCO3+	1.174e-09	1.042e-09	-8.930	-8.982	-0.052	(0)
CdCO3	3.180e-10	3.191e-10	-9.498	-9.496	0.001	(0)
CdCl+	3.098e-10	2.749e-10	-9.509	-9.561	-0.052	6.43
Cd(CO3)2-2	2.014e-10	1.249e-10	-9.696	-9.903	-0.208	(0)
CdOH+	8.681e-11	7.703e-11	-10.061	-10.113	-0.052	(0)
CdOHCl	2.948e-11	2.958e-11	-10.530	-10.529	0.001	(0)
CdSO4	1.996e-11	2.002e-11	-10.700	-10.698	0.001	77.21
CdF+	1.262e-11	1.120e-11	-10.899	-10.951	-0.052	(0)
CdBr+	2.907e-12	2.580e-12	-11.536	-11.588	-0.052	(0)
CdNO3+	1.564e-12	1.388e-12	-11.806	-11.858	-0.052	17.54

CdCl2	1.014e-12	1.017e-12	-11.994	-11.993	0.001	23.14
Cd(OH)2	9.107e-13	9.137e-13	-12.041	-12.039	0.001	(0)
CdF2	7.689e-15	7.714e-15	-14.114	-14.113	0.001	(0)
Cd(SO4)2-2	7.418e-15	4.600e-15	-14.130	-14.337	-0.208	-104.33
CdCl3-	6.548e-16	5.810e-16	-15.184	-15.236	-0.052	68.19
CdBr2	7.544e-17	7.568e-17	-16.122	-16.121	0.001	(0)
Cd(OH)3-	2.901e-17	2.574e-17	-16.538	-16.589	-0.052	(0)
Cd2OH+3	3.512e-18	1.198e-18	-17.454	-17.922	-0.467	(0)
Cd(OH)4-2	9.289e-23	5.760e-23	-22.032	-22.240	-0.208	(0)
Cl	1.045e-03					
Cl-	9.959e-04	8.820e-04	-3.002	-3.055	-0.053	18.20
NaCl	4.871e-05	4.887e-05	-4.312	-4.311	0.001	(0)
BaCl+	2.564e-08	2.275e-08	-7.591	-7.643	-0.052	(0)
CuCl2-	9.271e-10	8.219e-10	-9.033	-9.085	-0.052	(0)
CdCl+	3.098e-10	2.749e-10	-9.509	-9.561	-0.052	6.43
ZnOHCl	1.097e-10	1.100e-10	-9.960	-9.958	0.001	(0)
FeCl+	9.747e-11	8.649e-11	-10.011	-10.063	-0.052	(0)
ZnCl+	4.337e-11	3.845e-11	-10.363	-10.415	-0.052	-12.22
MnCl+	3.314e-11	2.949e-11	-10.480	-10.530	-0.051	-2.62
CdOHCl	2.948e-11	2.958e-11	-10.530	-10.529	0.001	(0)
CuCl3-2	1.843e-12	1.157e-12	-11.734	-11.937	-0.202	(0)
CdCl2	1.014e-12	1.017e-12	-11.994	-11.993	0.001	23.14
PbCl+	6.651e-14	5.902e-14	-13.177	-13.229	-0.052	8.08
CuCl+	4.647e-14	4.120e-14	-13.333	-13.385	-0.052	0.28
ZnCl2	3.565e-14	3.576e-14	-13.448	-13.447	0.001	98.71
MnCl2	1.132e-14	1.136e-14	-13.946	-13.945	0.001	83.81
CdCl3-	6.548e-16	5.810e-16	-15.184	-15.236	-0.052	68.19
PbCl2	7.963e-17	7.989e-17	-16.099	-16.098	0.001	35.11
ZnCl3-	4.034e-17	3.576e-17	-16.394	-16.447	-0.052	17.12
CuCl2	1.982e-17	1.988e-17	-16.703	-16.702	0.001	32.98
MnCl3-	3.100e-18	2.759e-18	-17.509	-17.559	-0.051	43.39
PbCl3-	6.375e-20	5.657e-20	-19.196	-19.247	-0.052	66.24
ZnCl4-2	2.554e-20	1.603e-20	-19.593	-19.795	-0.202	145.76
FeCl+2	8.479e-22	5.321e-22	-21.072	-21.274	-0.202	(0)
CuCl3-	7.238e-23	6.417e-23	-22.140	-22.193	-0.052	(0)
PbCl4-2	3.903e-23	2.420e-23	-22.409	-22.616	-0.208	101.94
FeCl2+	2.230e-24	1.984e-24	-23.652	-23.702	-0.051	(0)
CuCl4-2	4.705e-28	2.952e-28	-27.327	-27.530	-0.202	(0)
FeCl3	1.745e-28	1.750e-28	-27.758	-27.757	0.001	(0)
Cu(1)	4.737e-09					
Cu+	3.808e-09	3.354e-09	-8.419	-8.474	-0.055	(0)
CuCl2-	9.271e-10	8.219e-10	-9.033	-9.085	-0.052	(0)
CuCl3-2	1.843e-12	1.157e-12	-11.734	-11.937	-0.202	(0)
Cu(2)	3.433e-08					
Cu(OH)2	2.093e-08	2.100e-08	-7.679	-7.678	0.001	(0)
CuCO3	1.057e-08	1.060e-08	-7.976	-7.975	0.001	(0)
Cu(CO3)2-2	2.664e-09	1.652e-09	-8.574	-8.782	-0.208	(0)
CuHCO3+	9.145e-11	8.115e-11	-10.039	-10.091	-0.052	(0)
CuOH+	4.516e-11	4.003e-11	-10.345	-10.398	-0.052	(0)
Cu+2	2.504e-11	1.594e-11	-10.601	-10.797	-0.196	-26.37
Cu(OH)3-	3.581e-13	3.177e-13	-12.446	-12.498	-0.052	(0)
CuF+	9.109e-14	8.083e-14	-13.041	-13.092	-0.052	(0)
CuSO4	6.953e-14	6.976e-14	-13.158	-13.156	0.001	13.30
CuCl+	4.647e-14	4.120e-14	-13.333	-13.385	-0.052	0.28
Cu2(OH)2+2	1.343e-15	8.327e-16	-14.872	-15.080	-0.208	(0)
Cu(OH)4-2	2.567e-17	1.592e-17	-16.591	-16.798	-0.208	(0)
CuCl2	1.982e-17	1.988e-17	-16.703	-16.702	0.001	32.98
CuCl3-	7.238e-23	6.417e-23	-22.140	-22.193	-0.052	(0)
CuCl4-2	4.705e-28	2.952e-28	-27.327	-27.530	-0.202	(0)
F	3.177e-04					
F-	3.099e-04	2.742e-04	-3.509	-3.562	-0.053	-1.22
MgF+	6.323e-06	5.617e-06	-5.199	-5.251	-0.051	-10.51
NaF	1.438e-06	1.443e-06	-5.842	-5.841	0.001	7.33
BF(OH)3-	6.024e-09	5.346e-09	-8.220	-8.272	-0.052	(0)
HF	1.684e-09	1.689e-09	-8.774	-8.772	0.001	12.58
FeF+	2.195e-10	1.948e-10	-9.659	-9.710	-0.052	(0)
ZnF+	6.694e-11	5.940e-11	-10.174	-10.226	-0.052	(0)
AlF3	2.075e-11	2.082e-11	-10.683	-10.682	0.001	(0)

MnF+	1.750e-11	1.557e-11	-10.757	-10.808	-0.051	(0)
CdF+	1.262e-11	1.120e-11	-10.899	-10.951	-0.052	(0)
AlF2+	6.753e-12	6.020e-12	-11.170	-11.220	-0.050	(0)
AlF4-	2.559e-12	2.273e-12	-11.592	-11.643	-0.051	(0)
HF2-	2.029e-12	1.801e-12	-11.693	-11.745	-0.052	22.22
BF2(OH)2-	7.033e-13	6.241e-13	-12.153	-12.205	-0.052	(0)
CuF+	9.109e-14	8.083e-14	-13.041	-13.092	-0.052	(0)
AlF+2	6.877e-14	4.341e-14	-13.163	-13.362	-0.200	(0)
PbF+	8.848e-15	7.852e-15	-14.053	-14.105	-0.052	(0)
CdF2	7.689e-15	7.714e-15	-14.114	-14.113	0.001	(0)
FeF2+	1.056e-16	9.402e-17	-15.976	-16.027	-0.051	(0)
PbF2	4.382e-17	4.396e-17	-16.358	-16.357	0.001	(0)
FeF3	4.097e-17	4.110e-17	-16.388	-16.386	0.001	(0)
FeF+2	1.345e-17	8.437e-18	-16.871	-17.074	-0.202	(0)
BF3OH-	8.160e-19	7.241e-19	-18.088	-18.140	-0.052	(0)
PbF3-	9.840e-20	8.732e-20	-19.007	-19.059	-0.052	(0)
PbF4-2	1.848e-23	1.146e-23	-22.733	-22.941	-0.208	(0)
BF4-	3.622e-24	3.214e-24	-23.441	-23.493	-0.052	(0)
Fe(2)	4.110e-07					
FeCO3	2.103e-07	2.110e-07	-6.677	-6.676	0.001	(0)
Fe+2	1.116e-07	7.104e-08	-6.953	-7.149	-0.196	-21.77
FeHCO3+	8.129e-08	7.214e-08	-7.090	-7.142	-0.052	(0)
FeOH+	7.212e-09	6.419e-09	-8.142	-8.193	-0.051	(0)
FeSO4	2.752e-10	2.761e-10	-9.560	-9.559	0.001	17.19
FeF+	2.195e-10	1.948e-10	-9.659	-9.710	-0.052	(0)
FeCl+	9.747e-11	8.649e-11	-10.011	-10.063	-0.052	(0)
FeHPO4	4.715e-11	4.730e-11	-10.326	-10.325	0.001	(0)
Fe(OH)2	1.589e-11	1.594e-11	-10.799	-10.797	0.001	(0)
FeH2PO4+	4.243e-13	3.782e-13	-12.372	-12.422	-0.050	(0)
Fe(OH)3-	1.700e-13	1.513e-13	-12.770	-12.820	-0.051	(0)
FeHSO4+	8.195e-18	7.272e-18	-17.086	-17.138	-0.052	(0)
Fe(3)	1.371e-07					
Fe(OH)3	1.048e-07	1.051e-07	-6.980	-6.978	0.001	(0)
Fe(OH)4-	2.894e-08	2.580e-08	-7.538	-7.588	-0.050	(0)
Fe(OH)2+	3.380e-09	3.013e-09	-8.471	-8.521	-0.050	(0)
FeOH+2	5.408e-14	3.394e-14	-13.267	-13.469	-0.202	(0)
FeF2+	1.056e-16	9.402e-17	-15.976	-16.027	-0.051	(0)
FeF3	4.097e-17	4.110e-17	-16.388	-16.386	0.001	(0)
FeF+2	1.345e-17	8.437e-18	-16.871	-17.074	-0.202	(0)
Fe+3	4.782e-20	1.891e-20	-19.320	-19.723	-0.403	(0)
FeSO4+	5.125e-21	4.561e-21	-20.290	-20.341	-0.051	(0)
FeHPO4+	1.012e-21	9.007e-22	-20.995	-21.045	-0.051	(0)
FeCl+2	8.479e-22	5.321e-22	-21.072	-21.274	-0.202	(0)
FeH2PO4+2	8.563e-23	5.406e-23	-22.067	-22.267	-0.200	(0)
Fe(SO4)2-	2.397e-24	2.127e-24	-23.620	-23.672	-0.052	(0)
FeCl2+	2.230e-24	1.984e-24	-23.652	-23.702	-0.051	(0)
Fe2(OH)2+4	1.953e-25	2.886e-26	-24.709	-25.540	-0.830	(0)
FeCl3	1.745e-28	1.750e-28	-27.758	-27.757	0.001	(0)
FeHSO4+2	7.842e-29	4.862e-29	-28.106	-28.313	-0.208	(0)
Fe3(OH)4+5	3.072e-31	1.549e-32	-30.513	-31.810	-1.297	(0)
H(0)	3.421e-21					
H2	1.711e-21	1.716e-21	-20.767	-20.765	0.001	28.60
K	8.447e-05					
K+	8.446e-05	7.476e-05	-4.073	-4.126	-0.053	9.14
KSO4-	1.286e-08	1.146e-08	-7.891	-7.941	-0.050	34.23
KHPO4-	2.735e-11	2.438e-11	-10.563	-10.613	-0.050	38.09
Mg	5.574e-04					
Mg+2	4.722e-04	3.005e-04	-3.326	-3.522	-0.196	-21.62
MgHCO3+	4.060e-05	3.599e-05	-4.392	-4.444	-0.052	5.59
MgCO3	3.634e-05	3.646e-05	-4.440	-4.438	0.001	-17.09
MgF+	6.323e-06	5.617e-06	-5.199	-5.251	-0.051	-10.51
MgSO4	1.554e-06	1.559e-06	-5.808	-5.807	0.001	5.90
MgOH+	3.578e-07	3.202e-07	-6.446	-6.495	-0.048	(0)
MgHPO4	3.836e-08	3.848e-08	-7.416	-7.415	0.001	(0)
MgPO4-	2.645e-08	2.357e-08	-7.578	-7.628	-0.050	(0)
MgH2PO4+	1.206e-10	1.075e-10	-9.919	-9.969	-0.050	(0)
Mn(2)	1.018e-07					
MnCO3	8.046e-08	8.072e-08	-7.094	-7.093	0.001	(0)

Mn+2	1.289e-08	8.208e-09	-7.890	-8.086	-0.196	-19.61
MnHCO3+	8.347e-09	7.429e-09	-8.078	-8.129	-0.051	(0)
MnOH+	6.853e-11	6.100e-11	-10.164	-10.215	-0.051	(0)
MnCl+	3.314e-11	2.949e-11	-10.480	-10.530	-0.051	-2.62
MnSO4	3.184e-11	3.194e-11	-10.497	-10.496	0.001	21.79
MnF+	1.750e-11	1.557e-11	-10.757	-10.808	-0.051	(0)
MnCl2	1.132e-14	1.136e-14	-13.946	-13.945	0.001	83.81
Mn(NO3)2	1.042e-15	1.045e-15	-14.982	-14.981	0.001	40.59
MnCl3-	3.100e-18	2.759e-18	-17.509	-17.559	-0.051	43.39
Mn(OH)3-	2.314e-18	2.059e-18	-17.636	-17.686	-0.051	(0)
Mn(3)	2.094e-33					
Mn+3	2.094e-33	8.279e-34	-32.679	-33.082	-0.403	(0)
N(5)	2.030e-04					
NO3-	2.030e-04	1.792e-04	-3.693	-3.747	-0.054	29.73
BaNO3+	2.031e-10	1.802e-10	-9.692	-9.744	-0.052	(0)
CdNO3+	1.564e-12	1.388e-12	-11.806	-11.858	-0.052	17.54
PbNO3+	4.809e-15	4.268e-15	-14.318	-14.370	-0.052	(0)
Mn(NO3)2	1.042e-15	1.045e-15	-14.982	-14.981	0.001	40.59
Na	1.041e-02					
Na+	1.029e-02	9.146e-03	-1.988	-2.039	-0.051	-1.27
NaHCO3	5.155e-05	5.172e-05	-4.288	-4.286	0.001	1.80
NaCl	4.871e-05	4.887e-05	-4.312	-4.311	0.001	(0)
NaCO3-	2.593e-05	2.301e-05	-4.586	-4.638	-0.052	-0.74
NaF	1.438e-06	1.443e-06	-5.842	-5.841	0.001	7.33
NaSO4-	1.101e-06	9.812e-07	-5.958	-6.008	-0.050	14.43
NaHPO4-	3.346e-09	2.983e-09	-8.475	-8.525	-0.050	34.46
NaOH	2.642e-18	2.651e-18	-17.578	-17.577	0.001	(0)
O(0)	0.000e+00					
O2	0.000e+00	0.000e+00	-50.293	-50.291	0.001	30.53
P	3.878e-07					
HPO4-2	2.666e-07	1.673e-07	-6.574	-6.777	-0.202	6.98
MgHPO4	3.836e-08	3.848e-08	-7.416	-7.415	0.001	(0)
MgPO4-	2.645e-08	2.357e-08	-7.578	-7.628	-0.050	(0)
CaHPO4	2.415e-08	2.423e-08	-7.617	-7.616	0.001	(0)
CaPO4-	1.669e-08	1.487e-08	-7.778	-7.828	-0.050	(0)
H2PO4-	1.192e-08	1.062e-08	-7.924	-7.974	-0.050	33.27
NaHPO4-	3.346e-09	2.983e-09	-8.475	-8.525	-0.050	34.46
MgH2PO4+	1.206e-10	1.075e-10	-9.919	-9.969	-0.050	(0)
CaH2PO4+	8.062e-11	7.186e-11	-10.094	-10.143	-0.050	(0)
PO4-3	5.795e-11	1.961e-11	-10.237	-10.708	-0.471	-22.67
FeHPO4	4.715e-11	4.730e-11	-10.326	-10.325	0.001	(0)
KHPO4-	2.735e-11	2.438e-11	-10.563	-10.613	-0.050	38.09
FeH2PO4+	4.243e-13	3.782e-13	-12.372	-12.422	-0.050	(0)
H3PO4	6.335e-15	6.356e-15	-14.198	-14.197	0.001	47.50
FeHPO4+	1.012e-21	9.007e-22	-20.995	-21.045	-0.051	(0)
FeH2PO4+2	8.563e-23	5.406e-23	-22.067	-22.267	-0.200	(0)
Pb	5.218e-09					
PbCO3	3.453e-09	3.464e-09	-8.462	-8.460	0.001	(0)
Pb(CO3)2-2	1.737e-09	1.077e-09	-8.760	-8.968	-0.208	(0)
PbHCO3+	1.464e-11	1.299e-11	-10.835	-10.886	-0.052	(0)
PbOH+	8.884e-12	7.883e-12	-11.051	-11.103	-0.052	(0)
Pb+2	2.597e-12	1.610e-12	-11.586	-11.793	-0.208	-15.29
Pb(OH)2	7.676e-13	7.701e-13	-12.115	-12.113	0.001	(0)
PbCl+	6.651e-14	5.902e-14	-13.177	-13.229	-0.052	8.08
PbSO4	1.911e-14	1.917e-14	-13.719	-13.717	0.001	(0)
PbF+	8.848e-15	7.852e-15	-14.053	-14.105	-0.052	(0)
PbNO3+	4.809e-15	4.268e-15	-14.318	-14.370	-0.052	(0)
Pb(OH)3-	2.502e-15	2.220e-15	-14.602	-14.654	-0.052	(0)
PbBr+	5.956e-16	5.285e-16	-15.225	-15.277	-0.052	(0)
PbCl2	7.963e-17	7.989e-17	-16.099	-16.098	0.001	35.11
PbF2	4.382e-17	4.396e-17	-16.358	-16.357	0.001	(0)
Pb(SO4)2-2	3.436e-18	2.131e-18	-17.464	-17.672	-0.208	(0)
Pb(OH)4-2	2.059e-18	1.277e-18	-17.686	-17.894	-0.208	(0)
PbF3-	9.840e-20	8.732e-20	-19.007	-19.059	-0.052	(0)
PbCl3-	6.375e-20	5.657e-20	-19.196	-19.247	-0.052	66.24
PbBr2	1.298e-21	1.302e-21	-20.887	-20.885	0.001	(0)
Pb2OH+3	8.330e-22	2.842e-22	-21.079	-21.546	-0.467	(0)
PbCl4-2	3.903e-23	2.420e-23	-22.409	-22.616	-0.208	101.94

PbF4-2	1.848e-23	1.146e-23	-22.733	-22.941	-0.208	(0)
Pb3(OH)4+2	4.573e-26	2.836e-26	-25.340	-25.547	-0.208	(0)
S(6)	3.751e-05					
SO4-2	3.378e-05	2.117e-05	-4.471	-4.674	-0.203	15.05
MgSO4	1.554e-06	1.559e-06	-5.808	-5.807	0.001	5.90
NaSO4-	1.101e-06	9.812e-07	-5.958	-6.008	-0.050	14.43
CaSO4	9.725e-07	9.756e-07	-6.012	-6.011	0.001	7.56
BaSO4	8.450e-08	8.477e-08	-7.073	-7.072	0.001	(0)
KSO4-	1.286e-08	1.146e-08	-7.891	-7.941	-0.050	34.23
FeSO4	2.752e-10	2.761e-10	-9.560	-9.559	0.001	17.19
ZnSO4	7.524e-11	7.548e-11	-10.124	-10.122	0.001	21.44
MnSO4	3.184e-11	3.194e-11	-10.497	-10.496	0.001	21.79
CdSO4	1.996e-11	2.002e-11	-10.700	-10.698	0.001	77.21
HSO4-	9.595e-12	8.515e-12	-11.018	-11.070	-0.052	40.47
CuSO4	6.953e-14	6.976e-14	-13.158	-13.156	0.001	13.30
CaHSO4+	2.951e-14	2.618e-14	-13.530	-13.582	-0.052	(0)
Zn(SO4)2-2	2.067e-14	1.282e-14	-13.685	-13.892	-0.208	-11.29
PbSO4	1.911e-14	1.917e-14	-13.719	-13.717	0.001	(0)
Cd(SO4)2-2	7.418e-15	4.600e-15	-14.130	-14.337	-0.208	-104.33
FeHSO4+	8.195e-18	7.272e-18	-17.086	-17.138	-0.052	(0)
Pb(SO4)2-2	3.436e-18	2.131e-18	-17.464	-17.672	-0.208	(0)
AlSO4+	1.208e-18	1.073e-18	-17.918	-17.969	-0.051	(0)
FeSO4+	5.125e-21	4.561e-21	-20.290	-20.341	-0.051	(0)
Al(SO4)2-	8.152e-22	7.242e-22	-21.089	-21.140	-0.051	(0)
Fe(SO4)2-	2.397e-24	2.127e-24	-23.620	-23.672	-0.052	(0)
AlHSO4+2	6.205e-28	3.848e-28	-27.207	-27.415	-0.208	(0)
FeHSO4+2	7.842e-29	4.862e-29	-28.106	-28.313	-0.208	(0)
Zn	2.015e-06					
Zn(CO3)2-2	1.582e-06	9.811e-07	-5.801	-6.008	-0.208	(0)
ZnCO3	3.695e-07	3.707e-07	-6.432	-6.431	0.001	(0)
Zn+2	2.391e-08	1.501e-08	-7.621	-7.824	-0.202	-25.21
ZnHCO3+	2.162e-08	1.918e-08	-7.665	-7.717	-0.052	(0)
Zn(OH)2	1.187e-08	1.191e-08	-7.925	-7.924	0.001	(0)
ZnOH+	5.309e-09	4.711e-09	-8.275	-8.327	-0.052	(0)
ZnOHCl	1.097e-10	1.100e-10	-9.960	-9.958	0.001	(0)
ZnSO4	7.524e-11	7.548e-11	-10.124	-10.122	0.001	21.44
ZnF+	6.694e-11	5.940e-11	-10.174	-10.226	-0.052	(0)
ZnCl+	4.337e-11	3.845e-11	-10.363	-10.415	-0.052	-12.22
Zn(OH)3-	1.066e-11	9.456e-12	-10.972	-11.024	-0.052	(0)
ZnCl2	3.565e-14	3.576e-14	-13.448	-13.447	0.001	98.71
ZnBr+	2.410e-14	2.139e-14	-13.618	-13.670	-0.052	(0)
Zn(SO4)2-2	2.067e-14	1.282e-14	-13.685	-13.892	-0.208	-11.29
Zn(OH)4-2	6.069e-16	3.763e-16	-15.217	-15.424	-0.208	(0)
ZnCl3-	4.034e-17	3.576e-17	-16.394	-16.447	-0.052	17.12
ZnBr2	4.600e-20	4.614e-20	-19.337	-19.336	0.001	(0)
ZnCl4-2	2.554e-20	1.603e-20	-19.593	-19.795	-0.202	145.76

----------Distribution of alkalinity----------

Total alkalinity (eq/kgw) = 1.218e-02

Species	Alkalinity	Molality	Alk/Mol
HCO3-	1.139e-02	1.139e-02	1.00
CO3-2	3.922e-04	1.961e-04	2.00
CaCO3	1.099e-04	5.496e-05	2.00
MgCO3	7.268e-05	3.634e-05	2.00
NaCO3-	5.185e-05	2.593e-05	2.00
NaHCO3	5.155e-05	5.155e-05	1.00
MgHCO3+	4.060e-05	4.060e-05	1.00
CaHCO3+	3.806e-05	3.806e-05	1.00
Al(OH)4-	9.171e-06	2.293e-06	4.00
H2BO3-	8.085e-06	8.085e-06	1.00
Zn(CO3)2-2	6.329e-06	1.582e-06	4.00
OH-	3.276e-06	3.276e-06	1.00
BaCO3	1.055e-06	5.273e-07	2.00
BaHCO3+	9.256e-07	9.256e-07	1.00
ZnCO3	7.390e-07	3.695e-07	2.00

FeCO3	4.206e-07	2.103e-07	2.00
MgOH+	3.578e-07	3.578e-07	1.00
HPO4-2	2.666e-07	2.666e-07	1.00
MnCO3	1.609e-07	8.046e-08	2.00
Fe(OH)3	1.048e-07	1.048e-07	1.00
FeHCO3+	8.129e-08	8.129e-08	1.00
Fe(OH)4-	5.788e-08	2.894e-08	2.00
MgPO4-	5.289e-08	2.645e-08	2.00
Cu(OH)2	4.187e-08	2.093e-08	2.00
MgHPO4	3.836e-08	3.836e-08	1.00
CaPO4-	3.338e-08	1.669e-08	2.00
CaHPO4	2.415e-08	2.415e-08	1.00
Zn(OH)2	2.374e-08	1.187e-08	2.00
ZnHCO3+	2.162e-08	2.162e-08	1.00
CuCO3	2.113e-08	1.057e-08	2.00
Al(OH)3	1.256e-08	4.186e-09	3.00
CaOH+	1.201e-08	1.201e-08	1.00
Cu(CO3)2-2	1.066e-08	2.664e-09	4.00
MnHCO3+	8.347e-09	8.347e-09	1.00
FeOH+	7.212e-09	7.212e-09	1.00
Pb(CO3)2-2	6.949e-09	1.737e-09	4.00
PbCO3	6.906e-09	3.453e-09	2.00
ZnOH+	5.309e-09	5.309e-09	1.00
H+	-4.413e-09	4.413e-09	-1.00
NaHPO4-	3.346e-09	3.346e-09	1.00
HF	-1.684e-09	1.684e-09	-1.00
CdHCO3+	1.174e-09	1.174e-09	1.00
Cd(CO3)2-2	8.058e-10	2.014e-10	4.00
CdCO3	6.361e-10	3.180e-10	2.00
Al(OH)2+	2.245e-10	1.122e-10	2.00
PO4-3	1.159e-10	5.795e-11	2.00
ZnOHCl	1.097e-10	1.097e-10	1.00
CuHCO3+	9.145e-11	9.145e-11	1.00
CdOH+	8.681e-11	8.681e-11	1.00
BaOH+	7.636e-11	7.636e-11	1.00
MnOH+	6.853e-11	6.853e-11	1.00
FeHPO4	4.715e-11	4.715e-11	1.00
CuOH+	4.516e-11	4.516e-11	1.00
Zn(OH)3-	3.197e-11	1.066e-11	3.00
Fe(OH)2	3.179e-11	1.589e-11	2.00
CdOHCl	2.948e-11	2.948e-11	1.00
KHPO4-	2.735e-11	2.735e-11	1.00
PbHCO3+	1.464e-11	1.464e-11	1.00
HSO4-	-9.595e-12	9.595e-12	-1.00
PbOH+	8.884e-12	8.884e-12	1.00
HF2-	-2.029e-12	2.029e-12	-1.00
Cd(OH)2	1.821e-12	9.107e-13	2.00
Pb(OH)2	1.535e-12	7.676e-13	2.00
Cu(OH)3-	1.074e-12	3.581e-13	3.00
BF2(OH)2-	-7.033e-13	7.033e-13	-1.00
Fe(OH)3-	5.099e-13	1.700e-13	3.00
AlOH+2	6.929e-14	6.929e-14	1.00
FeOH+2	-5.408e-14	5.408e-14	-1.00
CaHSO4+	-2.951e-14	2.951e-14	-1.00
Pb(OH)3-	7.505e-15	2.502e-15	3.00
H3PO4	-6.335e-15	6.335e-15	-1.00
Cu2(OH)2+2	2.686e-15	1.343e-15	2.00
Zn(OH)4-2	2.428e-15	6.069e-16	4.00
FeF2+	-2.113e-16	1.056e-16	-2.00
Cu(OH)4-2	1.027e-16	2.567e-17	4.00
Cd(OH)3-	8.702e-17	2.901e-17	3.00
FeF3	-8.193e-17	4.097e-17	-2.00
FeF+2	-2.689e-17	1.345e-17	-2.00
Pb(OH)4-2	8.237e-18	2.059e-18	4.00
FeHSO4+	-8.195e-18	8.195e-18	-1.00
Mn(OH)3-	6.941e-18	2.314e-18	3.00
Cd2OH+3	3.512e-18	3.512e-18	1.00
NaOH	2.642e-18	2.642e-18	1.00

BF3OH-	-1.632e-18	8.160e-19	-2.00
Fe+3	-9.563e-20	4.782e-20	-2.00
FeSO4+	-1.025e-20	5.125e-21	-2.00
FeCl+2	-1.696e-21	8.479e-22	-2.00
FeHPO4+	-1.012e-21	1.012e-21	-1.00
Pb2OH+3	8.330e-22	8.330e-22	1.00
Cd(OH)4-2	3.716e-22	9.289e-23	4.00
FeH2PO4+2	-1.713e-22	8.563e-23	-2.00
BF4-	-1.087e-23	3.622e-24	-3.00
Fe(SO4)2-	-4.794e-24	2.397e-24	-2.00
FeCl2+	-4.459e-24	2.230e-24	-2.00
Fe2(OH)2+4	-3.905e-25	1.953e-25	-2.00
Pb3(OH)4+2	1.829e-25	4.573e-26	4.00
AlHSO4+2	-6.205e-28	6.205e-28	-1.00
FeCl3	-3.490e-28	1.745e-28	-2.00
FeHSO4+2	-2.352e-28	7.842e-29	-3.00
Fe3(OH)4+5	-6.143e-31	3.072e-31	-2.00

----------Saturation indices----------

Phase	SI**	log IAP	log K(299 K, 1 atm)	
Al(OH)3(a)	-2.29	8.39	10.69	Al(OH)3
Alunite	-11.88	-13.49	-1.61	KAl3(SO4)2(OH)6
Anglesite	-8.69	-16.47	-7.78	PbSO4
Anhydrite	-3.97	-8.27	-4.30	CaSO4
Aragonite	0.85	-7.50	-8.35	CaCO3
BaCl2	-13.42	-11.21	2.21	BaCl2
BaCl2:2H2O	-11.43	-11.21	0.22	BaCl2:2H2O
BaCl2:H2O	-12.03	-11.21	0.83	BaCl2:H2O
Barite	0.06	-9.77	-9.83	BaSO4
Calcite	0.99	-7.50	-8.49	CaCO3
Cd(OH)2	-5.34	8.31	13.65	Cd(OH)2
CdSO4	-13.00	-13.16	-0.16	CdSO4
Cerussite	-2.59	-15.70	-13.11	PbCO3
CO2(g)	-2.56	-4.05	-1.49	CO2
Dolomite	2.20	-14.93	-17.13	CaMg(CO3)2
Fe(OH)3(a)	0.59	5.48	4.89	Fe(OH)3
Fluorite	-0.14	-10.72	-10.58	CaF2
Gibbsite	0.38	8.39	8.01	Al(OH)3
Goethite	6.54	5.48	-1.06	FeOOH
Gypsum	-3.68	-8.27	-4.58	CaSO4:2H2O
H2(g)	-17.66	-20.77	-3.11	H2
H2O(g)	-1.46	-0.00	1.46	H2O
Halite	-6.66	-5.09	1.57	NaCl
Hausmannite	-16.85	43.75	60.60	Mn3O4
Hematite	15.09	10.95	-4.14	Fe2O3
Hydroxyapatite	-1.12	-4.69	-3.57	Ca5(PO4)3OH
Jarosite-K	-12.90	-22.25	-9.34	KFe3(SO4)2(OH)6
Manganite	-7.82	17.52	25.34	MnOOH
Melanterite	-9.64	-11.82	-2.19	FeSO4:7H2O
O2(g)	-47.39	-50.29	-2.90	O2
Otavite	-0.30	-12.40	-12.10	CdCO3
Pb(OH)2	-3.08	5.01	8.09	Pb(OH)2
Pyrochroite	-6.49	8.71	15.20	Mn(OH)2
Pyrolusite	-14.78	26.32	41.10	MnO2:H2O
Rhodochrosite	-0.86	-11.99	-11.14	MnCO3
Siderite	-0.16	-11.06	-10.90	FeCO3
Smithsonite	-1.71	-11.73	-10.02	ZnCO3
Sylvite	-8.09	-7.18	0.91	KCl
Vivianite	-6.86	-42.86	-36.00	Fe3(PO4)2:8H2O
Witherite	-0.45	-9.00	-8.56	BaCO3
Zn(OH)2(e)	-2.52	8.98	11.50	Zn(OH)2

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
For ideal gases, phi = 1.

Initial solution 25.

----------Solution composition----------

Elements	Molality	Moles
Al	1.810e-06	1.810e-06
Alkalinity	4.047e-03	4.047e-03
B	1.243e-05	1.243e-05
Ba	7.139e-06	7.139e-06
Br	6.761e-06	6.761e-06
Ca	1.350e-03	1.350e-03
Cd	6.853e-09	6.853e-09
Cl	1.704e-03	1.704e-03
Cu	2.173e-08	2.173e-08
F	5.529e-05	5.529e-05
Fe	8.822e-07	8.822e-07
K	1.382e-04	1.382e-04
Mg	5.860e-04	5.860e-04
Mn	1.173e-06	1.173e-06
N(5)	4.193e-04	4.193e-04
Na	2.211e-03	2.211e-03
P	3.294e-06	3.294e-06
Pb	2.511e-09	2.511e-09
S(6)	1.791e-04	1.791e-04
Zn	1.654e-06	1.654e-06

----------Description of solution----------

pH	= 7.500
pe	= 0.441
Specific Conductance (µS/cm, 25°C)	= 627
Density (g/cm³)	= 0.99743
Volume (L)	= 1.00306
Activity of water	= 1.000
Ionic strength (mol/kgw)	= 8.258e-03
Mass of water (kg)	= 1.000e+00
Total carbon (mol/kg)	= 4.273e-03
Total CO2 (mol/kg)	= 4.273e-03
Temperature (°C)	= 24.93
Electrical balance (eq)	= -3.459e-04
Percent error, 100*(Cat-|An|)/(Cat+|An|)	= -2.77
Iterations	= 10 (265 overall)
Total H	= 1.110165e+02
Total O	= 5.552081e+01

----------Distribution of species----------

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma	mole V cm³/mol
OH-	3.506e-07	3.183e-07	-6.455	-6.497	-0.042	-4.05
H+	3.440e-08	3.162e-08	-7.463	-7.500	-0.037	0.00
H2O	5.551e+01	9.998e-01	1.744	-0.000	0.000	18.07
Al	1.810e-06					
Al(OH)4-	1.775e-06	1.615e-06	-5.751	-5.792	-0.041	(0)
Al(OH)3	2.708e-08	2.713e-08	-7.567	-7.567	0.001	(0)
Al(OH)2+	6.418e-09	5.854e-09	-8.193	-8.233	-0.040	(0)
AlF2+	9.981e-10	9.104e-10	-9.001	-9.041	-0.040	(0)
AlF3	5.594e-10	5.604e-10	-9.252	-9.251	0.001	(0)
AlF+2	5.367e-11	3.716e-11	-10.270	-10.430	-0.160	(0)
AlOH+2	3.433e-11	2.377e-11	-10.464	-10.624	-0.160	-27.58
AlF4-	1.199e-11	1.091e-11	-10.921	-10.962	-0.041	(0)
Al+3	1.621e-13	7.603e-14	-12.790	-13.119	-0.329	-41.92
AlSO4+	2.760e-14	2.512e-14	-13.559	-13.600	-0.041	(0)
Al(SO4)2-	9.125e-17	8.305e-17	-16.040	-16.081	-0.041	(0)
AlHSO4+2	1.029e-22	7.040e-23	-21.988	-22.152	-0.165	(0)
B	1.243e-05					
H3BO3	1.218e-05	1.221e-05	-4.914	-4.913	0.001	39.23

H2BO3-	2.440e-07	2.219e-07	-6.613	-6.654	-0.041	(0)
BF(OH)3-	2.611e-10	2.375e-10	-9.583	-9.624	-0.041	(0)
BF2(OH)2-	4.328e-14	3.936e-14	-13.364	-13.405	-0.041	(0)
BF3OH-	7.348e-20	6.683e-20	-19.134	-19.175	-0.041	(0)
BF4-	4.630e-25	4.211e-25	-24.334	-24.376	-0.041	(0)
Ba	7.139e-06					
Ba+2	6.689e-06	4.582e-06	-5.175	-5.339	-0.164	-12.56
BaSO4	2.397e-07	2.401e-07	-6.620	-6.620	0.001	(0)
BaHCO3+	1.728e-07	1.572e-07	-6.762	-6.804	-0.041	(0)
BaCl+	2.425e-08	2.205e-08	-7.615	-7.657	-0.041	(0)
BaCO3	1.253e-08	1.256e-08	-7.902	-7.901	0.001	-10.70
BaNO3+	2.411e-10	2.193e-10	-9.618	-9.659	-0.041	(0)
BaOH+	5.386e-12	4.908e-12	-11.269	-11.309	-0.040	(0)
Br	6.761e-06					
Br-	6.761e-06	6.130e-06	-5.170	-5.213	-0.043	24.61
CdBr+	3.818e-12	3.472e-12	-11.418	-11.459	-0.041	(0)
ZnBr+	8.990e-13	8.176e-13	-12.046	-12.087	-0.041	(0)
PbBr+	1.002e-14	9.112e-15	-13.999	-14.040	-0.041	(0)
CdBr2	1.141e-16	1.143e-16	-15.943	-15.942	0.001	(0)
ZnBr2	1.992e-18	1.995e-18	-17.701	-17.700	0.001	(0)
PbBr2	2.611e-20	2.616e-20	-19.583	-19.582	0.001	(0)
C(4)	4.273e-03					
HCO3-	3.932e-03	3.587e-03	-2.405	-2.445	-0.040	24.75
CO2	2.548e-04	2.553e-04	-3.594	-3.593	0.001	34.43
CaHCO3+	4.436e-05	4.052e-05	-4.353	-4.392	-0.039	9.71
MgHCO3+	1.782e-05	1.620e-05	-4.749	-4.790	-0.041	5.52
CaCO3	7.884e-06	7.899e-06	-5.103	-5.102	0.001	-14.60
CO3-2	7.672e-06	5.312e-06	-5.115	-5.275	-0.160	-5.05
NaHCO3	4.011e-06	4.019e-06	-5.397	-5.396	0.001	1.80
MgCO3	1.951e-06	1.955e-06	-5.710	-5.709	0.001	-17.09
ZnCO3	5.364e-07	5.374e-07	-6.271	-6.270	0.001	(0)
ZnHCO3+	2.518e-07	2.290e-07	-6.599	-6.640	-0.041	(0)
MnCO3	2.210e-07	2.214e-07	-6.656	-6.655	0.001	(0)
NaCO3-	2.158e-07	1.963e-07	-6.666	-6.707	-0.041	-0.95
MnHCO3+	1.841e-07	1.677e-07	-6.735	-6.775	-0.040	(0)
FeHCO3+	1.742e-07	1.584e-07	-6.759	-6.800	-0.041	(0)
BaHCO3+	1.728e-07	1.572e-07	-6.762	-6.804	-0.041	(0)
Zn(CO3)2-2	8.922e-08	6.104e-08	-7.050	-7.214	-0.165	(0)
FeCO3	5.616e-08	5.627e-08	-7.251	-7.250	0.001	(0)
BaCO3	1.253e-08	1.256e-08	-7.902	-7.901	0.001	-10.70
PbCO3	2.328e-09	2.333e-09	-8.633	-8.632	0.001	(0)
CuCO3	1.477e-09	1.480e-09	-8.831	-8.830	0.001	(0)
(CO2)2	1.191e-09	1.194e-09	-8.924	-8.923	0.001	68.86
CdHCO3+	4.775e-10	4.342e-10	-9.321	-9.362	-0.041	(0)
CuHCO3+	1.025e-10	9.326e-11	-9.989	-10.030	-0.041	(0)
PbHCO3+	7.918e-11	7.201e-11	-10.101	-10.143	-0.041	(0)
Pb(CO3)2-2	4.550e-11	3.113e-11	-10.342	-10.507	-0.165	(0)
CdCO3	1.612e-11	1.615e-11	-10.793	-10.792	0.001	(0)
Cu(CO3)2-2	1.447e-11	9.897e-12	-10.840	-11.005	-0.165	(0)
Cd(CO3)2-2	3.966e-13	2.713e-13	-12.402	-12.566	-0.165	(0)
Ca	1.350e-03					
Ca+2	1.281e-03	8.864e-04	-2.892	-3.052	-0.160	-17.95
CaHCO3+	4.436e-05	4.052e-05	-4.353	-4.392	-0.039	9.71
CaSO4	1.644e-05	1.648e-05	-4.784	-4.783	0.001	7.50
CaCO3	7.884e-06	7.899e-06	-5.103	-5.102	0.001	-14.60
CaHPO4	5.566e-07	5.577e-07	-6.254	-6.254	0.001	(0)
CaPO4-	4.568e-08	4.167e-08	-7.340	-7.380	-0.040	(0)
CaH2PO4+	1.454e-08	1.326e-08	-7.838	-7.877	-0.040	(0)
CaOH+	5.114e-09	4.651e-09	-8.291	-8.332	-0.041	(0)
CaHSO4+	3.762e-12	3.421e-12	-11.425	-11.466	-0.041	(0)
Cd	6.853e-09					
Cd+2	5.596e-09	3.828e-09	-8.252	-8.417	-0.165	-18.57
CdCl+	6.157e-10	5.599e-10	-9.211	-9.252	-0.041	5.91
CdHCO3+	4.775e-10	4.342e-10	-9.321	-9.362	-0.041	(0)
CdSO4	1.152e-10	1.154e-10	-9.939	-9.938	0.001	78.08
CdCO3	1.612e-11	1.615e-11	-10.793	-10.792	0.001	(0)
CdOH+	1.101e-11	1.002e-11	-10.958	-10.999	-0.041	(0)
CdOHCl	7.287e-12	7.301e-12	-11.137	-11.137	0.001	(0)

CdNO3+	4.028e-12	3.663e-12	-11.395	-11.436	-0.041	17.58
CdBr+	3.818e-12	3.472e-12	-11.418	-11.459	-0.041	(0)
CdCl2	3.568e-12	3.575e-12	-11.448	-11.447	0.001	23.14
CdF+	2.591e-12	2.357e-12	-11.586	-11.628	-0.041	(0)
Cd(CO3)2-2	3.966e-13	2.713e-13	-12.402	-12.566	-0.165	(0)
Cd(SO4)2-2	1.935e-13	1.324e-13	-12.713	-12.878	-0.165	-105.52
Cd(OH)2	1.706e-14	1.709e-14	-13.768	-13.767	0.001	(0)
CdCl3-	3.795e-15	3.451e-15	-14.421	-14.462	-0.041	69.42
CdF2	2.889e-16	2.895e-16	-15.539	-15.538	0.001	(0)
CdBr2	1.141e-16	1.143e-16	-15.943	-15.942	0.001	(0)
Cd2OH+3	4.416e-19	1.880e-19	-18.355	-18.726	-0.371	(0)
Cd(OH)3-	6.668e-20	6.064e-20	-19.176	-19.217	-0.041	(0)
Cd(OH)4-2	2.498e-26	1.709e-26	-25.602	-25.767	-0.165	(0)
Cl	1.704e-03					
Cl-	1.686e-03	1.532e-03	-2.773	-2.815	-0.042	18.13
NaCl	1.821e-05	1.825e-05	-4.740	-4.739	0.001	(0)
BaCl+	2.425e-08	2.205e-08	-7.615	-7.657	-0.041	(0)
CuCl2-	8.046e-09	7.314e-09	-8.094	-8.136	-0.041	(0)
MnCl+	3.593e-09	3.274e-09	-8.445	-8.485	-0.040	-3.06
ZnCl+	2.293e-09	2.084e-09	-8.640	-8.681	-0.041	-13.95
FeCl+	1.027e-09	9.337e-10	-8.989	-9.030	-0.041	(0)
ZnOHCl	8.117e-10	8.132e-10	-9.091	-9.090	0.001	(0)
CdCl+	6.157e-10	5.599e-10	-9.211	-9.252	-0.041	5.91
CuCl3-2	2.574e-11	1.775e-11	-10.589	-10.751	-0.161	(0)
CdOHCl	7.287e-12	7.301e-12	-11.137	-11.137	0.001	(0)
CdCl2	3.568e-12	3.575e-12	-11.448	-11.447	0.001	23.14
ZnCl2	3.336e-12	3.342e-12	-11.477	-11.476	0.001	102.16
MnCl2	2.185e-12	2.189e-12	-11.661	-11.660	0.001	85.97
PbCl+	1.692e-12	1.539e-12	-11.772	-11.813	-0.041	7.99
CuCl+	2.345e-13	2.132e-13	-12.630	-12.671	-0.041	0.71
ZnCl3-	6.316e-15	5.742e-15	-14.200	-14.241	-0.041	16.97
CdCl3-	3.795e-15	3.451e-15	-14.421	-14.462	-0.041	69.42
PbCl2	3.733e-15	3.740e-15	-14.428	-14.427	0.001	34.97
MnCl3-	1.014e-15	9.237e-16	-14.994	-15.034	-0.040	43.42
CuCl2	1.749e-16	1.752e-16	-15.757	-15.756	0.001	30.93
ZnCl4-2	6.388e-18	4.406e-18	-17.195	-17.356	-0.161	145.40
PbCl3-	5.002e-18	4.549e-18	-17.301	-17.342	-0.041	66.00
FeCl+2	7.760e-21	5.353e-21	-20.110	-20.271	-0.161	(0)
PbCl4-2	4.873e-21	3.333e-21	-20.312	-20.477	-0.165	101.56
CuCl3-	1.046e-21	9.512e-22	-20.980	-21.022	-0.041	(0)
FeCl2+	4.028e-23	3.671e-23	-22.395	-22.435	-0.040	(0)
CuCl4-2	1.057e-26	7.291e-27	-25.976	-26.137	-0.161	(0)
FeCl3	5.612e-27	5.623e-27	-26.251	-26.250	0.001	(0)
Cu(1)	1.896e-08					
Cu+	1.088e-08	9.856e-09	-7.963	-8.006	-0.043	(0)
CuCl2-	8.046e-09	7.314e-09	-8.094	-8.136	-0.041	(0)
CuCl3-2	2.574e-11	1.775e-11	-10.589	-10.751	-0.161	(0)
Cu(2)	2.769e-09					
CuCO3	1.477e-09	1.480e-09	-8.831	-8.830	0.001	(0)
Cu(OH)2	1.081e-09	1.083e-09	-8.966	-8.965	0.001	(0)
CuHCO3+	1.025e-10	9.326e-11	-9.989	-10.030	-0.041	(0)
Cu+2	7.450e-11	5.188e-11	-10.128	-10.285	-0.157	-26.43
CuOH+	1.804e-11	1.640e-11	-10.744	-10.785	-0.041	(0)
Cu(CO3)2-2	1.447e-11	9.897e-12	-10.840	-11.005	-0.165	(0)
CuSO4	1.105e-12	1.107e-12	-11.957	-11.956	0.001	13.08
CuCl+	2.345e-13	2.132e-13	-12.630	-12.671	-0.041	0.71
CuF+	5.072e-14	4.613e-14	-13.295	-13.336	-0.041	(0)
Cu(OH)3-	2.270e-15	2.064e-15	-14.644	-14.685	-0.041	(0)
CuCl2	1.749e-16	1.752e-16	-15.757	-15.756	0.001	30.93
Cu2(OH)2+2	1.709e-16	1.169e-16	-15.767	-15.932	-0.165	(0)
Cu(OH)4-2	1.903e-20	1.302e-20	-19.720	-19.885	-0.165	(0)
CuCl3-	1.046e-21	9.512e-22	-20.980	-21.022	-0.041	(0)
CuCl4-2	1.057e-26	7.291e-27	-25.976	-26.137	-0.161	(0)
F	5.529e-05					
F-	5.386e-05	4.890e-05	-4.269	-4.311	-0.042	-1.26
MgF+	1.369e-06	1.246e-06	-5.864	-5.905	-0.041	-10.53
NaF	5.593e-08	5.604e-08	-7.252	-7.251	0.001	7.26
HF	2.312e-09	2.316e-09	-8.636	-8.635	0.001	12.50

AlF2+	9.981e-10	9.104e-10	-9.001	-9.041	-0.040	(0)
AlF3	5.594e-10	5.604e-10	-9.252	-9.251	0.001	(0)
ZnF+	3.848e-10	3.499e-10	-9.415	-9.456	-0.041	(0)
BF(OH)3-	2.611e-10	2.375e-10	-9.583	-9.624	-0.041	(0)
FeF+	2.374e-10	2.159e-10	-9.624	-9.666	-0.041	(0)
MnF+	1.948e-10	1.775e-10	-9.710	-9.751	-0.040	(0)
AlF+2	5.367e-11	3.716e-11	-10.270	-10.430	-0.160	(0)
AlF4-	1.199e-11	1.091e-11	-10.921	-10.962	-0.041	(0)
CdF+	2.591e-12	2.357e-12	-11.586	-11.628	-0.041	(0)
HF2-	4.776e-13	4.343e-13	-12.321	-12.362	-0.041	22.11
CuF+	5.072e-14	4.613e-14	-13.295	-13.336	-0.041	(0)
BF2(OH)2-	4.328e-14	3.936e-14	-13.364	-13.405	-0.041	(0)
PbF+	2.416e-14	2.198e-14	-13.617	-13.658	-0.041	(0)
CdF2	2.889e-16	2.895e-16	-15.539	-15.538	0.001	(0)
PbF2	2.190e-17	2.194e-17	-16.660	-16.659	0.001	(0)
FeF2+	1.916e-17	1.746e-17	-16.718	-16.758	-0.040	(0)
FeF+2	1.302e-17	8.978e-18	-16.886	-17.047	-0.161	(0)
FeF3	1.350e-18	1.353e-18	-17.870	-17.869	0.001	(0)
BF3OH-	7.348e-20	6.683e-20	-19.134	-19.175	-0.041	(0)
PbF3-	8.546e-21	7.772e-21	-20.068	-20.109	-0.041	(0)
BF4-	4.630e-25	4.211e-25	-24.334	-24.376	-0.041	(0)
PbF4-2	2.659e-25	1.819e-25	-24.575	-24.740	-0.165	(0)
Fe(2)	8.809e-07					
Fe+2	6.342e-07	4.416e-07	-6.198	-6.355	-0.157	-21.96
FeHCO3+	1.742e-07	1.584e-07	-6.759	-6.800	-0.041	(0)
FeCO3	5.616e-08	5.627e-08	-7.251	-7.250	0.001	(0)
FeSO4	8.186e-09	8.202e-09	-8.087	-8.086	0.001	19.04
FeOH+	4.819e-09	4.392e-09	-8.317	-8.357	-0.040	(0)
FeHPO4	2.016e-09	2.020e-09	-8.696	-8.695	0.001	(0)
FeCl+	1.027e-09	9.337e-10	-8.989	-9.030	-0.041	(0)
FeF+	2.374e-10	2.159e-10	-9.624	-9.666	-0.041	(0)
FeH2PO4+	1.420e-10	1.296e-10	-9.848	-9.888	-0.040	(0)
Fe(OH)2	1.172e-12	1.175e-12	-11.931	-11.930	0.001	(0)
FeHSO4+	1.874e-15	1.704e-15	-14.727	-14.768	-0.041	(0)
Fe(OH)3-	1.513e-15	1.379e-15	-14.820	-14.860	-0.040	(0)
Fe(3)	1.299e-09					
Fe(OH)3	9.977e-10	9.996e-10	-9.001	-9.000	0.001	(0)
Fe(OH)2+	2.699e-10	2.462e-10	-9.569	-9.609	-0.040	(0)
Fe(OH)4-	3.151e-11	2.874e-11	-10.502	-10.541	-0.040	(0)
FeOH+2	3.418e-14	2.358e-14	-13.466	-13.628	-0.161	(0)
FeF2+	1.916e-17	1.746e-17	-16.718	-16.758	-0.040	(0)
FeF+2	1.302e-17	8.978e-18	-16.886	-17.047	-0.161	(0)
FeF3	1.350e-18	1.353e-18	-17.870	-17.869	0.001	(0)
Fe+3	2.472e-19	1.160e-19	-18.607	-18.936	-0.329	(0)
FeSO4+	1.457e-19	1.328e-19	-18.837	-18.877	-0.040	(0)
FeHPO4+	3.926e-20	3.578e-20	-19.406	-19.446	-0.040	(0)
FeH2PO4+2	2.639e-20	1.827e-20	-19.579	-19.738	-0.160	(0)
FeCl+2	7.760e-21	5.353e-21	-20.110	-20.271	-0.161	(0)
Fe(SO4)2-	3.339e-22	3.037e-22	-21.476	-21.518	-0.041	(0)
FeCl2+	4.028e-23	3.671e-23	-22.395	-22.435	-0.040	(0)
Fe2(OH)2+4	6.850e-26	1.500e-26	-25.164	-25.824	-0.659	(0)
FeHSO4+2	1.644e-26	1.124e-26	-25.784	-25.949	-0.165	(0)
FeCl3	5.612e-27	5.623e-27	-26.251	-26.250	0.001	(0)
Fe3(OH)4+5	8.331e-33	7.767e-34	-32.079	-33.110	-1.030	(0)
H(0)	1.856e-19					
H2	9.278e-20	9.296e-20	-19.033	-19.032	0.001	28.61
K	1.382e-04					
K+	1.381e-04	1.254e-04	-3.860	-3.902	-0.042	9.06
KSO4-	1.009e-07	9.202e-08	-6.996	-7.036	-0.040	34.16
KHPO4-	3.079e-10	2.809e-10	-9.512	-9.551	-0.040	38.18
Mg	5.860e-04					
Mg+2	5.550e-04	3.861e-04	-3.256	-3.413	-0.158	-21.64
MgHCO3+	1.782e-05	1.620e-05	-4.749	-4.790	-0.041	5.52
MgSO4	9.431e-06	9.449e-06	-5.025	-5.025	0.001	5.83
MgCO3	1.951e-06	1.955e-06	-5.710	-5.709	0.001	-17.09
MgF+	1.369e-06	1.246e-06	-5.864	-5.905	-0.041	-10.53
MgHPO4	3.278e-07	3.284e-07	-6.484	-6.484	0.001	(0)
MgOH+	4.816e-08	4.404e-08	-7.317	-7.356	-0.039	(0)

MgPO4-	2.684e-08	2.448e-08	-7.571	-7.611	-0.040	(0)
MgH2PO4+	8.063e-09	7.355e-09	-8.093	-8.133	-0.040	(0)
Mn(2)	1.173e-06					
Mn+2	7.535e-07	5.247e-07	-6.123	-6.280	-0.157	-19.97
MnCO3	2.210e-07	2.214e-07	-6.656	-6.655	0.001	(0)
MnHCO3+	1.841e-07	1.677e-07	-6.735	-6.775	-0.040	(0)
MnSO4	9.726e-09	9.744e-09	-8.012	-8.011	0.001	22.57
MnCl+	3.593e-09	3.274e-09	-8.445	-8.485	-0.040	-3.06
MnOH+	4.652e-10	4.240e-10	-9.332	-9.373	-0.040	(0)
MnF+	1.948e-10	1.775e-10	-9.710	-9.751	-0.040	(0)
MnCl2	2.185e-12	2.189e-12	-11.661	-11.660	0.001	85.97
Mn(NO3)2	3.013e-13	3.019e-13	-12.521	-12.520	0.001	41.06
MnCl3-	1.014e-15	9.237e-16	-14.994	-15.034	-0.040	43.42
Mn(OH)3-	2.884e-19	2.628e-19	-18.540	-18.580	-0.040	(0)
Mn(3)	9.445e-32					
Mn+3	9.445e-32	4.430e-32	-31.025	-31.354	-0.329	(0)
N(5)	4.193e-04					
NO3-	4.193e-04	3.801e-04	-3.378	-3.420	-0.043	29.54
BaNO3+	2.411e-10	2.193e-10	-9.618	-9.659	-0.041	(0)
CdNO3+	4.028e-12	3.663e-12	-11.395	-11.436	-0.041	17.58
Mn(NO3)2	3.013e-13	3.019e-13	-12.521	-12.520	0.001	41.06
PbNO3+	1.562e-13	1.421e-13	-12.806	-12.847	-0.041	(0)
Na	2.211e-03					
Na+	2.187e-03	1.992e-03	-2.660	-2.701	-0.041	-1.40
NaCl	1.821e-05	1.825e-05	-4.740	-4.739	0.001	(0)
NaHCO3	4.011e-06	4.019e-06	-5.397	-5.396	0.001	1.80
NaSO4-	1.144e-06	1.043e-06	-5.942	-5.982	-0.040	14.25
NaCO3-	2.158e-07	1.963e-07	-6.666	-6.707	-0.041	-0.95
NaF	5.593e-08	5.604e-08	-7.252	-7.251	0.001	7.26
NaHPO4-	4.891e-09	4.462e-09	-8.311	-8.350	-0.040	34.06
NaOH	6.327e-20	6.339e-20	-19.199	-19.198	0.001	(0)
O(0)	0.000e+00					
O2	0.000e+00	0.000e+00	-54.340	-54.339	0.001	30.40
P	3.294e-06					
HPO4-2	1.666e-06	1.149e-06	-5.778	-5.940	-0.161	6.94
H2PO4-	6.418e-07	5.854e-07	-6.193	-6.233	-0.040	33.27
CaHPO4	5.566e-07	5.577e-07	-6.254	-6.254	0.001	(0)
MgHPO4	3.278e-07	3.284e-07	-6.484	-6.484	0.001	(0)
CaPO4-	4.568e-08	4.167e-08	-7.340	-7.380	-0.040	(0)
MgPO4-	2.684e-08	2.448e-08	-7.571	-7.611	-0.040	(0)
CaH2PO4+	1.454e-08	1.326e-08	-7.838	-7.877	-0.040	(0)
MgH2PO4+	8.063e-09	7.355e-09	-8.093	-8.133	-0.040	(0)
NaHPO4-	4.891e-09	4.462e-09	-8.311	-8.350	-0.040	34.06
FeHPO4	2.016e-09	2.020e-09	-8.696	-8.695	0.001	(0)
KHPO4-	3.079e-10	2.809e-10	-9.512	-9.551	-0.040	38.18
FeH2PO4+	1.420e-10	1.296e-10	-9.848	-9.888	-0.040	(0)
PO4-3	3.857e-11	1.636e-11	-10.414	-10.786	-0.373	-22.74
H3PO4	2.718e-12	2.723e-12	-11.566	-11.565	0.001	47.40
FeHPO4+	3.926e-20	3.578e-20	-19.406	-19.446	-0.040	(0)
FeH2PO4+2	2.639e-20	1.827e-20	-19.579	-19.738	-0.160	(0)
Pb	2.511e-09					
PbCO3	2.328e-09	2.333e-09	-8.633	-8.632	0.001	(0)
PbHCO3+	7.918e-11	7.201e-11	-10.101	-10.143	-0.041	(0)
Pb(CO3)2-2	4.550e-11	3.113e-11	-10.342	-10.507	-0.165	(0)
Pb+2	3.694e-11	2.527e-11	-10.432	-10.597	-0.165	-15.35
PbOH+	1.713e-11	1.558e-11	-10.766	-10.807	-0.041	(0)
PbCl+	1.692e-12	1.539e-12	-11.772	-11.813	-0.041	7.99
PbSO4	1.483e-12	1.486e-12	-11.829	-11.828	0.001	(0)
Pb(OH)2	1.913e-13	1.916e-13	-12.718	-12.718	0.001	(0)
PbNO3+	1.562e-13	1.421e-13	-12.806	-12.847	-0.041	(0)
PbF+	2.416e-14	2.198e-14	-13.617	-13.658	-0.041	(0)
PbBr+	1.002e-14	9.112e-15	-13.999	-14.040	-0.041	(0)
PbCl2	3.733e-15	3.740e-15	-14.428	-14.427	0.001	34.97
Pb(SO4)2-2	1.192e-15	8.157e-16	-14.924	-15.088	-0.165	(0)
Pb(OH)3-	7.649e-17	6.957e-17	-16.116	-16.158	-0.041	(0)
PbF2	2.190e-17	2.194e-17	-16.660	-16.659	0.001	(0)
PbCl3-	5.002e-18	4.549e-18	-17.301	-17.342	-0.041	66.00
PbBr2	2.611e-20	2.616e-20	-19.583	-19.582	0.001	(0)

Pb2OH+3	2.071e-20	8.815e-21	-19.684	-20.055	-0.371	(0)
PbF3-	8.546e-21	7.772e-21	-20.068	-20.109	-0.041	(0)
Pb(OH)4-2	7.365e-21	5.039e-21	-20.133	-20.298	-0.165	(0)
PbCl4-2	4.873e-21	3.333e-21	-20.312	-20.477	-0.165	101.56
PbF4-2	2.659e-25	1.819e-25	-24.575	-24.740	-0.165	(0)
Pb3(OH)4+2	3.076e-26	2.104e-26	-25.512	-25.677	-0.165	(0)
S(6)	1.791e-04					
SO4-2	1.517e-04	1.046e-04	-3.819	-3.981	-0.162	14.73
CaSO4	1.644e-05	1.648e-05	-4.784	-4.783	0.001	7.50
MgSO4	9.431e-06	9.449e-06	-5.025	-5.025	0.001	5.83
NaSO4-	1.144e-06	1.043e-06	-5.942	-5.982	-0.040	14.25
BaSO4	2.397e-07	2.401e-07	-6.620	-6.620	0.001	(0)
KSO4-	1.009e-07	9.202e-08	-6.996	-7.036	-0.040	34.16
ZnSO4	1.240e-08	1.242e-08	-7.907	-7.906	0.001	21.73
MnSO4	9.726e-09	9.744e-09	-8.012	-8.011	0.001	22.57
FeSO4	8.186e-09	8.202e-09	-8.087	-8.086	0.001	19.04
HSO4-	3.530e-10	3.210e-10	-9.452	-9.493	-0.041	40.33
CdSO4	1.152e-10	1.154e-10	-9.939	-9.938	0.001	78.08
Zn(SO4)2-2	1.545e-11	1.057e-11	-10.811	-10.976	-0.165	-12.92
CaHSO4+	3.762e-12	3.421e-12	-11.425	-11.466	-0.041	(0)
PbSO4	1.483e-12	1.486e-12	-11.829	-11.828	0.001	(0)
CuSO4	1.105e-12	1.107e-12	-11.957	-11.956	0.001	13.08
Cd(SO4)2-2	1.935e-13	1.324e-13	-12.713	-12.878	-0.165	-105.52
AlSO4+	2.760e-14	2.512e-14	-13.559	-13.600	-0.041	(0)
FeHSO4+	1.874e-15	1.704e-15	-14.727	-14.768	-0.041	(0)
Pb(SO4)2-2	1.192e-15	8.157e-16	-14.924	-15.088	-0.165	(0)
Al(SO4)2-	9.125e-17	8.305e-17	-16.040	-16.081	-0.041	(0)
FeSO4+	1.457e-19	1.328e-19	-18.837	-18.877	-0.040	(0)
Fe(SO4)2-	3.339e-22	3.037e-22	-21.476	-21.518	-0.041	(0)
AlHSO4+2	1.029e-22	7.040e-23	-21.988	-22.152	-0.165	(0)
FeHSO4+2	1.644e-26	1.124e-26	-25.784	-25.949	-0.165	(0)
Zn	1.654e-06					
Zn+2	7.351e-07	5.071e-07	-6.134	-6.295	-0.161	-25.17
ZnCO3	5.364e-07	5.374e-07	-6.271	-6.270	0.001	(0)
ZnHCO3+	2.518e-07	2.290e-07	-6.599	-6.640	-0.041	(0)
Zn(CO3)2-2	8.922e-08	6.104e-08	-7.050	-7.214	-0.165	(0)
ZnOH+	1.923e-08	1.749e-08	-7.716	-7.757	-0.041	(0)
ZnSO4	1.240e-08	1.242e-08	-7.907	-7.906	0.001	21.73
Zn(OH)2	6.369e-09	6.381e-09	-8.196	-8.195	0.001	(0)
ZnCl+	2.293e-09	2.084e-09	-8.640	-8.681	-0.041	-13.95
ZnOHCl	8.117e-10	8.132e-10	-9.091	-9.090	0.001	(0)
ZnF+	3.848e-10	3.499e-10	-9.415	-9.456	-0.041	(0)
Zn(SO4)2-2	1.545e-11	1.057e-11	-10.811	-10.976	-0.165	-12.92
ZnCl2	3.336e-12	3.342e-12	-11.477	-11.476	0.001	102.16
ZnBr+	8.990e-13	8.176e-13	-12.046	-12.087	-0.041	(0)
Zn(OH)3-	7.015e-13	6.380e-13	-12.154	-12.195	-0.041	(0)
ZnCl3-	6.316e-15	5.742e-15	-14.200	-14.241	-0.041	16.97
ZnCl4-2	6.388e-18	4.406e-18	-17.195	-17.356	-0.161	145.40
Zn(OH)4-2	4.673e-18	3.197e-18	-17.330	-17.495	-0.165	(0)
ZnBr2	1.992e-18	1.995e-18	-17.701	-17.700	0.001	(0)

----------Distribution of alkalinity----------

Total alkalinity (eq/kgw) = 4.047e-03

Species	Alkalinity	Molality	Alk/Mol
HCO3-	3.932e-03	3.932e-03	1.00
CaHCO3+	4.436e-05	4.436e-05	1.00
MgHCO3+	1.782e-05	1.782e-05	1.00
CaCO3	1.577e-05	7.884e-06	2.00
CO3-2	1.534e-05	7.672e-06	2.00
Al(OH)4-	7.098e-06	1.775e-06	4.00
NaHCO3	4.011e-06	4.011e-06	1.00
MgCO3	3.903e-06	1.951e-06	2.00
HPO4-2	1.666e-06	1.666e-06	1.00
ZnCO3	1.073e-06	5.364e-07	2.00
CaHPO4	5.566e-07	5.566e-07	1.00

MnCO3	4.419e-07	2.210e-07	2.00
NaCO3-	4.317e-07	2.158e-07	2.00
Zn(CO3)2-2	3.569e-07	8.922e-08	4.00
OH-	3.506e-07	3.506e-07	1.00
MgHPO4	3.278e-07	3.278e-07	1.00
ZnHCO3+	2.518e-07	2.518e-07	1.00
H2BO3-	2.440e-07	2.440e-07	1.00
MnHCO3+	1.841e-07	1.841e-07	1.00
FeHCO3+	1.742e-07	1.742e-07	1.00
BaHCO3+	1.728e-07	1.728e-07	1.00
FeCO3	1.123e-07	5.616e-08	2.00
CaPO4-	9.136e-08	4.568e-08	2.00
Al(OH)3	8.124e-08	2.708e-08	3.00
MgPO4-	5.368e-08	2.684e-08	2.00
MgOH+	4.816e-08	4.816e-08	1.00
H+	-3.440e-08	3.440e-08	-1.00
BaCO3	2.506e-08	1.253e-08	2.00
ZnOH+	1.923e-08	1.923e-08	1.00
Al(OH)2+	1.284e-08	6.418e-09	2.00
Zn(OH)2	1.274e-08	6.369e-09	2.00
CaOH+	5.114e-09	5.114e-09	1.00
NaHPO4-	4.891e-09	4.891e-09	1.00
FeOH+	4.819e-09	4.819e-09	1.00
PbCO3	4.657e-09	2.328e-09	2.00
CuCO3	2.954e-09	1.477e-09	2.00
HF	-2.312e-09	2.312e-09	-1.00
Cu(OH)2	2.163e-09	1.081e-09	2.00
FeHPO4	2.016e-09	2.016e-09	1.00
Fe(OH)3	9.977e-10	9.977e-10	1.00
ZnOHCl	8.117e-10	8.117e-10	1.00
CdHCO3+	4.775e-10	4.775e-10	1.00
MnOH+	4.652e-10	4.652e-10	1.00
HSO4-	-3.530e-10	3.530e-10	-1.00
KHPO4-	3.079e-10	3.079e-10	1.00
Pb(CO3)2-2	1.820e-10	4.550e-11	4.00
CuHCO3+	1.025e-10	1.025e-10	1.00
PbHCO3+	7.918e-11	7.918e-11	1.00
PO4-3	7.715e-11	3.857e-11	2.00
Fe(OH)4-	6.302e-11	3.151e-11	2.00
Cu(CO3)2-2	5.787e-11	1.447e-11	4.00
AlOH+2	3.433e-11	3.433e-11	1.00
CdCO3	3.225e-11	1.612e-11	2.00
CuOH+	1.804e-11	1.804e-11	1.00
PbOH+	1.713e-11	1.713e-11	1.00
CdOH+	1.101e-11	1.101e-11	1.00
CdOHCl	7.287e-12	7.287e-12	1.00
BaOH+	5.386e-12	5.386e-12	1.00
CaHSO4+	-3.762e-12	3.762e-12	-1.00
H3PO4	-2.718e-12	2.718e-12	-1.00
Fe(OH)2	2.345e-12	1.172e-12	2.00
Zn(OH)3-	2.105e-12	7.015e-13	3.00
Cd(CO3)2-2	1.587e-12	3.966e-13	4.00
HF2-	-4.776e-13	4.776e-13	-1.00
Pb(OH)2	3.825e-13	1.913e-13	2.00
BF2(OH)2-	-4.328e-14	4.328e-14	-1.00
FeOH+2	-3.418e-14	3.418e-14	-1.00
Cd(OH)2	3.412e-14	1.706e-14	2.00
Cu(OH)3-	6.809e-15	2.270e-15	3.00
Fe(OH)3-	4.539e-15	1.513e-15	3.00
FeHSO4+	-1.874e-15	1.874e-15	-1.00
Cu2(OH)2+2	3.418e-16	1.709e-16	2.00
Pb(OH)3-	2.295e-16	7.649e-17	3.00
FeF2+	-3.832e-17	1.916e-17	-2.00
FeF+2	-2.603e-17	1.302e-17	-2.00
Zn(OH)4-2	1.869e-17	4.673e-18	4.00
FeF3	-2.701e-18	1.350e-18	-2.00
Mn(OH)3-	8.652e-19	2.884e-19	3.00
Fe+3	-4.945e-19	2.472e-19	-2.00

Cd2OH+3	4.416e-19	4.416e-19	1.00
FeSO4+	-2.914e-19	1.457e-19	-2.00
Cd(OH)3-	2.000e-19	6.668e-20	3.00
BF3OH-	-1.470e-19	7.348e-20	-2.00
Cu(OH)4-2	7.613e-20	1.903e-20	4.00
NaOH	6.327e-20	6.327e-20	1.00
FeH2PO4+2	-5.278e-20	2.639e-20	-2.00
FeHPO4+	-3.926e-20	3.926e-20	-1.00
Pb(OH)4-2	2.946e-20	7.365e-21	4.00
Pb2OH+3	2.071e-20	2.071e-20	1.00
FeCl+2	-1.552e-20	7.760e-21	-2.00
Fe(SO4)2-	-6.679e-22	3.339e-22	-2.00
AlHSO4+2	-1.029e-22	1.029e-22	-1.00
FeCl2+	-8.056e-23	4.028e-23	-2.00
BF4-	-1.389e-24	4.630e-25	-3.00
Fe2(OH)2+4	-1.370e-25	6.850e-26	-2.00
Pb3(OH)4+2	1.230e-25	3.076e-26	4.00
Cd(OH)4-2	9.991e-26	2.498e-26	4.00
FeHSO4+2	-4.931e-26	1.644e-26	-3.00
FeCl3	-1.122e-26	5.612e-27	-2.00
Fe3(OH)4+5	-1.666e-32	8.331e-33	-2.00

----------Saturation indices----------

Phase	SI**	log IAP	log K(298 K, 1 atm)	
Al(OH)3(a)	-1.42	9.38	10.80	Al(OH)3
Alunite	-4.83	-6.22	-1.39	KAl3(SO4)2(OH)6
Anglesite	-6.79	-14.58	-7.79	PbSO4
Anhydrite	-2.76	-7.03	-4.28	CaSO4
Aragonite	0.01	-8.33	-8.34	CaCO3
BaCl2	-13.20	-10.97	2.23	BaCl2
BaCl2:2H2O	-11.18	-10.97	0.21	BaCl2:2H2O
BaCl2:H2O	-11.79	-10.97	0.82	BaCl2:H2O
Barite	0.52	-9.32	-9.84	BaSO4
Calcite	0.15	-8.33	-8.48	CaCO3
Cd(OH)2	-7.07	6.58	13.65	Cd(OH)2
CdSO4	-12.30	-12.40	-0.10	CdSO4
Cerussite	-2.74	-15.87	-13.13	PbCO3
CO2(g)	-2.13	-3.59	-1.47	CO2
Dolomite	0.07	-17.02	-17.09	CaMg(CO3)2
Fe(OH)3(a)	-1.33	3.56	4.89	Fe(OH)3
Fluorite	-1.07	-11.67	-10.60	CaF2
Gibbsite	1.27	9.38	8.11	Al(OH)3
Goethite	4.56	3.56	-1.00	FeOOH
Gypsum	-2.45	-7.03	-4.58	CaSO4:2H2O
H2(g)	-15.93	-19.03	-3.10	H2
H2O(g)	-1.50	-0.00	1.50	H2O
Halite	-7.09	-5.52	1.57	NaCl
Hausmannite	-19.01	42.04	61.05	Mn3O4
Hematite	11.13	7.13	-4.00	Fe2O3
Hydroxyapatite	0.33	-3.08	-3.41	Ca5(PO4)3OH
Jarosite-K	-14.47	-23.67	-9.20	KFe3(SO4)2(OH)6
Manganite	-8.68	16.66	25.34	MnOOH
Melanterite	-8.13	-10.34	-2.21	FeSO4:7H2O
O2(g)	-51.45	-54.34	-2.89	O2
Otavite	-1.59	-13.69	-12.10	CdCO3
Pb(OH)2	-3.75	4.40	8.15	Pb(OH)2
Pyrochroite	-6.48	8.72	15.20	Mn(OH)2
Pyrolusite	-16.79	24.60	41.39	MnO2:H2O
Rhodochrosite	-0.43	-11.55	-11.13	MnCO3
Siderite	-0.74	-11.63	-10.89	FeCO3
Smithsonite	-1.57	-11.57	-10.00	ZnCO3
Sylvite	-7.62	-6.72	0.90	KCl
Vivianite	-4.64	-40.64	-36.00	Fe3(PO4)2:8H2O
Witherite	-2.05	-10.61	-8.56	BaCO3
Zn(OH)2(e)	-2.80	8.70	11.50	Zn(OH)2

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
  For ideal gases, phi = 1.

Initial solution 26.

-----------------------------Solution composition------------------------------

Elements	Molality	Moles
Al	9.881e-07	9.881e-07
Alkalinity	4.719e-03	4.719e-03
B	1.211e-05	1.211e-05
Br	6.260e-06	6.260e-06
Ca	1.068e-03	1.068e-03
Cd	6.319e-09	6.319e-09
Cl	9.368e-04	9.368e-04
Cu	2.661e-08	2.661e-08
F	1.053e-04	1.053e-04
Fe	3.100e-06	3.100e-06
K	7.931e-05	7.931e-05
Mg	1.127e-03	1.127e-03
Mn	2.108e-06	2.108e-06
N(3)	2.286e-05	2.286e-05
N(5)	4.171e-04	4.171e-04
Na	1.288e-03	1.288e-03
P	2.810e-06	2.810e-06
Pb	3.090e-09	3.090e-09
S(6)	7.186e-05	7.186e-05
Zn	1.857e-06	1.857e-06

----------------------------Description of solution----------------------------

pH	= 7.200
pe	= 0.343
Specific Conductance (µS/cm, 26°C)	= 573
Density (g/cm³)	= 0.99727
Volume (L)	= 1.00323
Activity of water	= 1.000
Ionic strength (mol/kgw)	= 8.083e-03
Mass of water (kg)	= 1.000e+00
Total carbon (mol/kg)	= 5.293e-03
Total CO2 (mol/kg)	= 5.293e-03
Temperature (°C)	= 25.54
Electrical balance (eq)	= -5.779e-04
Percent error, 100*(Cat-|An|)/(Cat+|An|)	= -4.88
Iterations	= 11 (276 overall)
Total H	= 1.110172e+02
Total O	= 5.552314e+01

---------------------------------Redox couples---------------------------------

Redox couple	pe	Eh (volts)
N(3)/N(5)	7.6867	0.4555

----------------------------Distribution of species----------------------------

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma	mole V cm³/mol
OH-	1.839e-07	1.671e-07	-6.735	-6.777	-0.042	-4.02
H+	6.859e-08	6.310e-08	-7.164	-7.200	-0.036	0.00
H2O	5.551e+01	9.998e-01	1.744	-0.000	0.000	18.07
Al	9.881e-07					
Al(OH)4-	8.976e-07	8.177e-07	-6.047	-6.087	-0.041	(0)
Al(OH)3	2.712e-08	2.718e-08	-7.567	-7.566	0.001	(0)
AlF3	2.517e-08	2.522e-08	-7.599	-7.598	0.001	(0)
AlF2+	2.411e-08	2.201e-08	-7.618	-7.657	-0.040	(0)

Al(OH)2+	1.226e-08	1.119e-08	-7.912	-7.951	-0.040	(0)
AlF4-	1.003e-09	9.136e-10	-8.999	-9.039	-0.041	(0)
AlF+2	6.929e-10	4.812e-10	-9.159	-9.318	-0.158	(0)
AlOH+2	1.238e-10	8.595e-11	-9.907	-10.066	-0.158	-27.60
Al+3	1.118e-12	5.272e-13	-11.952	-12.278	-0.326	-41.96
AlSO4+	7.536e-14	6.865e-14	-13.123	-13.163	-0.041	(0)
Al(SO4)2-	9.769e-17	8.899e-17	-16.010	-16.051	-0.041	(0)
AlHSO4+2	5.623e-22	3.859e-22	-21.250	-21.413	-0.163	(0)
B	1.211e-05					
H3BO3	1.199e-05	1.201e-05	-4.921	-4.920	0.001	39.27
H2BO3-	1.216e-07	1.107e-07	-6.915	-6.956	-0.041	(0)
BF(OH)3-	4.808e-10	4.376e-10	-9.318	-9.359	-0.041	(0)
BF2(OH)2-	2.956e-13	2.690e-13	-12.529	-12.570	-0.041	(0)
BF3OH-	1.843e-18	1.677e-18	-17.735	-17.775	-0.041	(0)
BF4-	4.307e-23	3.920e-23	-22.366	-22.407	-0.041	(0)
Br	6.260e-06					
Br-	6.260e-06	5.681e-06	-5.203	-5.246	-0.042	24.64
CdBr+	3.399e-12	3.094e-12	-11.469	-11.509	-0.041	(0)
ZnBr+	1.107e-12	1.008e-12	-11.956	-11.997	-0.041	(0)
PbBr+	1.880e-14	1.711e-14	-13.726	-13.767	-0.041	(0)
CdBr2	9.445e-17	9.462e-17	-16.025	-16.024	0.001	(0)
ZnBr2	2.274e-18	2.279e-18	-17.643	-17.642	0.001	(0)
PbBr2	4.499e-20	4.507e-20	-19.347	-19.346	0.001	(0)
C(4)	5.293e-03					
HCO3-	4.603e-03	4.202e-03	-2.337	-2.377	-0.040	24.79
CO2	5.913e-04	5.924e-04	-3.228	-3.227	0.001	34.46
CaHCO3+	4.175e-05	3.816e-05	-4.379	-4.418	-0.039	9.74
MgHCO3+	4.052e-05	3.686e-05	-4.392	-4.433	-0.041	5.54
CO3-2	4.546e-06	3.157e-06	-5.342	-5.501	-0.158	-5.01
CaCO3	3.779e-06	3.786e-06	-5.423	-5.422	0.001	-14.60
NaHCO3	2.741e-06	2.746e-06	-5.562	-5.561	0.001	1.80
MgCO3	2.268e-06	2.272e-06	-5.644	-5.644	0.001	-17.09
FeHCO3+	7.197e-07	6.550e-07	-6.143	-6.184	-0.041	(0)
ZnCO3	4.240e-07	4.248e-07	-6.373	-6.372	0.001	(0)
MnHCO3+	4.112e-07	3.750e-07	-6.386	-6.426	-0.040	(0)
ZnHCO3+	3.919e-07	3.567e-07	-6.407	-6.448	-0.041	(0)
MnCO3	2.507e-07	2.511e-07	-6.601	-6.600	0.001	(0)
FeCO3	1.178e-07	1.181e-07	-6.929	-6.928	0.001	(0)
NaCO3-	7.737e-08	7.042e-08	-7.111	-7.152	-0.041	-0.89
Zn(CO3)2-2	4.178e-08	2.868e-08	-7.379	-7.542	-0.163	(0)
(CO2)2	6.544e-09	6.556e-09	-8.184	-8.183	0.001	68.92
PbCO3	2.777e-09	2.782e-09	-8.556	-8.556	0.001	(0)
CuCO3	1.286e-09	1.289e-09	-8.891	-8.890	0.001	(0)
CdHCO3+	5.389e-10	4.905e-10	-9.268	-9.309	-0.041	(0)
PbHCO3+	1.860e-10	1.693e-10	-9.731	-9.771	-0.041	(0)
CuHCO3+	1.759e-10	1.601e-10	-9.755	-9.796	-0.041	(0)
Pb(CO3)2-2	3.216e-11	2.207e-11	-10.493	-10.656	-0.163	(0)
CdCO3	9.240e-12	9.258e-12	-11.034	-11.033	0.001	(0)
Cu(CO3)2-2	7.465e-12	5.123e-12	-11.127	-11.290	-0.163	(0)
Cd(CO3)2-2	1.347e-13	9.243e-14	-12.871	-13.034	-0.163	(0)
Ca	1.068e-03					
Ca+2	1.017e-03	7.060e-04	-2.993	-3.151	-0.159	-17.95
CaHCO3+	4.175e-05	3.816e-05	-4.379	-4.418	-0.039	9.74
CaSO4	5.145e-06	5.155e-06	-5.289	-5.288	0.001	7.52
CaCO3	3.779e-06	3.786e-06	-5.423	-5.422	0.001	-14.60
CaHPO4	3.045e-07	3.051e-07	-6.516	-6.516	0.001	(0)
CaH2PO4+	1.581e-08	1.443e-08	-7.801	-7.841	-0.040	(0)
CaPO4-	1.266e-08	1.156e-08	-7.898	-7.937	-0.040	(0)
CaOH+	2.040e-09	1.857e-09	-8.690	-8.731	-0.041	(0)
CaHSO4+	2.367e-12	2.154e-12	-11.626	-11.667	-0.041	(0)
Cd	6.319e-09					
Cd+2	5.378e-09	3.691e-09	-8.269	-8.433	-0.163	-18.54
CdHCO3+	5.389e-10	4.905e-10	-9.268	-9.309	-0.041	(0)
CdCl+	3.284e-10	2.989e-10	-9.484	-9.524	-0.041	6.07
CdSO4	4.359e-11	4.367e-11	-10.361	-10.360	0.001	77.78
CdCO3	9.240e-12	9.258e-12	-11.034	-11.033	0.001	(0)
CdOH+	5.563e-12	5.064e-12	-11.255	-11.296	-0.041	(0)
CdF+	4.645e-12	4.228e-12	-11.333	-11.374	-0.041	(0)

CdNO3+	3.795e-12	3.454e-12	-11.421	-11.462	-0.041	17.56
CdBr+	3.399e-12	3.094e-12	-11.469	-11.509	-0.041	(0)
CdOHCl	1.975e-12	1.979e-12	-11.704	-11.704	0.001	(0)
CdCl2	1.055e-12	1.057e-12	-11.977	-11.976	0.001	23.14
Cd(CO3)2-2	1.347e-13	9.243e-14	-12.871	-13.034	-0.163	(0)
Cd(SO4)2-2	2.844e-14	1.952e-14	-13.546	-13.710	-0.163	-105.14
Cd(OH)2	4.132e-15	4.140e-15	-14.384	-14.383	0.001	(0)
CdF2	9.644e-16	9.662e-16	-15.016	-15.015	0.001	(0)
CdCl3-	6.251e-16	5.690e-16	-15.204	-15.245	-0.041	68.99
CdBr2	9.445e-17	9.462e-17	-16.025	-16.024	0.001	(0)
Cd2OH+3	2.121e-19	9.093e-20	-18.673	-19.041	-0.368	(0)
Cd(OH)3-	8.087e-21	7.361e-21	-20.092	-20.133	-0.041	(0)
Cd(OH)4-2	1.515e-27	1.040e-27	-26.820	-26.983	-0.163	(0)
Cl	9.368e-04					
Cl-	9.309e-04	8.464e-04	-3.031	-3.072	-0.041	18.14
NaCl	5.915e-06	5.926e-06	-5.228	-5.227	0.001	(0)
CuCl2-	4.526e-09	4.118e-09	-8.344	-8.385	-0.041	(0)
MnCl+	3.786e-09	3.453e-09	-8.422	-8.462	-0.040	-2.92
FeCl+	2.001e-09	1.821e-09	-8.699	-8.740	-0.041	(0)
ZnCl+	1.729e-09	1.573e-09	-8.762	-8.803	-0.041	-13.36
CdCl+	3.284e-10	2.989e-10	-9.484	-9.524	-0.041	6.07
ZnOHCl	2.989e-10	2.995e-10	-9.524	-9.524	0.001	(0)
CuCl3-2	8.000e-12	5.535e-12	-11.097	-11.257	-0.160	(0)
CdOHCl	1.975e-12	1.979e-12	-11.704	-11.704	0.001	(0)
PbCl+	1.903e-12	1.732e-12	-11.721	-11.762	-0.041	8.01
ZnCl2	1.395e-12	1.397e-12	-11.856	-11.855	0.001	100.98
MnCl2	1.273e-12	1.276e-12	-11.895	-11.894	0.001	85.23
CdCl2	1.055e-12	1.057e-12	-11.977	-11.976	0.001	23.14
CuCl+	1.954e-13	1.778e-13	-12.709	-12.750	-0.041	0.55
PbCl2	2.296e-15	2.300e-15	-14.639	-14.638	0.001	35.02
ZnCl3-	1.463e-15	1.331e-15	-14.835	-14.876	-0.041	17.03
CdCl3-	6.251e-16	5.690e-16	-15.204	-15.245	-0.041	68.99
MnCl3-	3.261e-16	2.974e-16	-15.487	-15.527	-0.040	43.40
CuCl2	8.113e-17	8.128e-17	-16.091	-16.090	0.001	31.64
PbCl3-	1.704e-18	1.551e-18	-17.768	-17.809	-0.041	66.07
ZnCl4-2	8.197e-19	5.671e-19	-18.086	-18.246	-0.160	145.48
FeCl+2	1.269e-20	8.782e-21	-19.896	-20.056	-0.160	(0)
PbCl4-2	9.196e-22	6.311e-22	-21.036	-21.200	-0.163	101.65
CuCl3-	2.709e-22	2.465e-22	-21.567	-21.608	-0.041	(0)
FeCl2+	3.579e-23	3.264e-23	-22.446	-22.486	-0.040	(0)
FeCl3	2.758e-27	2.763e-27	-26.559	-26.559	0.001	(0)
CuCl4-2	1.530e-27	1.059e-27	-26.815	-26.975	-0.160	(0)
Cu(1)	2.461e-08					
Cu+	2.008e-08	1.820e-08	-7.697	-7.740	-0.043	(0)
CuCl2-	4.526e-09	4.118e-09	-8.344	-8.385	-0.041	(0)
CuCl3-2	8.000e-12	5.535e-12	-11.097	-11.257	-0.160	(0)
Cu(2)	1.991e-09					
CuCO3	1.286e-09	1.289e-09	-8.891	-8.890	0.001	(0)
Cu(OH)2	3.980e-10	3.987e-10	-9.400	-9.399	0.001	(0)
CuHCO3+	1.759e-10	1.601e-10	-9.755	-9.796	-0.041	(0)
Cu+2	1.088e-10	7.601e-11	-9.963	-10.119	-0.156	-26.44
CuOH+	1.324e-11	1.204e-11	-10.878	-10.919	-0.041	(0)
Cu(CO3)2-2	7.465e-12	5.123e-12	-11.127	-11.290	-0.163	(0)
CuSO4	6.357e-13	6.369e-13	-12.197	-12.196	0.001	13.16
CuCl+	1.954e-13	1.778e-13	-12.709	-12.750	-0.041	0.55
CuF+	1.389e-13	1.265e-13	-12.857	-12.898	-0.041	(0)
Cu(OH)3-	4.183e-16	3.807e-16	-15.379	-15.419	-0.041	(0)
Cu2(OH)2+2	9.757e-17	6.697e-17	-16.011	-16.174	-0.163	(0)
CuCl2	8.113e-17	8.128e-17	-16.091	-16.090	0.001	31.64
Cu(OH)4-2	1.754e-21	1.204e-21	-20.756	-20.919	-0.163	(0)
CuCl3-	2.709e-22	2.465e-22	-21.567	-21.608	-0.041	(0)
CuCl4-2	1.530e-27	1.059e-27	-26.815	-26.975	-0.160	(0)
F	1.053e-04					
F-	1.001e-04	9.098e-05	-3.999	-4.041	-0.042	-1.26
MgF+	4.984e-06	4.540e-06	-5.302	-5.343	-0.041	-10.53
NaF	6.091e-08	6.103e-08	-7.215	-7.214	0.001	7.28
AlF3	2.517e-08	2.522e-08	-7.599	-7.598	0.001	(0)
AlF2+	2.411e-08	2.201e-08	-7.618	-7.657	-0.040	(0)

HF	8.677e-09	8.694e-09	-8.062	-8.061	0.001	12.52
FeF+	1.558e-09	1.418e-09	-8.807	-8.848	-0.041	(0)
AlF4-	1.003e-09	9.136e-10	-8.999	-9.039	-0.041	(0)
ZnF+	9.585e-10	8.724e-10	-9.018	-9.059	-0.041	(0)
AlF+2	6.929e-10	4.812e-10	-9.159	-9.318	-0.158	(0)
MnF+	6.911e-10	6.303e-10	-9.160	-9.200	-0.040	(0)
BF(OH)3-	4.808e-10	4.376e-10	-9.318	-9.359	-0.041	(0)
CdF+	4.645e-12	4.228e-12	-11.333	-11.374	-0.041	(0)
HF2-	3.348e-12	3.048e-12	-11.475	-11.516	-0.041	22.14
BF2(OH)2-	2.956e-13	2.690e-13	-12.529	-12.570	-0.041	(0)
CuF+	1.389e-13	1.265e-13	-12.857	-12.898	-0.041	(0)
PbF+	9.014e-14	8.205e-14	-13.045	-13.086	-0.041	(0)
CdF2	9.644e-16	9.662e-16	-15.016	-15.015	0.001	(0)
FeF2+	1.963e-16	1.790e-16	-15.707	-15.747	-0.040	(0)
PbF2	1.521e-16	1.524e-16	-15.818	-15.817	0.001	(0)
FeF+2	7.097e-17	4.911e-17	-16.149	-16.309	-0.160	(0)
FeF3	2.581e-17	2.586e-17	-16.588	-16.587	0.001	(0)
BF3OH-	1.843e-18	1.677e-18	-17.735	-17.775	-0.041	(0)
PbF3-	1.104e-19	1.005e-19	-18.957	-18.998	-0.041	(0)
BF4-	4.307e-23	3.920e-23	-22.366	-22.407	-0.041	(0)
PbF4-2	6.374e-24	4.375e-24	-23.196	-23.359	-0.163	(0)
Fe(2)	3.099e-06					
Fe+2	2.232e-06	1.559e-06	-5.651	-5.807	-0.156	-21.92
FeHCO3+	7.197e-07	6.550e-07	-6.143	-6.184	-0.041	(0)
FeCO3	1.178e-07	1.181e-07	-6.929	-6.928	0.001	(0)
FeSO4	1.143e-08	1.145e-08	-7.942	-7.941	0.001	18.41
FeOH+	8.916e-09	8.132e-09	-8.050	-8.090	-0.040	(0)
FeHPO4	4.833e-09	4.842e-09	-8.316	-8.315	0.001	(0)
FeCl+	2.001e-09	1.821e-09	-8.699	-8.740	-0.041	(0)
FeF+	1.558e-09	1.418e-09	-8.807	-8.848	-0.041	(0)
FeH2PO4+	6.765e-10	6.176e-10	-9.170	-9.209	-0.040	(0)
Fe(OH)2	1.147e-12	1.149e-12	-11.940	-11.940	0.001	(0)
FeHSO4+	5.226e-15	4.757e-15	-14.282	-14.323	-0.041	(0)
Fe(OH)3-	7.459e-16	6.803e-16	-15.127	-15.167	-0.040	(0)
Fe(3)	6.143e-10					
Fe(OH)3	3.985e-10	3.992e-10	-9.400	-9.399	0.001	(0)
Fe(OH)2+	2.093e-10	1.910e-10	-9.679	-9.719	-0.040	(0)
Fe(OH)4-	6.459e-12	5.896e-12	-11.190	-11.229	-0.040	(0)
FeOH+2	5.155e-14	3.567e-14	-13.288	-13.448	-0.160	(0)
FeF2+	1.963e-16	1.790e-16	-15.707	-15.747	-0.040	(0)
FeF+2	7.097e-17	4.911e-17	-16.149	-16.309	-0.160	(0)
FeF3	2.581e-17	2.586e-17	-16.588	-16.587	0.001	(0)
Fe+3	7.160e-19	3.378e-19	-18.145	-18.471	-0.326	(0)
FeSO4+	1.680e-19	1.533e-19	-18.775	-18.815	-0.040	(0)
FeH2PO4+2	1.035e-19	7.187e-20	-18.985	-19.143	-0.158	(0)
FeHPO4+	7.915e-20	7.219e-20	-19.102	-19.142	-0.040	(0)
FeCl+2	1.269e-20	8.782e-21	-19.896	-20.056	-0.160	(0)
Fe(SO4)2-	1.509e-22	1.374e-22	-21.821	-21.862	-0.041	(0)
FeCl2+	3.579e-23	3.264e-23	-22.446	-22.486	-0.040	(0)
Fe2(OH)2+4	1.510e-25	3.349e-26	-24.821	-25.475	-0.654	(0)
FeHSO4+2	3.772e-26	2.589e-26	-25.423	-25.587	-0.163	(0)
FeCl3	2.758e-27	2.763e-27	-26.559	-26.559	0.001	(0)
Fe3(OH)4+5	1.337e-32	1.272e-33	-31.874	-32.896	-1.022	(0)
H(0)	1.153e-18					
H2	5.766e-19	5.777e-19	-18.239	-18.238	0.001	28.61
K	7.931e-05					
K+	7.929e-05	7.207e-05	-4.101	-4.142	-0.041	9.08
KSO4-	2.290e-08	2.090e-08	-7.640	-7.680	-0.040	34.17
KHPO4-	1.201e-10	1.096e-10	-9.920	-9.960	-0.040	38.14
Mg	1.127e-03					
Mg+2	1.072e-03	7.479e-04	-2.970	-3.126	-0.156	-21.66
MgHCO3+	4.052e-05	3.686e-05	-4.392	-4.433	-0.041	5.54
MgSO4	7.256e-06	7.269e-06	-5.139	-5.138	0.001	5.86
MgF+	4.984e-06	4.540e-06	-5.302	-5.343	-0.041	-10.53
MgCO3	2.268e-06	2.272e-06	-5.644	-5.644	0.001	-17.09
MgHPO4	4.362e-07	4.370e-07	-6.360	-6.360	0.001	(0)
MgOH+	4.936e-08	4.518e-08	-7.307	-7.345	-0.039	(0)
MgH2PO4+	2.132e-08	1.947e-08	-7.671	-7.711	-0.040	(0)

MgPO4-	1.809e-08	1.652e-08	-7.743	-7.782	-0.040	(0)
Mn(2)	2.108e-06					
Mn+2	1.434e-06	1.001e-06	-5.843	-5.999	-0.156	-19.97
MnHCO3+	4.112e-07	3.750e-07	-6.386	-6.426	-0.040	(0)
MnCO3	2.507e-07	2.511e-07	-6.601	-6.600	0.001	(0)
MnSO4	7.343e-09	7.357e-09	-8.134	-8.133	0.001	22.31
MnCl+	3.786e-09	3.453e-09	-8.422	-8.462	-0.040	-2.92
MnF+	6.911e-10	6.303e-10	-9.160	-9.200	-0.040	(0)
MnOH+	4.673e-10	4.262e-10	-9.330	-9.370	-0.040	(0)
MnCl2	1.273e-12	1.276e-12	-11.895	-11.894	0.001	85.23
Mn(NO3)2	5.694e-13	5.705e-13	-12.245	-12.244	0.001	40.90
MnCl3-	3.261e-16	2.974e-16	-15.487	-15.527	-0.040	43.40
Mn(OH)3-	6.924e-20	6.315e-20	-19.160	-19.200	-0.040	(0)
Mn(3)	1.563e-31					
Mn+3	1.563e-31	7.375e-32	-30.806	-31.132	-0.326	(0)
N(3)	2.286e-05					
NO2-	2.286e-05	2.074e-05	-4.641	-4.683	-0.042	25.05
N(5)	4.171e-04					
NO3-	4.171e-04	3.785e-04	-3.380	-3.422	-0.042	29.60
CdNO3+	3.795e-12	3.454e-12	-11.421	-11.462	-0.041	17.56
Mn(NO3)2	5.694e-13	5.705e-13	-12.245	-12.244	0.001	40.90
PbNO3+	3.119e-13	2.839e-13	-12.506	-12.547	-0.041	(0)
Na	1.288e-03					
Na+	1.279e-03	1.166e-03	-2.893	-2.933	-0.040	-1.37
NaCl	5.915e-06	5.926e-06	-5.228	-5.227	0.001	(0)
NaHCO3	2.741e-06	2.746e-06	-5.562	-5.561	0.001	1.80
NaSO4-	2.626e-07	2.397e-07	-6.581	-6.620	-0.040	14.22
NaCO3-	7.737e-08	7.042e-08	-7.111	-7.152	-0.041	-0.89
NaF	6.091e-08	6.103e-08	-7.215	-7.214	0.001	7.28
NaHPO4-	1.943e-09	1.773e-09	-8.712	-8.751	-0.040	34.03
NaOH	1.944e-20	1.948e-20	-19.711	-19.710	0.001	(0)
O(0)	0.000e+00					
O2	0.000e+00	0.000e+00	-55.730	-55.730	0.001	30.44
P	2.810e-06					
HPO4-2	1.128e-06	7.803e-07	-5.948	-6.108	-0.160	6.91
H2PO4-	8.660e-07	7.906e-07	-6.062	-6.102	-0.040	33.26
MgHPO4	4.362e-07	4.370e-07	-6.360	-6.360	0.001	(0)
CaHPO4	3.045e-07	3.051e-07	-6.516	-6.516	0.001	(0)
MgH2PO4+	2.132e-08	1.947e-08	-7.671	-7.711	-0.040	(0)
MgPO4-	1.809e-08	1.652e-08	-7.743	-7.782	-0.040	(0)
CaH2PO4+	1.581e-08	1.443e-08	-7.801	-7.841	-0.040	(0)
CaPO4-	1.266e-08	1.156e-08	-7.898	-7.937	-0.040	(0)
FeHPO4	4.833e-09	4.842e-09	-8.316	-8.315	0.001	(0)
NaHPO4-	1.943e-09	1.773e-09	-8.712	-8.751	-0.040	34.03
FeH2PO4+	6.765e-10	6.176e-10	-9.170	-9.209	-0.040	(0)
KHPO4-	1.201e-10	1.096e-10	-9.920	-9.960	-0.040	38.14
PO4-3	1.319e-11	5.635e-12	-10.880	-11.249	-0.369	-22.80
H3PO4	7.378e-12	7.391e-12	-11.132	-11.131	0.001	47.44
FeH2PO4+2	1.035e-19	7.187e-20	-18.985	-19.143	-0.158	(0)
FeHPO4+	7.915e-20	7.219e-20	-19.102	-19.142	-0.040	(0)
Pb	3.090e-09					
PbCO3	2.777e-09	2.782e-09	-8.556	-8.556	0.001	(0)
PbHCO3+	1.860e-10	1.693e-10	-9.731	-9.771	-0.041	(0)
Pb+2	7.389e-11	5.071e-11	-10.131	-10.295	-0.163	-15.36
Pb(CO3)2-2	3.216e-11	2.207e-11	-10.493	-10.656	-0.163	(0)
PbOH+	1.721e-11	1.567e-11	-10.764	-10.805	-0.041	(0)
PbCl+	1.903e-12	1.732e-12	-11.721	-11.762	-0.041	8.01
PbSO4	1.164e-12	1.166e-12	-11.934	-11.933	0.001	(0)
PbNO3+	3.119e-13	2.839e-13	-12.506	-12.547	-0.041	(0)
Pb(OH)2	9.641e-14	9.659e-14	-13.016	-13.015	0.001	(0)
PbF+	9.014e-14	8.205e-14	-13.045	-13.086	-0.041	(0)
PbBr+	1.880e-14	1.711e-14	-13.726	-13.767	-0.041	(0)
PbCl2	2.296e-15	2.300e-15	-14.639	-14.638	0.001	35.02
Pb(SO4)2-2	3.646e-16	2.502e-16	-15.438	-15.602	-0.163	(0)
PbF2	1.521e-16	1.524e-16	-15.818	-15.817	0.001	(0)
Pb(OH)3-	1.931e-17	1.757e-17	-16.714	-16.755	-0.041	(0)
PbCl3-	1.704e-18	1.551e-18	-17.768	-17.809	-0.041	66.07
PbF3-	1.104e-19	1.005e-19	-18.957	-18.998	-0.041	(0)

PbBr2	4.499e-20	4.507e-20	-19.347	-19.346	0.001	(0)
Pb2OH+3	4.149e-20	1.779e-20	-19.382	-19.750	-0.368	(0)
Pb(OH)4-2	9.296e-22	6.380e-22	-21.032	-21.195	-0.163	(0)
PbCl4-2	9.196e-22	6.311e-22	-21.036	-21.200	-0.163	101.65
PbF4-2	6.374e-24	4.375e-24	-23.196	-23.359	-0.163	(0)
Pb3(OH)4+2	1.712e-26	1.175e-26	-25.766	-25.930	-0.163	(0)
S(6)	7.186e-05					
SO4-2	5.914e-05	4.089e-05	-4.228	-4.388	-0.160	14.80
MgSO4	7.256e-06	7.269e-06	-5.139	-5.138	0.001	5.86
CaSO4	5.145e-06	5.155e-06	-5.289	-5.288	0.001	7.52
NaSO4-	2.626e-07	2.397e-07	-6.581	-6.620	-0.040	14.22
KSO4-	2.290e-08	2.090e-08	-7.640	-7.680	-0.040	34.17
FeSO4	1.143e-08	1.145e-08	-7.942	-7.941	0.001	18.41
MnSO4	7.343e-09	7.357e-09	-8.134	-8.133	0.001	22.31
ZnSO4	6.478e-09	6.490e-09	-8.189	-8.188	0.001	21.63
HSO4-	2.789e-10	2.538e-10	-9.555	-9.595	-0.041	40.37
CdSO4	4.359e-11	4.367e-11	-10.361	-10.360	0.001	77.78
Zn(SO4)2-2	3.130e-12	2.148e-12	-11.504	-11.668	-0.163	-12.41
CaHSO4+	2.367e-12	2.154e-12	-11.626	-11.667	-0.041	(0)
PbSO4	1.164e-12	1.166e-12	-11.934	-11.933	0.001	(0)
CuSO4	6.357e-13	6.369e-13	-12.197	-12.196	0.001	13.16
AlSO4+	7.536e-14	6.865e-14	-13.123	-13.163	-0.041	(0)
Cd(SO4)2-2	2.844e-14	1.952e-14	-13.546	-13.710	-0.163	-105.14
FeHSO4+	5.226e-15	4.757e-15	-14.282	-14.323	-0.041	(0)
Pb(SO4)2-2	3.646e-16	2.502e-16	-15.438	-15.602	-0.163	(0)
Al(SO4)2-	9.769e-17	8.899e-17	-16.010	-16.051	-0.041	(0)
FeSO4+	1.680e-19	1.533e-19	-18.775	-18.815	-0.040	(0)
AlHSO4+2	5.623e-22	3.859e-22	-21.250	-21.413	-0.163	(0)
Fe(SO4)2-	1.509e-22	1.374e-22	-21.821	-21.862	-0.041	(0)
FeHSO4+2	3.772e-26	2.589e-26	-25.423	-25.587	-0.163	(0)
Zn	1.857e-06					
Zn+2	9.745e-07	6.743e-07	-6.011	-6.171	-0.160	-25.21
ZnCO3	4.240e-07	4.248e-07	-6.373	-6.372	0.001	(0)
ZnHCO3+	3.919e-07	3.567e-07	-6.407	-6.448	-0.041	(0)
Zn(CO3)2-2	4.178e-08	2.868e-08	-7.379	-7.542	-0.163	(0)
ZnOH+	1.341e-08	1.220e-08	-7.873	-7.913	-0.041	(0)
ZnSO4	6.478e-09	6.490e-09	-8.189	-8.188	0.001	21.63
Zn(OH)2	2.128e-09	2.131e-09	-8.672	-8.671	0.001	(0)
ZnCl+	1.729e-09	1.573e-09	-8.762	-8.803	-0.041	-13.36
ZnF+	9.585e-10	8.724e-10	-9.018	-9.059	-0.041	(0)
ZnOHCl	2.989e-10	2.995e-10	-9.524	-9.524	0.001	(0)
Zn(SO4)2-2	3.130e-12	2.148e-12	-11.504	-11.668	-0.163	-12.41
ZnCl2	1.395e-12	1.397e-12	-11.856	-11.855	0.001	100.98
ZnBr+	1.107e-12	1.008e-12	-11.956	-11.997	-0.041	(0)
Zn(OH)3-	1.173e-13	1.068e-13	-12.931	-12.971	-0.041	(0)
ZnCl3-	1.463e-15	1.331e-15	-14.835	-14.876	-0.041	17.03
ZnBr2	2.274e-18	2.279e-18	-17.643	-17.642	0.001	(0)
ZnCl4-2	8.197e-19	5.671e-19	-18.086	-18.246	-0.160	145.48
Zn(OH)4-2	3.909e-19	2.682e-19	-18.408	-18.571	-0.163	(0)

----------Distribution of alkalinity----------

Total alkalinity (eq/kgw) = 4.719e-03

Species	Alkalinity	Molality	Alk/Mol
HCO3-	4.603e-03	4.603e-03	1.00
CaHCO3+	4.175e-05	4.175e-05	1.00
MgHCO3+	4.052e-05	4.052e-05	1.00
CO3-2	9.093e-06	4.546e-06	2.00
CaCO3	7.558e-06	3.779e-06	2.00
MgCO3	4.536e-06	2.268e-06	2.00
Al(OH)4-	3.590e-06	8.976e-07	4.00
NaHCO3	2.741e-06	2.741e-06	1.00
HPO4-2	1.128e-06	1.128e-06	1.00
ZnCO3	8.480e-07	4.240e-07	2.00
FeHCO3+	7.197e-07	7.197e-07	1.00
MnCO3	5.013e-07	2.507e-07	2.00

MgHPO4	4.362e-07	4.362e-07	1.00
MnHCO3+	4.112e-07	4.112e-07	1.00
ZnHCO3+	3.919e-07	3.919e-07	1.00
CaHPO4	3.045e-07	3.045e-07	1.00
FeCO3	2.357e-07	1.178e-07	2.00
OH-	1.839e-07	1.839e-07	1.00
Zn(CO3)2-2	1.671e-07	4.178e-08	4.00
NaCO3-	1.547e-07	7.737e-08	2.00
H2BO3-	1.216e-07	1.216e-07	1.00
Al(OH)3	8.137e-08	2.712e-08	3.00
H+	-6.859e-08	6.859e-08	-1.00
MgOH+	4.936e-08	4.936e-08	1.00
MgPO4-	3.618e-08	1.809e-08	2.00
CaPO4-	2.532e-08	1.266e-08	2.00
Al(OH)2+	2.451e-08	1.226e-08	2.00
ZnOH+	1.341e-08	1.341e-08	1.00
FeOH+	8.916e-09	8.916e-09	1.00
HF	-8.677e-09	8.677e-09	-1.00
PbCO3	5.555e-09	2.777e-09	2.00
FeHPO4	4.833e-09	4.833e-09	1.00
Zn(OH)2	4.255e-09	2.128e-09	2.00
CuCO3	2.573e-09	1.286e-09	2.00
CaOH+	2.040e-09	2.040e-09	1.00
NaHPO4-	1.943e-09	1.943e-09	1.00
Cu(OH)2	7.960e-10	3.980e-10	2.00
CdHCO3+	5.389e-10	5.389e-10	1.00
MnOH+	4.673e-10	4.673e-10	1.00
Fe(OH)3	3.985e-10	3.985e-10	1.00
ZnOHCl	2.989e-10	2.989e-10	1.00
HSO4-	-2.789e-10	2.789e-10	-1.00
PbHCO3+	1.860e-10	1.860e-10	1.00
CuHCO3+	1.759e-10	1.759e-10	1.00
Pb(CO3)2-2	1.286e-10	3.216e-11	4.00
AlOH+2	1.238e-10	1.238e-10	1.00
KHPO4-	1.201e-10	1.201e-10	1.00
Cu(CO3)2-2	2.986e-11	7.465e-12	4.00
PO4-3	2.639e-11	1.319e-11	2.00
CdCO3	1.848e-11	9.240e-12	2.00
PbOH+	1.721e-11	1.721e-11	1.00
CuOH+	1.324e-11	1.324e-11	1.00
Fe(OH)4-	1.292e-11	6.459e-12	2.00
H3PO4	-7.378e-12	7.378e-12	-1.00
CdOH+	5.563e-12	5.563e-12	1.00
HF2-	-3.348e-12	3.348e-12	-1.00
CaHSO4+	-2.367e-12	2.367e-12	-1.00
Fe(OH)2	2.295e-12	1.147e-12	2.00
CdOHCl	1.975e-12	1.975e-12	1.00
Cd(CO3)2-2	5.387e-13	1.347e-13	4.00
Zn(OH)3-	3.520e-13	1.173e-13	3.00
BF2(OH)2-	-2.956e-13	2.956e-13	-1.00
Pb(OH)2	1.928e-13	9.641e-14	2.00
FeOH+2	-5.155e-14	5.155e-14	-1.00
Cd(OH)2	8.265e-15	4.132e-15	2.00
FeHSO4+	-5.226e-15	5.226e-15	-1.00
Fe(OH)3-	2.238e-15	7.459e-16	3.00
Cu(OH)3-	1.255e-15	4.183e-16	3.00
FeF2+	-3.926e-16	1.963e-16	-2.00
Cu2(OH)2+2	1.951e-16	9.757e-17	2.00
FeF+2	-1.419e-16	7.097e-17	-2.00
Pb(OH)3-	5.792e-17	1.931e-17	3.00
FeF3	-5.162e-17	2.581e-17	-2.00
BF3OH-	-3.685e-18	1.843e-18	-2.00
Zn(OH)4-2	1.563e-18	3.909e-19	4.00
Fe+3	-1.432e-18	7.160e-19	-2.00
FeSO4+	-3.361e-19	1.680e-19	-2.00
Cd2OH+3	2.121e-19	2.121e-19	1.00
Mn(OH)3-	2.077e-19	6.924e-20	3.00
FeH2PO4+2	-2.070e-19	1.035e-19	-2.00

FeHPO4+	-7.915e-20	7.915e-20	-1.00
Pb2OH+3	4.149e-20	4.149e-20	1.00
FeCl+2	-2.539e-20	1.269e-20	-2.00
Cd(OH)3-	2.426e-20	8.087e-21	3.00
NaOH	1.944e-20	1.944e-20	1.00
Cu(OH)4-2	7.016e-21	1.754e-21	4.00
Pb(OH)4-2	3.718e-21	9.296e-22	4.00
AlHSO4+2	-5.623e-22	5.623e-22	-1.00
Fe(SO4)2-	-3.019e-22	1.509e-22	-2.00
BF4-	-1.292e-22	4.307e-23	-3.00
FeCl2+	-7.158e-23	3.579e-23	-2.00
Fe2(OH)2+4	-3.019e-25	1.510e-25	-2.00
FeHSO4+2	-1.132e-25	3.772e-26	-3.00
Pb3(OH)4+2	6.850e-26	1.712e-26	4.00
Cd(OH)4-2	6.059e-27	1.515e-27	4.00
FeCl3	-5.515e-27	2.758e-27	-2.00
Fe3(OH)4+5	-2.675e-32	1.337e-32	-2.00

----------Saturation indices----------

Phase	SI**	log IAP	log K(298 K, 1 atm)	
Al(OH)3(a)	-1.44	9.32	10.76	Al(OH)3
Alunite	-5.09	-6.55	-1.47	KAl3(SO4)2(OH)6
Anglesite	-6.90	-14.68	-7.79	PbSO4
Anhydrite	-3.26	-7.54	-4.28	CaSO4
Aragonite	-0.31	-8.65	-8.34	CaCO3
Calcite	-0.17	-8.65	-8.48	CaCO3
Cd(OH)2	-7.68	5.97	13.65	Cd(OH)2
CdSO4	-12.70	-12.82	-0.12	CdSO4
Cerussite	-2.67	-15.80	-13.12	PbCO3
CO2(g)	-1.75	-3.23	-1.47	CO2
Dolomite	-0.18	-17.28	-17.10	CaMg(CO3)2
Fe(OH)3(a)	-1.76	3.13	4.89	Fe(OH)3
Fluorite	-0.64	-11.23	-10.59	CaF2
Gibbsite	1.24	9.32	8.08	Al(OH)3
Goethite	4.15	3.13	-1.02	FeOOH
Gypsum	-2.96	-7.54	-4.58	CaSO4:2H2O
H2(g)	-15.14	-18.24	-3.10	H2
H2O(g)	-1.49	-0.00	1.49	H2O
Halite	-7.58	-6.01	1.57	NaCl
Hausmannite	-20.61	40.29	60.90	Mn3O4
Hematite	10.31	6.26	-4.05	Fe2O3
Hydroxyapatite	-1.81	-5.28	-3.47	Ca5(PO4)3OH
Jarosite-K	-15.88	-25.13	-9.25	KFe3(SO4)2(OH)6
Manganite	-9.40	15.94	25.34	MnOOH
Melanterite	-7.99	-10.20	-2.20	FeSO4:7H2O
O2(g)	-52.83	-55.73	-2.90	O2
Otavite	-1.83	-13.93	-12.10	CdCO3
Pb(OH)2	-4.03	4.10	8.13	Pb(OH)2
Pyrochroite	-6.80	8.40	15.20	Mn(OH)2
Pyrolusite	-17.81	23.49	41.29	MnO2:H2O
Rhodochrosite	-0.37	-11.50	-11.13	MnCO3
Siderite	-0.41	-11.31	-10.89	FeCO3
Smithsonite	-1.67	-11.67	-10.01	ZnCO3
Sylvite	-8.12	-7.21	0.90	KCl
Vivianite	-3.92	-39.92	-36.00	Fe3(PO4)2:8H2O
Zn(OH)2(e)	-3.27	8.23	11.50	Zn(OH)2

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
For ideal gases, phi = 1.

Initial solution 27.

----------Solution composition----------

Elements	Molality	Moles

Al	1.557e-06	1.557e-06
Alkalinity	2.375e-03	2.375e-03
B	1.260e-05	1.260e-05
Ba	1.173e-05	1.173e-05
Br	6.009e-06	6.009e-06
Ca	3.519e-04	3.519e-04
Cd	8.721e-09	8.721e-09
Cl	8.379e-04	8.379e-04
Cu	9.570e-08	9.570e-08
F	6.107e-05	6.107e-05
Fe	4.522e-07	4.522e-07
K	1.919e-04	1.919e-04
Mg	6.887e-04	6.887e-04
Mn	1.231e-06	1.231e-06
N(3)	1.428e-06	1.428e-06
N(5)	1.087e-03	1.087e-03
Na	1.049e-03	1.049e-03
P	9.688e-08	9.688e-08
Pb	2.221e-09	2.221e-09
S(6)	5.102e-05	5.102e-05
Zn	2.376e-06	2.376e-06

----------Description of solution----------

pH	= 4.600
pe	= 0.223
Specific Conductance (µS/cm, 25°C)	= 411
Density (g/cm³)	= 0.99858
Volume (L)	= 1.00730
Activity of water	= 0.998
Ionic strength (mol/kgw)	= 4.968e-03
Mass of water (kg)	= 1.000e+00
Total carbon (mol/kg)	= 1.286e-01
Total CO2 (mol/kg)	= 1.286e-01
Temperature (°C)	= 24.63
Electrical balance (eq)	= -1.113e-03
Percent error, 100*(Cat-|An|)/(Cat+|An|)	= -14.28
Iterations	= 11 (287 overall)
Total H	= 1.110149e+02
Total O	= 5.576934e+01

----------Redox couples----------

Redox couple	pe	Eh (volts)
N(3)/N(5)	11.1461	0.6585

----------Distribution of species----------

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma	mole V cm³/mol
H+	2.690e-05	2.512e-05	-4.570	-4.600	-0.030	0.00
OH-	4.219e-10	3.908e-10	-9.375	-9.408	-0.033	-4.08
H2O	5.551e+01	9.977e-01	1.744	-0.001	0.000	18.07
Al	1.557e-06					
AlF2+	9.466e-07	8.795e-07	-6.024	-6.056	-0.032	(0)
AlF3	5.507e-07	5.513e-07	-6.259	-6.259	0.000	(0)
AlF+2	4.736e-08	3.529e-08	-7.325	-7.452	-0.128	(0)
AlF4-	1.178e-08	1.093e-08	-7.929	-7.961	-0.033	(0)
Al+3	1.315e-10	7.100e-11	-9.881	-10.149	-0.268	-42.01
AlOH+2	3.670e-11	2.735e-11	-10.435	-10.563	-0.128	-27.62
Al(OH)2+	8.872e-12	8.243e-12	-11.052	-11.084	-0.032	(0)
AlSO4+	8.079e-12	7.496e-12	-11.093	-11.125	-0.033	(0)
Al(OH)3	4.689e-14	4.694e-14	-13.329	-13.328	0.000	(0)
Al(SO4)2-	8.555e-15	7.938e-15	-14.068	-14.100	-0.033	(0)
Al(OH)4-	3.769e-15	3.497e-15	-14.424	-14.456	-0.033	(0)
AlHSO4+2	2.251e-17	1.664e-17	-16.648	-16.779	-0.131	(0)

B	1.260e-05					
H3BO3	1.260e-05	1.262e-05	-4.900	-4.899	0.000	39.20
H2BO3-	3.096e-10	2.871e-10	-9.509	-9.542	-0.033	(0)
BF(OH)3-	2.688e-10	2.492e-10	-9.571	-9.603	-0.033	(0)
BF2(OH)2-	3.614e-11	3.351e-11	-10.442	-10.475	-0.033	(0)
BF3OH-	5.003e-14	4.639e-14	-13.301	-13.334	-0.033	(0)
BF4-	2.558e-16	2.372e-16	-15.592	-15.625	-0.033	(0)
Ba	1.173e-05					
Ba+2	1.137e-05	8.415e-06	-4.944	-5.075	-0.131	-12.64
BaHCO3+	1.902e-07	1.763e-07	-6.721	-6.754	-0.033	(0)
BaSO4	1.413e-07	1.415e-07	-6.850	-6.849	0.000	(0)
BaCl+	2.192e-08	2.033e-08	-7.659	-7.692	-0.033	(0)
BaNO3+	1.149e-09	1.066e-09	-8.940	-8.972	-0.033	(0)
BaCO3	1.766e-11	1.768e-11	-10.753	-10.752	0.000	-10.70
BaOH+	1.220e-14	1.133e-14	-13.914	-13.946	-0.032	(0)
Br	6.009e-06					
Br-	6.009e-06	5.561e-06	-5.221	-5.255	-0.034	24.58
CdBr+	5.092e-12	4.722e-12	-11.293	-11.326	-0.033	(0)
ZnBr+	2.262e-12	2.097e-12	-11.646	-11.678	-0.033	(0)
PbBr+	2.301e-13	2.133e-13	-12.638	-12.671	-0.033	(0)
CdBr2	1.406e-16	1.408e-16	-15.852	-15.851	0.000	(0)
ZnBr2	4.638e-18	4.644e-18	-17.334	-17.333	0.000	(0)
PbBr2	5.576e-19	5.583e-19	-18.254	-18.253	0.000	(0)
C(4)	1.286e-01					
CO2	1.256e-01	1.258e-01	-0.901	-0.900	0.000	34.41
HCO3-	2.381e-03	2.212e-03	-2.623	-2.655	-0.032	24.70
(CO2)2	2.865e-04	2.868e-04	-3.543	-3.542	0.000	68.83
MgHCO3+	1.394e-05	1.292e-05	-4.856	-4.889	-0.033	5.50
CaHCO3+	7.700e-06	7.161e-06	-5.114	-5.145	-0.032	9.69
NaHCO3	1.205e-06	1.206e-06	-5.919	-5.919	0.000	1.80
ZnHCO3+	4.306e-07	3.992e-07	-6.366	-6.399	-0.033	(0)
BaHCO3+	1.902e-07	1.763e-07	-6.721	-6.754	-0.033	(0)
MnHCO3+	1.676e-07	1.556e-07	-6.776	-6.808	-0.032	(0)
FeHCO3+	6.812e-08	6.317e-08	-7.167	-7.199	-0.033	(0)
CO3-2	5.500e-09	4.099e-09	-8.260	-8.387	-0.128	-5.15
MgCO3	1.942e-09	1.945e-09	-8.712	-8.711	0.000	-17.09
CaCO3	1.742e-09	1.744e-09	-8.759	-8.758	0.000	-14.60
PbHCO3+	1.242e-09	1.151e-09	-8.906	-8.939	-0.033	(0)
ZnCO3	1.171e-09	1.173e-09	-8.931	-8.931	0.000	(0)
CdHCO3+	4.323e-10	4.008e-10	-9.364	-9.397	-0.033	(0)
CuHCO3+	2.826e-10	2.621e-10	-9.549	-9.582	-0.033	(0)
MnCO3	2.568e-10	2.571e-10	-9.590	-9.590	0.000	(0)
NaCO3-	7.817e-11	7.248e-11	-10.107	-10.140	-0.033	-1.01
PbCO3	4.662e-11	4.668e-11	-10.331	-10.331	0.000	(0)
FeCO3	2.805e-11	2.808e-11	-10.552	-10.552	0.000	(0)
BaCO3	1.766e-11	1.768e-11	-10.753	-10.752	0.000	-10.70
CuCO3	5.197e-12	5.203e-12	-11.284	-11.284	0.000	(0)
Zn(CO3)2-2	1.390e-13	1.027e-13	-12.857	-12.988	-0.131	(0)
CdCO3	1.864e-14	1.866e-14	-13.730	-13.729	0.000	(0)
Pb(CO3)2-2	6.501e-16	4.806e-16	-15.187	-15.318	-0.131	(0)
Cu(CO3)2-2	3.632e-17	2.685e-17	-16.440	-16.571	-0.131	(0)
Cd(CO3)2-2	3.271e-19	2.418e-19	-18.485	-18.617	-0.131	(0)
Ca	3.519e-04					
Ca+2	3.427e-04	2.552e-04	-3.465	-3.593	-0.128	-18.02
CaHCO3+	7.700e-06	7.161e-06	-5.114	-5.145	-0.032	9.69
CaSO4	1.516e-06	1.518e-06	-5.819	-5.819	0.000	7.49
CaCO3	1.742e-09	1.744e-09	-8.759	-8.758	0.000	-14.60
CaH2PO4+	6.095e-10	5.663e-10	-9.215	-9.247	-0.032	(0)
CaHSO4+	2.689e-10	2.493e-10	-9.570	-9.603	-0.033	(0)
CaHPO4	2.990e-11	2.994e-11	-10.524	-10.524	0.000	(0)
CaOH+	1.814e-12	1.682e-12	-11.741	-11.774	-0.033	(0)
CaPO4-	3.014e-15	2.800e-15	-14.521	-14.553	-0.032	(0)
Cd	8.721e-09					
Cd+2	7.752e-09	5.731e-09	-8.111	-8.242	-0.131	-18.64
CdCl+	4.553e-10	4.222e-10	-9.342	-9.375	-0.033	5.80
CdHCO3+	4.323e-10	4.008e-10	-9.364	-9.397	-0.033	(0)
CdSO4	5.525e-11	5.532e-11	-10.258	-10.257	0.000	78.23
CdNO3+	1.579e-11	1.464e-11	-10.802	-10.834	-0.033	17.57

CdBr+	5.092e-12	4.722e-12	-11.293	-11.326	-0.033	(0)
CdF+	3.876e-12	3.594e-12	-11.412	-11.444	-0.033	(0)
CdCl2	1.356e-12	1.357e-12	-11.868	-11.867	0.000	23.14
Cd(SO4)2-2	2.758e-14	2.039e-14	-13.559	-13.691	-0.131	-105.77
CdOH+	1.987e-14	1.842e-14	-13.702	-13.735	-0.033	(0)
CdCO3	1.864e-14	1.866e-14	-13.730	-13.729	0.000	(0)
CdOHCl	6.864e-15	6.872e-15	-14.163	-14.163	0.000	(0)
CdCl3-	7.094e-16	6.578e-16	-15.149	-15.182	-0.033	69.62
CdF2	4.492e-16	4.497e-16	-15.348	-15.347	0.000	(0)
CdBr2	1.406e-16	1.408e-16	-15.852	-15.851	0.000	(0)
Cd(CO3)2-2	3.271e-19	2.418e-19	-18.485	-18.617	-0.131	(0)
Cd(OH)2	4.034e-20	4.039e-20	-19.394	-19.394	0.000	(0)
Cd2OH+3	1.025e-21	5.194e-22	-20.989	-21.284	-0.295	(0)
Cd(OH)3-	1.941e-28	1.800e-28	-27.712	-27.745	-0.033	(0)
Cd(OH)4-2	8.620e-38	6.372e-38	-37.065	-37.196	-0.131	(0)
Cl	8.379e-04					
Cl-	8.334e-04	7.723e-04	-3.079	-3.112	-0.033	18.10
NaCl	4.456e-06	4.461e-06	-5.351	-5.351	0.000	(0)
BaCl+	2.192e-08	2.033e-08	-7.659	-7.692	-0.033	(0)
CuCl2-	1.507e-08	1.397e-08	-7.822	-7.855	-0.033	(0)
ZnCl+	3.163e-09	2.932e-09	-8.500	-8.533	-0.033	-14.25
MnCl+	2.675e-09	2.484e-09	-8.573	-8.605	-0.032	-3.15
CdCl+	4.553e-10	4.222e-10	-9.342	-9.375	-0.033	5.80
FeCl+	3.284e-10	3.045e-10	-9.484	-9.516	-0.033	(0)
CuCl3-2	2.297e-11	1.707e-11	-10.639	-10.768	-0.129	(0)
PbCl+	2.153e-11	1.997e-11	-10.667	-10.700	-0.033	7.97
ZnCl2	2.365e-12	2.368e-12	-11.626	-11.626	0.000	102.75
ZnOHCl	1.455e-12	1.457e-12	-11.837	-11.837	0.000	(0)
CdCl2	1.356e-12	1.357e-12	-11.868	-11.867	0.000	23.14
MnCl2	8.366e-13	8.375e-13	-12.077	-12.077	0.000	86.34
CuCl+	5.206e-13	4.826e-13	-12.284	-12.316	-0.033	0.76
PbCl2	2.458e-14	2.461e-14	-13.609	-13.609	0.000	34.94
CdOHCl	6.864e-15	6.872e-15	-14.163	-14.163	0.000	(0)
ZnCl3-	2.208e-15	2.047e-15	-14.656	-14.689	-0.033	16.95
CdCl3-	7.094e-16	6.578e-16	-15.149	-15.182	-0.033	69.62
CuCl2	1.991e-16	1.994e-16	-15.701	-15.700	0.000	30.59
MnCl3-	1.919e-16	1.782e-16	-15.717	-15.749	-0.032	43.41
PbCl3-	1.625e-17	1.506e-17	-16.789	-16.822	-0.033	65.94
ZnCl4-2	1.063e-18	7.902e-19	-17.973	-18.102	-0.129	145.27
PbCl4-2	7.511e-21	5.552e-21	-20.124	-20.256	-0.131	101.43
FeCl+2	1.385e-21	1.030e-21	-20.859	-20.987	-0.129	(0)
CuCl3-	5.854e-22	5.427e-22	-21.233	-21.265	-0.033	(0)
FeCl2+	3.870e-24	3.594e-24	-23.412	-23.444	-0.032	(0)
CuCl4-2	2.802e-27	2.083e-27	-26.553	-26.681	-0.129	(0)
FeCl3	2.772e-28	2.776e-28	-27.557	-27.557	0.000	(0)
Cu(1)	9.509e-08					
Cu+	8.000e-08	7.399e-08	-7.097	-7.131	-0.034	(0)
CuCl2-	1.507e-08	1.397e-08	-7.822	-7.855	-0.033	(0)
CuCl3-2	2.297e-11	1.707e-11	-10.639	-10.768	-0.129	(0)
Cu(2)	6.064e-10					
Cu+2	3.161e-10	2.364e-10	-9.500	-9.626	-0.126	-26.48
CuHCO3+	2.826e-10	2.621e-10	-9.549	-9.582	-0.033	(0)
CuCO3	5.197e-12	5.203e-12	-11.284	-11.284	0.000	(0)
CuSO4	1.613e-12	1.615e-12	-11.792	-11.792	0.000	13.04
CuCl+	5.206e-13	4.826e-13	-12.284	-12.316	-0.033	0.76
CuF+	2.303e-13	2.136e-13	-12.638	-12.670	-0.033	(0)
CuOH+	1.013e-13	9.390e-14	-12.994	-13.027	-0.033	(0)
Cu(OH)2	7.784e-15	7.793e-15	-14.109	-14.108	0.000	(0)
CuCl2	1.991e-16	1.994e-16	-15.701	-15.700	0.000	30.59
Cu(CO3)2-2	3.632e-17	2.685e-17	-16.440	-16.571	-0.131	(0)
Cu2(OH)2+2	5.031e-21	3.719e-21	-20.298	-20.430	-0.131	(0)
CuCl3-	5.854e-22	5.427e-22	-21.233	-21.265	-0.033	(0)
Cu(OH)3-	2.011e-23	1.865e-23	-22.696	-22.729	-0.033	(0)
CuCl4-2	2.802e-27	2.083e-27	-26.553	-26.681	-0.129	(0)
Cu(OH)4-2	2.000e-31	1.478e-31	-30.699	-30.830	-0.131	(0)
F	6.107e-05					
F-	5.378e-05	4.982e-05	-4.269	-4.303	-0.033	-1.28
HF	1.862e-06	1.864e-06	-5.730	-5.730	0.000	12.48

MgF+	1.762e-06	1.635e-06	-5.754	-5.787	-0.033	-10.54
AlF2+	9.466e-07	8.795e-07	-6.024	-6.056	-0.032	(0)
AlF3	5.507e-07	5.513e-07	-6.259	-6.259	0.000	(0)
AlF+2	4.736e-08	3.529e-08	-7.325	-7.452	-0.128	(0)
NaF	2.771e-08	2.774e-08	-7.557	-7.557	0.000	7.25
AlF4-	1.178e-08	1.093e-08	-7.929	-7.961	-0.033	(0)
ZnF+	1.083e-09	1.004e-09	-8.965	-8.998	-0.033	(0)
HF2-	3.832e-10	3.553e-10	-9.417	-9.449	-0.033	22.08
MnF+	2.931e-10	2.721e-10	-9.533	-9.565	-0.032	(0)
BF(OH)3-	2.688e-10	2.492e-10	-9.571	-9.603	-0.033	(0)
FeF+	1.534e-10	1.423e-10	-9.814	-9.847	-0.033	(0)
BF2(OH)2-	3.614e-11	3.351e-11	-10.442	-10.475	-0.033	(0)
CdF+	3.876e-12	3.594e-12	-11.412	-11.444	-0.033	(0)
PbF+	6.261e-13	5.806e-13	-12.203	-12.236	-0.033	(0)
CuF+	2.303e-13	2.136e-13	-12.638	-12.670	-0.033	(0)
BF3OH-	5.003e-14	4.639e-14	-13.301	-13.334	-0.033	(0)
PbF2	5.898e-16	5.905e-16	-15.229	-15.229	0.000	(0)
CdF2	4.492e-16	4.497e-16	-15.348	-15.347	0.000	(0)
BF4-	2.558e-16	2.372e-16	-15.592	-15.625	-0.033	(0)
FeF2+	7.456e-18	6.923e-18	-17.127	-17.160	-0.032	(0)
FeF+2	4.717e-18	3.506e-18	-17.326	-17.455	-0.129	(0)
FeF3	5.453e-19	5.459e-19	-18.263	-18.263	0.000	(0)
PbF3-	2.298e-19	2.131e-19	-18.639	-18.671	-0.033	(0)
PbF4-2	6.873e-24	5.081e-24	-23.163	-23.294	-0.131	(0)
Fe(2)	4.522e-07					
Fe+2	3.819e-07	2.856e-07	-6.418	-6.544	-0.126	-22.04
FeHCO3+	6.812e-08	6.317e-08	-7.167	-7.199	-0.033	(0)
FeSO4	1.690e-09	1.692e-09	-8.772	-8.772	0.000	19.36
FeCl+	3.284e-10	3.045e-10	-9.484	-9.516	-0.033	(0)
FeF+	1.534e-10	1.423e-10	-9.814	-9.847	-0.033	(0)
FeCO3	2.805e-11	2.808e-11	-10.552	-10.552	0.000	(0)
FeH2PO4+	1.346e-11	1.250e-11	-10.871	-10.903	-0.032	(0)
FeOH+	3.758e-12	3.489e-12	-11.425	-11.457	-0.032	(0)
FeHSO4+	3.009e-13	2.790e-13	-12.522	-12.554	-0.033	(0)
FeHPO4	2.447e-13	2.450e-13	-12.611	-12.611	0.000	(0)
Fe(OH)2	1.141e-18	1.142e-18	-17.943	-17.942	0.000	(0)
Fe(OH)3-	1.809e-24	1.680e-24	-23.743	-23.775	-0.032	(0)
Fe(3)	1.851e-16					
Fe(OH)2+	1.564e-16	1.453e-16	-15.806	-15.838	-0.032	(0)
FeOH+2	1.508e-17	1.121e-17	-16.822	-16.951	-0.129	(0)
FeF2+	7.456e-18	6.923e-18	-17.127	-17.160	-0.032	(0)
FeF+2	4.717e-18	3.506e-18	-17.326	-17.455	-0.129	(0)
Fe(OH)3	7.310e-19	7.318e-19	-18.136	-18.136	0.000	(0)
FeF3	5.453e-19	5.459e-19	-18.263	-18.263	0.000	(0)
Fe+3	8.270e-20	4.466e-20	-19.082	-19.350	-0.268	(0)
FeSO4+	1.755e-20	1.629e-20	-19.756	-19.788	-0.032	(0)
FeH2PO4+2	1.409e-21	1.050e-21	-20.851	-20.979	-0.128	(0)
FeCl+2	1.385e-21	1.030e-21	-20.859	-20.987	-0.129	(0)
Fe(OH)4-	2.811e-23	2.612e-23	-22.551	-22.583	-0.032	(0)
Fe(SO4)2-	1.288e-23	1.194e-23	-22.890	-22.923	-0.033	(0)
FeCl2+	3.870e-24	3.594e-24	-23.412	-23.444	-0.032	(0)
FeHPO4+	2.756e-24	2.559e-24	-23.560	-23.592	-0.032	(0)
FeHSO4+2	1.483e-24	1.096e-24	-23.829	-23.960	-0.131	(0)
FeCl3	2.772e-28	2.776e-28	-27.557	-27.557	0.000	(0)
Fe2(OH)2+4	1.149e-32	3.433e-33	-31.940	-32.464	-0.525	(0)
Fe3(OH)4+5	0.000e+00	0.000e+00	-45.147	-45.967	-0.820	(0)
H(0)	3.207e-13					
H2	1.604e-13	1.605e-13	-12.795	-12.794	0.000	28.61
K	1.919e-04					
K+	1.918e-04	1.777e-04	-3.717	-3.750	-0.033	9.03
KSO4-	4.479e-08	4.162e-08	-7.349	-7.381	-0.032	34.13
KHPO4-	8.035e-14	7.466e-14	-13.095	-13.127	-0.032	38.18
Mg	6.887e-04					
Mg+2	6.691e-04	5.001e-04	-3.174	-3.301	-0.126	-21.69
MgHCO3+	1.394e-05	1.292e-05	-4.856	-4.889	-0.033	5.50
MgSO4	3.891e-06	3.895e-06	-5.410	-5.409	0.000	5.82
MgF+	1.762e-06	1.635e-06	-5.754	-5.787	-0.033	-10.54
MgCO3	1.942e-09	1.945e-09	-8.712	-8.711	0.000	-17.09

MgH2PO4+	1.521e-09	1.413e-09	-8.818	-8.850	-0.032	(0)
MgHPO4	7.923e-11	7.932e-11	-10.101	-10.101	0.000	(0)
MgOH+	7.494e-11	6.975e-11	-10.125	-10.156	-0.031	(0)
MgPO4-	7.967e-15	7.402e-15	-14.099	-14.131	-0.032	(0)
Mn(2)	1.231e-06					
Mn+2	1.056e-06	7.896e-07	-5.976	-6.103	-0.126	-20.26
MnHCO3+	1.676e-07	1.556e-07	-6.776	-6.808	-0.032	(0)
MnSO4	4.672e-09	4.677e-09	-8.331	-8.330	0.000	22.71
MnCl+	2.675e-09	2.484e-09	-8.573	-8.605	-0.032	-3.15
MnF+	2.931e-10	2.721e-10	-9.533	-9.565	-0.032	(0)
MnCO3	2.568e-10	2.571e-10	-9.590	-9.590	0.000	(0)
Mn(NO3)2	3.180e-12	3.184e-12	-11.498	-11.497	0.000	41.14
MnOH+	8.424e-13	7.822e-13	-12.074	-12.107	-0.032	(0)
MnCl2	8.366e-13	8.375e-13	-12.077	-12.077	0.000	86.34
MnCl3-	1.919e-16	1.782e-16	-15.717	-15.749	-0.032	43.41
Mn(OH)3-	8.446e-28	7.843e-28	-27.073	-27.106	-0.032	(0)
Mn(3)	7.153e-32					
Mn+3	7.153e-32	3.863e-32	-31.146	-31.413	-0.268	(0)
N(3)	1.428e-06					
NO2-	1.428e-06	1.322e-06	-5.845	-5.879	-0.034	24.98
N(5)	1.087e-03					
NO3-	1.087e-03	1.006e-03	-2.964	-2.997	-0.034	29.49
BaNO3+	1.149e-09	1.066e-09	-8.940	-8.972	-0.033	(0)
CdNO3+	1.579e-11	1.464e-11	-10.802	-10.834	-0.033	17.57
PbNO3+	1.052e-11	9.752e-12	-10.978	-11.011	-0.033	(0)
Mn(NO3)2	3.180e-12	3.184e-12	-11.498	-11.497	0.000	41.14
Na	1.049e-03					
Na+	1.043e-03	9.677e-04	-2.982	-3.014	-0.032	-1.44
NaCl	4.456e-06	4.461e-06	-5.351	-5.351	0.000	(0)
NaHCO3	1.205e-06	1.206e-06	-5.919	-5.919	0.000	1.80
NaSO4-	1.747e-07	1.623e-07	-6.758	-6.790	-0.032	14.08
NaF	2.771e-08	2.774e-08	-7.557	-7.557	0.000	7.25
NaCO3-	7.817e-11	7.248e-11	-10.107	-10.140	-0.033	-1.01
NaHPO4-	4.375e-13	4.065e-13	-12.359	-12.391	-0.032	33.81
NaOH	3.778e-23	3.782e-23	-22.423	-22.422	0.000	(0)
O(0)	0.000e+00					
O2	0.000e+00	0.000e+00	-66.913	-66.913	0.000	30.37
P	9.688e-08					
H2PO4-	9.401e-08	8.735e-08	-7.027	-7.059	-0.032	33.26
MgH2PO4+	1.521e-09	1.413e-09	-8.818	-8.850	-0.032	(0)
CaH2PO4+	6.095e-10	5.663e-10	-9.215	-9.247	-0.032	(0)
H3PO4	3.212e-10	3.216e-10	-9.493	-9.493	0.000	47.39
HPO4-2	2.898e-10	2.155e-10	-9.538	-9.667	-0.129	6.87
MgHPO4	7.923e-11	7.932e-11	-10.101	-10.101	0.000	(0)
CaHPO4	2.990e-11	2.994e-11	-10.524	-10.524	0.000	(0)
FeH2PO4+	1.346e-11	1.250e-11	-10.871	-10.903	-0.032	(0)
NaHPO4-	4.375e-13	4.065e-13	-12.359	-12.391	-0.032	33.81
FeHPO4	2.447e-13	2.450e-13	-12.611	-12.611	0.000	(0)
KHPO4-	8.035e-14	7.466e-14	-13.095	-13.127	-0.032	38.18
MgPO4-	7.967e-15	7.402e-15	-14.099	-14.131	-0.032	(0)
CaPO4-	3.014e-15	2.800e-15	-14.521	-14.553	-0.032	(0)
PO4-3	7.587e-18	3.838e-18	-17.120	-17.416	-0.296	-22.88
FeH2PO4+2	1.409e-21	1.050e-21	-20.851	-20.979	-0.128	(0)
FeHPO4+	2.756e-24	2.559e-24	-23.560	-23.592	-0.032	(0)
Pb	2.221e-09					
PbHCO3+	1.242e-09	1.151e-09	-8.906	-8.939	-0.033	(0)
Pb+2	8.865e-10	6.554e-10	-9.052	-9.184	-0.131	-15.41
PbCO3	4.662e-11	4.668e-11	-10.331	-10.331	0.000	(0)
PbCl+	2.153e-11	1.997e-11	-10.667	-10.700	-0.033	7.97
PbSO4	1.235e-11	1.236e-11	-10.908	-10.908	0.000	(0)
PbNO3+	1.052e-11	9.752e-12	-10.978	-11.011	-0.033	(0)
PbF+	6.261e-13	5.806e-13	-12.203	-12.236	-0.033	(0)
PbOH+	5.474e-13	5.076e-13	-12.262	-12.294	-0.033	(0)
PbBr+	2.301e-13	2.133e-13	-12.638	-12.671	-0.033	(0)
PbCl2	2.458e-14	2.461e-14	-13.609	-13.609	0.000	34.94
Pb(SO4)2-2	2.944e-15	2.176e-15	-14.531	-14.662	-0.131	(0)
Pb(CO3)2-2	6.501e-16	4.806e-16	-15.187	-15.318	-0.131	(0)
PbF2	5.898e-16	5.905e-16	-15.229	-15.229	0.000	(0)

PbCl3-	1.625e-17	1.506e-17	-16.789	-16.822	-0.033	65.94
Pb(OH)2	7.835e-18	7.844e-18	-17.106	-17.105	0.000	(0)
PbBr2	5.576e-19	5.583e-19	-18.254	-18.253	0.000	(0)
PbF3-	2.298e-19	2.131e-19	-18.639	-18.671	-0.033	(0)
Pb2OH+3	1.470e-20	7.447e-21	-19.833	-20.128	-0.295	(0)
PbCl4-2	7.511e-21	5.552e-21	-20.124	-20.256	-0.131	101.43
PbF4-2	6.873e-24	5.081e-24	-23.163	-23.294	-0.131	(0)
Pb(OH)3-	3.858e-24	3.577e-24	-23.414	-23.446	-0.033	(0)
Pb(OH)4-2	4.403e-31	3.255e-31	-30.356	-30.487	-0.131	(0)
Pb3(OH)4+2	1.182e-33	8.738e-34	-32.927	-33.059	-0.131	(0)
S(6)	5.102e-05					
SO4-2	4.515e-05	3.354e-05	-4.345	-4.474	-0.129	14.61
MgSO4	3.891e-06	3.895e-06	-5.410	-5.409	0.000	5.82
CaSO4	1.516e-06	1.518e-06	-5.819	-5.819	0.000	7.49
NaSO4-	1.747e-07	1.623e-07	-6.758	-6.790	-0.032	14.08
BaSO4	1.413e-07	1.415e-07	-6.850	-6.849	0.000	(0)
HSO4-	8.764e-08	8.126e-08	-7.057	-7.090	-0.033	40.29
KSO4-	4.479e-08	4.162e-08	-7.349	-7.381	-0.032	34.13
ZnSO4	1.123e-08	1.124e-08	-7.950	-7.949	0.000	21.77
MnSO4	4.672e-09	4.677e-09	-8.331	-8.330	0.000	22.71
FeSO4	1.690e-09	1.692e-09	-8.772	-8.772	0.000	19.36
CaHSO4+	2.689e-10	2.493e-10	-9.570	-9.603	-0.033	(0)
CdSO4	5.525e-11	5.532e-11	-10.258	-10.257	0.000	78.23
PbSO4	1.235e-11	1.236e-11	-10.908	-10.908	0.000	(0)
AlSO4+	8.079e-12	7.496e-12	-11.093	-11.125	-0.033	(0)
Zn(SO4)2-2	4.159e-12	3.074e-12	-11.381	-11.512	-0.131	-13.27
CuSO4	1.613e-12	1.615e-12	-11.792	-11.792	0.000	13.04
FeHSO4+	3.009e-13	2.790e-13	-12.522	-12.554	-0.033	(0)
Cd(SO4)2-2	2.758e-14	2.039e-14	-13.559	-13.691	-0.131	-105.77
Al(SO4)2-	8.555e-15	7.938e-15	-14.068	-14.100	-0.033	(0)
Pb(SO4)2-2	2.944e-15	2.176e-15	-14.531	-14.662	-0.131	(0)
AlHSO4+2	2.251e-17	1.664e-17	-16.648	-16.779	-0.131	(0)
FeSO4+	1.755e-20	1.629e-20	-19.756	-19.788	-0.032	(0)
Fe(SO4)2-	1.288e-23	1.194e-23	-22.890	-22.923	-0.033	(0)
FeHSO4+2	1.483e-24	1.096e-24	-23.829	-23.960	-0.131	(0)
Zn	2.376e-06					
Zn+2	1.929e-06	1.434e-06	-5.715	-5.844	-0.129	-25.21
ZnHCO3+	4.306e-07	3.992e-07	-6.366	-6.399	-0.033	(0)
ZnSO4	1.123e-08	1.124e-08	-7.950	-7.949	0.000	21.77
ZnCl+	3.163e-09	2.932e-09	-8.500	-8.533	-0.033	-14.25
ZnCO3	1.171e-09	1.173e-09	-8.931	-8.931	0.000	(0)
ZnF+	1.083e-09	1.004e-09	-8.965	-8.998	-0.033	(0)
ZnOH+	6.548e-11	6.072e-11	-10.184	-10.217	-0.033	(0)
Zn(SO4)2-2	4.159e-12	3.074e-12	-11.381	-11.512	-0.131	-13.27
ZnCl2	2.365e-12	2.368e-12	-11.626	-11.626	0.000	102.75
ZnBr+	2.262e-12	2.097e-12	-11.646	-11.678	-0.033	(0)
ZnOHCl	1.455e-12	1.457e-12	-11.837	-11.837	0.000	(0)
Zn(CO3)2-2	1.390e-13	1.027e-13	-12.857	-12.988	-0.131	(0)
Zn(OH)2	2.845e-14	2.848e-14	-13.546	-13.545	0.000	(0)
ZnCl3-	2.208e-15	2.047e-15	-14.656	-14.689	-0.033	16.95
ZnBr2	4.638e-18	4.644e-18	-17.334	-17.333	0.000	(0)
ZnCl4-2	1.063e-18	7.902e-19	-17.973	-18.102	-0.129	145.27
Zn(OH)3-	3.858e-21	3.577e-21	-20.414	-20.446	-0.033	(0)
Zn(OH)4-2	3.046e-29	2.252e-29	-28.516	-28.647	-0.131	(0)

----------Distribution of alkalinity----------

Total alkalinity (eq/kgw) = 2.375e-03

Species	Alkalinity	Molality	Alk/Mol
HCO3-	2.381e-03	2.381e-03	1.00
H+	-2.690e-05	2.690e-05	-1.00
MgHCO3+	1.394e-05	1.394e-05	1.00
CaHCO3+	7.700e-06	7.700e-06	1.00
HF	-1.862e-06	1.862e-06	-1.00
NaHCO3	1.205e-06	1.205e-06	1.00
ZnHCO3+	4.306e-07	4.306e-07	1.00

BaHCO3+	1.902e-07	1.902e-07	1.00
MnHCO3+	1.676e-07	1.676e-07	1.00
HSO4-	-8.764e-08	8.764e-08	-1.00
FeHCO3+	6.812e-08	6.812e-08	1.00
CO3-2	1.100e-08	5.500e-09	2.00
MgCO3	3.885e-09	1.942e-09	2.00
CaCO3	3.484e-09	1.742e-09	2.00
ZnCO3	2.342e-09	1.171e-09	2.00
PbHCO3+	1.242e-09	1.242e-09	1.00
MnCO3	5.135e-10	2.568e-10	2.00
CdHCO3+	4.323e-10	4.323e-10	1.00
OH-	4.219e-10	4.219e-10	1.00
HF2-	-3.832e-10	3.832e-10	-1.00
H3PO4	-3.212e-10	3.212e-10	-1.00
H2BO3-	3.096e-10	3.096e-10	1.00
HPO4-2	2.898e-10	2.898e-10	1.00
CuHCO3+	2.826e-10	2.826e-10	1.00
CaHSO4+	-2.689e-10	2.689e-10	-1.00
NaCO3-	1.563e-10	7.817e-11	2.00
PbCO3	9.325e-11	4.662e-11	2.00
MgHPO4	7.923e-11	7.923e-11	1.00
MgOH+	7.494e-11	7.494e-11	1.00
ZnOH+	6.548e-11	6.548e-11	1.00
FeCO3	5.610e-11	2.805e-11	2.00
AlOH+2	3.670e-11	3.670e-11	1.00
BF2(OH)2-	-3.614e-11	3.614e-11	-1.00
BaCO3	3.533e-11	1.766e-11	2.00
CaHPO4	2.990e-11	2.990e-11	1.00
Al(OH)2+	1.774e-11	8.872e-12	2.00
CuCO3	1.039e-11	5.197e-12	2.00
FeOH+	3.758e-12	3.758e-12	1.00
CaOH+	1.814e-12	1.814e-12	1.00
ZnOHCl	1.455e-12	1.455e-12	1.00
MnOH+	8.424e-13	8.424e-13	1.00
Zn(CO3)2-2	5.559e-13	1.390e-13	4.00
PbOH+	5.474e-13	5.474e-13	1.00
NaHPO4-	4.375e-13	4.375e-13	1.00
FeHSO4+	-3.009e-13	3.009e-13	-1.00
FeHPO4	2.447e-13	2.447e-13	1.00
Al(OH)3	1.407e-13	4.689e-14	3.00
CuOH+	1.013e-13	1.013e-13	1.00
BF3OH-	-1.001e-13	5.003e-14	-2.00
KHPO4-	8.035e-14	8.035e-14	1.00
Zn(OH)2	5.689e-14	2.845e-14	2.00
CdCO3	3.727e-14	1.864e-14	2.00
CdOH+	1.987e-14	1.987e-14	1.00
MgPO4-	1.593e-14	7.967e-15	2.00
Cu(OH)2	1.557e-14	7.784e-15	2.00
Al(OH)4-	1.508e-14	3.769e-15	4.00
BaOH+	1.220e-14	1.220e-14	1.00
CdOHCl	6.864e-15	6.864e-15	1.00
CaPO4-	6.028e-15	3.014e-15	2.00
Pb(CO3)2-2	2.600e-15	6.501e-16	4.00
BF4-	-7.673e-16	2.558e-16	-3.00
Cu(CO3)2-2	1.453e-16	3.632e-17	4.00
AlHSO4+2	-2.251e-17	2.251e-17	-1.00
Pb(OH)2	1.567e-17	7.835e-18	2.00
PO4-3	1.517e-17	7.587e-18	2.00
FeOH+2	-1.508e-17	1.508e-17	-1.00
FeF2+	-1.491e-17	7.456e-18	-2.00
FeF+2	-9.434e-18	4.717e-18	-2.00
Fe(OH)2	2.282e-18	1.141e-18	2.00
Cd(CO3)2-2	1.308e-18	3.271e-19	4.00
FeF3	-1.091e-18	5.453e-19	-2.00
Fe(OH)3	7.310e-19	7.310e-19	1.00
Fe+3	-1.654e-19	8.270e-20	-2.00
Cd(OH)2	8.068e-20	4.034e-20	2.00
FeSO4+	-3.509e-20	1.755e-20	-2.00

Pb2OH+3	1.470e-20	1.470e-20	1.00
Zn(OH)3-	1.157e-20	3.858e-21	3.00
Cu2(OH)2+2	1.006e-20	5.031e-21	2.00
FeH2PO4+2	-2.818e-21	1.409e-21	-2.00
FeCl+2	-2.770e-21	1.385e-21	-2.00
Cd2OH+3	1.025e-21	1.025e-21	1.00
Cu(OH)3-	6.034e-23	2.011e-23	3.00
Fe(OH)4-	5.623e-23	2.811e-23	2.00
NaOH	3.778e-23	3.778e-23	1.00
Fe(SO4)2-	-2.575e-23	1.288e-23	-2.00
Pb(OH)3-	1.157e-23	3.858e-24	3.00
FeCl2+	-7.741e-24	3.870e-24	-2.00
Fe(OH)3-	5.427e-24	1.809e-24	3.00
FeHSO4+2	-4.448e-24	1.483e-24	-3.00
FeHPO4+	-2.756e-24	2.756e-24	-1.00
Mn(OH)3-	2.534e-27	8.446e-28	3.00
Cd(OH)3-	5.824e-28	1.941e-28	3.00
FeCl3	-5.545e-28	2.772e-28	-2.00
Zn(OH)4-2	1.219e-28	3.046e-29	4.00
Pb(OH)4-2	1.761e-30	4.403e-31	4.00
Cu(OH)4-2	7.998e-31	2.000e-31	4.00
Fe2(OH)2+4	-2.299e-32	1.149e-32	-2.00
Pb3(OH)4+2	4.728e-33	1.182e-33	4.00
Cd(OH)4-2	3.448e-37	8.620e-38	4.00
Fe3(OH)4+5	-0.000e+00	0.000e+00	-2.00

-----------------------------Saturation indices-------------------------------

Phase	SI**	log IAP	log K(297 K, 1 atm)	
Al(OH)3(a)	-7.18	3.65	10.82	Al(OH)3
Alunite	-14.20	-15.55	-1.35	KAl3(SO4)2(OH)6
Anglesite	-5.87	-13.66	-7.79	PbSO4
Anhydrite	-3.79	-8.07	-4.27	CaSO4
Aragonite	-3.65	-11.98	-8.33	CaCO3
BaCl2	-13.53	-11.30	2.23	BaCl2
BaCl2:2H2O	-11.51	-11.30	0.20	BaCl2:2H2O
BaCl2:H2O	-12.12	-11.30	0.82	BaCl2:H2O
Barite	0.30	-9.55	-9.85	BaSO4
Calcite	-3.50	-11.98	-8.48	CaCO3
Cd(OH)2	-12.69	0.96	13.65	Cd(OH)2
CdSO4	-12.63	-12.72	-0.09	CdSO4
Cerussite	-4.44	-17.57	-13.13	PbCO3
CO2(g)	0.56	-0.90	-1.46	CO2
Dolomite	-6.59	-23.67	-17.08	CaMg(CO3)2
Fe(OH)3(a)	-10.44	-5.55	4.89	Fe(OH)3
Fluorite	-1.59	-12.20	-10.60	CaF2
Gibbsite	-4.48	3.65	8.13	Al(OH)3
Goethite	-4.57	-5.55	-0.99	FeOOH
Gypsum	-3.49	-8.07	-4.58	CaSO4:2H2O
H2(g)	-9.69	-12.79	-3.10	H2
H2O(g)	-1.51	-0.00	1.51	H2O
Halite	-7.70	-6.13	1.57	NaCl
Hausmannite	-42.19	18.93	61.12	Mn3O4
Hematite	-7.12	-11.10	-3.98	Fe2O3
Hydroxyapatite	-25.18	-28.57	-3.39	Ca5(PO4)3OH
Jarosite-K	-33.97	-43.16	-9.18	KFe3(SO4)2(OH)6
Manganite	-17.42	7.92	25.34	MnOOH
Melanterite	-8.81	-11.03	-2.21	FeSO4:7H2O
O2(g)	-64.02	-66.91	-2.89	O2
Otavite	-4.53	-16.63	-12.10	CdCO3
Pb(OH)2	-8.15	0.01	8.16	Pb(OH)2
Pyrochroite	-12.10	3.10	15.20	Mn(OH)2
Pyrolusite	-28.70	12.74	41.44	MnO2:H2O
Rhodochrosite	-3.36	-14.49	-11.13	MnCO3
Siderite	-4.04	-14.93	-10.89	FeCO3
Smithsonite	-4.23	-14.23	-10.00	ZnCO3
Sylvite	-7.76	-6.86	0.90	KCl

Vivianite	-18.47	-54.47	-36.00	Fe3(PO4)2:8H2O
Witherite	-4.90	-13.46	-8.56	BaCO3
Zn(OH)2(e)	-8.15	3.35	11.50	Zn(OH)2

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
For ideal gases, phi = 1.

Initial solution 28.

-----------------------------Solution composition------------------------------

Elements	Molality	Moles
Al	9.516e-07	9.516e-07
Alkalinity	2.064e-03	2.064e-03
B	1.261e-05	1.261e-05
Ba	1.682e-05	1.682e-05
Br	5.633e-06	5.633e-06
Ca	5.066e-04	5.066e-04
Cd	9.165e-09	9.165e-09
Cl	4.683e-04	4.683e-04
Cu	4.140e-08	4.140e-08
F	5.738e-05	5.738e-05
Fe	5.727e-07	5.727e-07
K	1.151e-04	1.151e-04
Mg	4.986e-04	4.986e-04
Mn	2.148e-07	2.148e-07
N(3)	7.141e-07	7.141e-07
N(5)	6.834e-04	6.834e-04
Na	7.178e-04	7.178e-04
P	2.906e-07	2.906e-07
Pb	3.427e-09	3.427e-09
S(6)	3.644e-05	3.644e-05
Zn	1.812e-06	1.812e-06

----------------------------Description of solution----------------------------

pH	= 5.000
pe	= 0.253
Specific Conductance (µS/cm, 25°C)	= 320
Density (g/cm³)	= 0.99763
Volume (L)	= 1.00453
Activity of water	= 0.999
Ionic strength (mol/kgw)	= 4.128e-03
Mass of water (kg)	= 1.000e+00
Total carbon (mol/kg)	= 4.529e-02
Total CO2 (mol/kg)	= 4.529e-02
Temperature (°C)	= 25.06
Electrical balance (eq)	= -4.676e-04
Percent error, 100*(Cat-|An|)/(Cat+|An|)	= -7.55
Iterations	= 10 (297 overall)
Total H	= 1.110146e+02
Total O	= 5.560111e+01

---------------------------------Redox couples---------------------------------

Redox couple	pe	Eh (volts)
N(3)/N(5)	10.7724	0.6374

----------------------------Distribution of species----------------------------

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma	mole V cm³/mol
H+	1.065e-05	1.000e-05	-4.972	-5.000	-0.028	0.00
OH-	1.090e-09	1.016e-09	-8.963	-8.993	-0.031	-4.07
H2O	5.551e+01	9.992e-01	1.744	-0.000	0.000	18.07

Al	9.516e-07					
AlF2+	5.789e-07	5.410e-07	-6.237	-6.267	-0.029	(0)
AlF3	3.368e-07	3.371e-07	-6.473	-6.472	0.000	(0)
AlF+2	2.859e-08	2.180e-08	-7.544	-7.661	-0.118	(0)
AlF4-	7.115e-09	6.641e-09	-8.148	-8.178	-0.030	(0)
Al+3	7.794e-11	4.404e-11	-10.108	-10.356	-0.248	-42.08
AlOH+2	5.754e-11	4.388e-11	-10.240	-10.358	-0.118	-27.66
Al(OH)2+	3.697e-11	3.455e-11	-10.432	-10.462	-0.029	(0)
AlSO4+	3.675e-12	3.430e-12	-11.435	-11.465	-0.030	(0)
Al(OH)3	5.104e-13	5.108e-13	-12.292	-12.292	0.000	(0)
Al(OH)4-	1.032e-13	9.628e-14	-12.987	-13.016	-0.030	(0)
Al(SO4)2-	2.861e-15	2.670e-15	-14.544	-14.573	-0.030	(0)
AlHSO4+2	4.018e-18	3.043e-18	-17.396	-17.517	-0.121	(0)
B	1.261e-05					
H3BO3	1.261e-05	1.262e-05	-4.899	-4.899	0.000	39.24
H2BO3-	7.794e-10	7.271e-10	-9.108	-9.138	-0.030	(0)
BF(OH)3-	2.667e-10	2.488e-10	-9.574	-9.604	-0.030	(0)
BF2(OH)2-	1.416e-11	1.321e-11	-10.849	-10.879	-0.030	(0)
BF3OH-	7.679e-15	7.164e-15	-14.115	-14.145	-0.030	(0)
BF4-	1.549e-17	1.445e-17	-16.810	-16.840	-0.030	(0)
Ba	1.682e-05					
Ba+2	1.640e-05	1.244e-05	-4.785	-4.905	-0.120	-12.64
BaHCO3+	2.459e-07	2.294e-07	-6.609	-6.639	-0.030	(0)
BaSO4	1.533e-07	1.534e-07	-6.815	-6.814	0.000	(0)
BaCl+	1.826e-08	1.703e-08	-7.739	-7.769	-0.030	(0)
BaNO3+	1.068e-09	9.966e-10	-8.971	-9.001	-0.030	(0)
BaCO3	5.796e-11	5.801e-11	-10.237	-10.236	0.000	-10.70
BaOH+	4.508e-14	4.211e-14	-13.346	-13.376	-0.030	(0)
Br	5.633e-06					
Br-	5.633e-06	5.247e-06	-5.249	-5.280	-0.031	24.59
CdBr+	5.292e-12	4.937e-12	-11.276	-11.307	-0.030	(0)
ZnBr+	1.693e-12	1.580e-12	-11.771	-11.801	-0.030	(0)
PbBr+	3.598e-13	3.356e-13	-12.444	-12.474	-0.030	(0)
CdBr2	1.390e-16	1.392e-16	-15.857	-15.856	0.000	(0)
ZnBr2	3.296e-18	3.299e-18	-17.482	-17.482	0.000	(0)
PbBr2	8.221e-19	8.229e-19	-18.085	-18.085	0.000	(0)
C(4)	4.529e-02					
CO2	4.315e-02	4.319e-02	-1.365	-1.365	0.000	34.44
HCO3-	2.055e-03	1.921e-03	-2.687	-2.717	-0.029	24.73
(CO2)2	3.427e-05	3.430e-05	-4.465	-4.465	0.000	68.87
CaHCO3+	9.896e-06	9.255e-06	-5.005	-5.034	-0.029	9.70
MgHCO3+	8.957e-06	8.355e-06	-5.048	-5.078	-0.030	5.51
NaHCO3	7.203e-07	7.210e-07	-6.142	-6.142	0.000	1.80
ZnHCO3+	2.966e-07	2.767e-07	-6.528	-6.558	-0.030	(0)
BaHCO3+	2.459e-07	2.294e-07	-6.609	-6.639	-0.030	(0)
FeHCO3+	7.762e-08	7.242e-08	-7.110	-7.140	-0.030	(0)
MnHCO3+	2.628e-08	2.455e-08	-7.580	-7.610	-0.030	(0)
CO3-2	1.182e-08	9.018e-09	-7.927	-8.045	-0.118	-5.14
CaCO3	5.718e-09	5.723e-09	-8.243	-8.242	0.000	-14.60
MgCO3	3.199e-09	3.202e-09	-8.495	-8.495	0.000	-17.09
ZnCO3	2.057e-09	2.059e-09	-8.687	-8.686	0.000	(0)
PbHCO3+	1.775e-09	1.656e-09	-8.751	-8.781	-0.030	(0)
CdHCO3+	4.143e-10	3.865e-10	-9.383	-9.413	-0.030	(0)
PbCO3	1.699e-10	1.701e-10	-9.770	-9.769	0.000	(0)
CuHCO3+	1.270e-10	1.185e-10	-9.896	-9.926	-0.030	(0)
NaCO3-	1.206e-10	1.125e-10	-9.919	-9.949	-0.030	-0.98
MnCO3	1.026e-10	1.027e-10	-9.989	-9.988	0.000	(0)
FeCO3	8.149e-11	8.156e-11	-10.089	-10.088	0.000	(0)
BaCO3	5.796e-11	5.801e-11	-10.237	-10.236	0.000	-10.70
CuCO3	5.956e-12	5.962e-12	-11.225	-11.225	0.000	(0)
Zn(CO3)2-2	5.242e-13	3.971e-13	-12.280	-12.401	-0.121	(0)
CdCO3	4.554e-14	4.559e-14	-13.342	-13.341	0.000	(0)
Pb(CO3)2-2	5.087e-15	3.853e-15	-14.294	-14.414	-0.121	(0)
Cu(CO3)2-2	8.936e-17	6.769e-17	-16.049	-16.170	-0.121	(0)
Cd(CO3)2-2	1.716e-18	1.300e-18	-17.765	-17.886	-0.121	(0)
Ca	5.066e-04					
Ca+2	4.950e-04	3.773e-04	-3.305	-3.423	-0.118	-18.03
CaHCO3+	9.896e-06	9.255e-06	-5.005	-5.034	-0.029	9.70

CaSO4	1.651e-06	1.652e-06	-5.782	-5.782	0.000	7.50
CaCO3	5.718e-09	5.723e-09	-8.243	-8.242	0.000	-14.60
CaH2PO4+	2.717e-09	2.539e-09	-8.566	-8.595	-0.029	(0)
CaHPO4	3.376e-10	3.379e-10	-9.472	-9.471	0.000	(0)
CaHSO4+	1.165e-10	1.087e-10	-9.934	-9.964	-0.030	(0)
CaOH+	6.707e-12	6.257e-12	-11.173	-11.204	-0.030	(0)
CaPO4-	8.565e-14	8.004e-14	-13.067	-13.097	-0.029	(0)
Cd	9.165e-09					
Cd+2	8.402e-09	6.364e-09	-8.076	-8.196	-0.121	-18.64
CdHCO3+	4.143e-10	3.865e-10	-9.383	-9.413	-0.030	(0)
CdCl+	2.835e-10	2.644e-10	-9.548	-9.578	-0.030	5.90
CdSO4	4.514e-11	4.518e-11	-10.345	-10.345	0.000	78.02
CdNO3+	1.089e-11	1.016e-11	-10.963	-10.993	-0.030	17.55
CdBr+	5.292e-12	4.937e-12	-11.276	-11.307	-0.030	(0)
CdF+	4.250e-12	3.965e-12	-11.372	-11.402	-0.030	(0)
CdCl2	4.792e-13	4.797e-13	-12.319	-12.319	0.000	23.14
CdOH+	5.694e-14	5.312e-14	-13.245	-13.275	-0.030	(0)
CdCO3	4.554e-14	4.559e-14	-13.342	-13.341	0.000	(0)
Cd(SO4)2-2	1.609e-14	1.219e-14	-13.793	-13.914	-0.121	-105.51
CdOHCl	1.092e-14	1.093e-14	-13.962	-13.961	0.000	(0)
CdF2	4.924e-16	4.929e-16	-15.308	-15.307	0.000	(0)
CdCl3-	1.413e-16	1.318e-16	-15.850	-15.880	-0.030	69.31
CdBr2	1.390e-16	1.392e-16	-15.857	-15.856	0.000	(0)
Cd(CO3)2-2	1.716e-18	1.300e-18	-17.765	-17.886	-0.121	(0)
Cd(OH)2	2.835e-19	2.838e-19	-18.547	-18.547	0.000	(0)
Cd2OH+3	3.091e-21	1.654e-21	-20.510	-20.781	-0.271	(0)
Cd(OH)3-	3.410e-27	3.182e-27	-26.467	-26.497	-0.030	(0)
Cd(OH)4-2	3.740e-36	2.833e-36	-35.427	-35.548	-0.121	(0)
Cl	4.683e-04					
Cl-	4.666e-04	4.350e-04	-3.331	-3.361	-0.030	18.11
NaCl	1.738e-06	1.739e-06	-5.760	-5.760	0.000	(0)
BaCl+	1.826e-08	1.703e-08	-7.739	-7.769	-0.030	(0)
CuCl2-	2.316e-09	2.160e-09	-8.635	-8.665	-0.030	(0)
ZnCl+	1.441e-09	1.344e-09	-8.841	-8.872	-0.030	-13.83
CdCl+	2.835e-10	2.644e-10	-9.548	-9.578	-0.030	5.90
MnCl+	2.721e-10	2.542e-10	-9.565	-9.595	-0.030	-3.05
FeCl+	2.427e-10	2.264e-10	-9.615	-9.645	-0.030	(0)
PbCl+	2.018e-11	1.882e-11	-10.695	-10.725	-0.030	7.98
CuCl3-2	1.958e-12	1.490e-12	-11.708	-11.827	-0.119	(0)
ZnOHCl	1.646e-12	1.647e-12	-11.784	-11.783	0.000	(0)
ZnCl2	6.117e-13	6.123e-13	-12.213	-12.213	0.000	101.91
CdCl2	4.792e-13	4.797e-13	-12.319	-12.319	0.000	23.14
CuCl+	1.550e-13	1.446e-13	-12.810	-12.840	-0.030	0.65
MnCl2	4.822e-14	4.827e-14	-13.317	-13.316	0.000	85.81
PbCl2	1.295e-14	1.296e-14	-13.888	-13.887	0.000	34.98
CdOHCl	1.092e-14	1.093e-14	-13.962	-13.961	0.000	(0)
ZnCl3-	3.205e-16	2.990e-16	-15.494	-15.524	-0.030	16.99
CdCl3-	1.413e-16	1.318e-16	-15.850	-15.880	-0.030	69.31
CuCl2	3.376e-17	3.380e-17	-16.472	-16.471	0.000	31.09
MnCl3-	6.192e-18	5.784e-18	-17.208	-17.238	-0.030	43.38
PbCl3-	4.804e-18	4.482e-18	-17.318	-17.349	-0.030	65.99
ZnCl4-2	8.569e-20	6.522e-20	-19.067	-19.186	-0.119	145.30
PbCl4-2	1.233e-21	9.337e-22	-20.909	-21.030	-0.121	101.48
FeCl+2	1.119e-21	8.515e-22	-20.951	-21.070	-0.119	(0)
CuCl3-	5.599e-23	5.222e-23	-22.252	-22.282	-0.030	(0)
FeCl2+	1.768e-24	1.651e-24	-23.752	-23.782	-0.030	(0)
CuCl4-2	1.498e-28	1.140e-28	-27.824	-27.943	-0.119	(0)
FeCl3	7.178e-29	7.185e-29	-28.144	-28.144	0.000	(0)
Cu(1)	4.110e-08					
Cu+	3.878e-08	3.610e-08	-7.411	-7.442	-0.031	(0)
CuCl2-	2.316e-09	2.160e-09	-8.635	-8.665	-0.030	(0)
CuCl3-2	1.958e-12	1.490e-12	-11.708	-11.827	-0.119	(0)
Cu(2)	2.949e-10					
Cu+2	1.609e-10	1.231e-10	-9.793	-9.910	-0.116	-26.51
CuHCO3+	1.270e-10	1.185e-10	-9.896	-9.926	-0.030	(0)
CuCO3	5.956e-12	5.962e-12	-11.225	-11.225	0.000	(0)
CuSO4	6.182e-13	6.188e-13	-12.209	-12.208	0.000	13.10
CuCl+	1.550e-13	1.446e-13	-12.810	-12.840	-0.030	0.65

CuOH+	1.319e-13	1.230e-13	-12.880	-12.910	-0.030	(0)
CuF+	1.189e-13	1.109e-13	-12.925	-12.955	-0.030	(0)
Cu(OH)2	2.565e-14	2.568e-14	-13.591	-13.590	0.000	(0)
Cu(CO3)2-2	8.936e-17	6.769e-17	-16.049	-16.170	-0.121	(0)
CuCl2	3.376e-17	3.380e-17	-16.472	-16.471	0.000	31.09
Cu2(OH)2+2	8.792e-21	6.660e-21	-20.056	-20.177	-0.121	(0)
Cu(OH)3-	1.657e-22	1.546e-22	-21.781	-21.811	-0.030	(0)
CuCl3-	5.599e-23	5.222e-23	-22.252	-22.282	-0.030	(0)
CuCl4-2	1.498e-28	1.140e-28	-27.824	-27.943	-0.119	(0)
Cu(OH)4-2	4.069e-30	3.082e-30	-29.391	-29.511	-0.121	(0)
F	5.738e-05					
F-	5.309e-05	4.949e-05	-4.275	-4.305	-0.031	-1.28
MgF+	1.303e-06	1.217e-06	-5.885	-5.915	-0.030	-10.55
HF	7.423e-07	7.430e-07	-6.129	-6.129	0.000	12.50
AlF2+	5.789e-07	5.410e-07	-6.237	-6.267	-0.029	(0)
AlF3	3.368e-07	3.371e-07	-6.473	-6.472	0.000	(0)
AlF+2	2.859e-08	2.180e-08	-7.544	-7.661	-0.118	(0)
NaF	1.900e-08	1.902e-08	-7.721	-7.721	0.000	7.26
AlF4-	7.115e-09	6.641e-09	-8.148	-8.178	-0.030	(0)
ZnF+	8.583e-10	8.007e-10	-9.066	-9.097	-0.030	(0)
BF(OH)3-	2.667e-10	2.488e-10	-9.574	-9.604	-0.030	(0)
FeF+	2.000e-10	1.866e-10	-9.699	-9.729	-0.030	(0)
HF2-	1.513e-10	1.412e-10	-9.820	-9.850	-0.030	22.09
MnF+	5.257e-11	4.911e-11	-10.279	-10.309	-0.030	(0)
BF2(OH)2-	1.416e-11	1.321e-11	-10.849	-10.879	-0.030	(0)
CdF+	4.250e-12	3.965e-12	-11.372	-11.402	-0.030	(0)
PbF+	1.024e-12	9.551e-13	-11.990	-12.020	-0.030	(0)
CuF+	1.189e-13	1.109e-13	-12.925	-12.955	-0.030	(0)
BF3OH-	7.679e-15	7.164e-15	-14.115	-14.145	-0.030	(0)
PbF2	9.642e-16	9.651e-16	-15.016	-15.015	0.000	(0)
CdF2	4.924e-16	4.929e-16	-15.308	-15.307	0.000	(0)
BF4-	1.549e-17	1.445e-17	-16.810	-16.840	-0.030	(0)
FeF2+	1.072e-17	1.001e-17	-16.970	-16.999	-0.030	(0)
FeF+2	6.673e-18	5.078e-18	-17.176	-17.294	-0.119	(0)
FeF3	7.848e-19	7.855e-19	-18.105	-18.105	0.000	(0)
PbF3-	3.709e-19	3.460e-19	-18.431	-18.461	-0.030	(0)
PbF4-2	1.082e-23	8.196e-24	-22.966	-23.086	-0.121	(0)
Fe(2)	5.727e-07					
Fe+2	4.929e-07	3.770e-07	-6.307	-6.424	-0.116	-22.03
FeHCO3+	7.762e-08	7.242e-08	-7.110	-7.140	-0.030	(0)
FeSO4	1.650e-09	1.652e-09	-8.782	-8.782	0.000	18.91
FeCl+	2.427e-10	2.264e-10	-9.615	-9.645	-0.030	(0)
FeF+	2.000e-10	1.866e-10	-9.699	-9.729	-0.030	(0)
FeCO3	8.149e-11	8.156e-11	-10.089	-10.088	0.000	(0)
FeH2PO4+	5.312e-11	4.964e-11	-10.275	-10.304	-0.029	(0)
FeOH+	1.281e-11	1.197e-11	-10.892	-10.922	-0.030	(0)
FeHPO4	2.447e-12	2.449e-12	-11.611	-11.611	0.000	(0)
FeHSO4+	1.164e-13	1.086e-13	-12.934	-12.964	-0.030	(0)
Fe(OH)2	1.022e-17	1.023e-17	-16.991	-16.990	0.000	(0)
Fe(OH)3-	4.068e-23	3.800e-23	-22.391	-22.420	-0.030	(0)
Fe(3)	1.577e-15					
Fe(OH)2+	1.486e-15	1.389e-15	-14.828	-14.857	-0.029	(0)
FeOH+2	5.503e-17	4.188e-17	-16.259	-16.378	-0.119	(0)
Fe(OH)3	1.791e-17	1.792e-17	-16.747	-16.747	0.000	(0)
FeF2+	1.072e-17	1.001e-17	-16.970	-16.999	-0.030	(0)
FeF+2	6.673e-18	5.078e-18	-17.176	-17.294	-0.119	(0)
FeF3	7.848e-19	7.855e-19	-18.105	-18.105	0.000	(0)
Fe+3	1.145e-19	6.469e-20	-18.941	-19.189	-0.248	(0)
FeSO4+	1.871e-20	1.748e-20	-19.728	-19.757	-0.030	(0)
FeH2PO4+2	5.997e-21	4.574e-21	-20.222	-20.340	-0.118	(0)
Fe(OH)4-	1.752e-21	1.637e-21	-20.756	-20.786	-0.029	(0)
FeCl+2	1.119e-21	8.515e-22	-20.951	-21.070	-0.119	(0)
FeHPO4+	3.047e-23	2.846e-23	-22.516	-22.546	-0.030	(0)
Fe(SO4)2-	1.009e-23	9.413e-24	-22.996	-23.026	-0.030	(0)
FeCl2+	1.768e-24	1.651e-24	-23.752	-23.782	-0.030	(0)
FeHSO4+2	6.179e-25	4.680e-25	-24.209	-24.330	-0.121	(0)
FeCl3	7.178e-29	7.185e-29	-28.144	-28.144	0.000	(0)
Fe2(OH)2+4	1.431e-31	4.709e-32	-30.844	-31.327	-0.483	(0)

Fe3(OH)4+5	0.000e+00	0.000e+00	-43.113	-43.867	-0.754	(0)
H(0)	4.409e-14					
H2	2.205e-14	2.207e-14	-13.657	-13.656	0.000	28.61
K	1.151e-04					
K+	1.151e-04	1.073e-04	-3.939	-3.969	-0.030	9.04
KSO4-	1.987e-08	1.857e-08	-7.702	-7.731	-0.029	34.14
KHPO4-	3.653e-13	3.413e-13	-12.437	-12.467	-0.029	38.14
Mg	4.986e-04					
Mg+2	4.862e-04	3.717e-04	-3.313	-3.430	-0.117	-21.72
MgHCO3+	8.957e-06	8.355e-06	-5.048	-5.078	-0.030	5.51
MgSO4	2.146e-06	2.148e-06	-5.668	-5.668	0.000	5.84
MgF+	1.303e-06	1.217e-06	-5.885	-5.915	-0.030	-10.55
MgH2PO4+	3.409e-09	3.185e-09	-8.467	-8.497	-0.029	(0)
MgCO3	3.199e-09	3.202e-09	-8.495	-8.495	0.000	-17.09
MgHPO4	4.497e-10	4.501e-10	-9.347	-9.347	0.000	(0)
MgOH+	1.449e-10	1.356e-10	-9.839	-9.868	-0.029	(0)
MgPO4-	1.138e-13	1.064e-13	-12.944	-12.973	-0.029	(0)
Mn(2)	2.148e-07					
Mn+2	1.875e-07	1.434e-07	-6.727	-6.843	-0.116	-20.35
MnHCO3+	2.628e-08	2.455e-08	-7.580	-7.610	-0.030	(0)
MnSO4	6.278e-10	6.284e-10	-9.202	-9.202	0.000	22.52
MnCl+	2.721e-10	2.542e-10	-9.565	-9.595	-0.030	-3.05
MnCO3	1.026e-10	1.027e-10	-9.989	-9.988	0.000	(0)
MnF+	5.257e-11	4.911e-11	-10.279	-10.309	-0.030	(0)
MnOH+	3.963e-13	3.702e-13	-12.402	-12.432	-0.030	(0)
Mn(NO3)2	2.311e-13	2.313e-13	-12.636	-12.636	0.000	41.02
MnCl2	4.822e-14	4.827e-14	-13.317	-13.316	0.000	85.81
MnCl3-	6.192e-18	5.784e-18	-17.208	-17.238	-0.030	43.38
Mn(OH)3-	2.428e-27	2.267e-27	-26.615	-26.644	-0.030	(0)
Mn(3)	1.417e-32					
Mn+3	1.417e-32	8.006e-33	-31.849	-32.097	-0.248	(0)
N(3)	7.141e-07					
NO2-	7.141e-07	6.652e-07	-6.146	-6.177	-0.031	25.00
N(5)	6.834e-04					
NO3-	6.834e-04	6.366e-04	-3.165	-3.196	-0.031	29.53
BaNO3+	1.068e-09	9.966e-10	-8.971	-9.001	-0.030	(0)
PbNO3+	1.095e-11	1.022e-11	-10.960	-10.991	-0.030	(0)
CdNO3+	1.089e-11	1.016e-11	-10.963	-10.993	-0.030	17.55
Mn(NO3)2	2.311e-13	2.313e-13	-12.636	-12.636	0.000	41.02
Na	7.178e-04					
Na+	7.153e-04	6.678e-04	-3.146	-3.175	-0.030	-1.43
NaCl	1.738e-06	1.739e-06	-5.760	-5.760	0.000	(0)
NaHCO3	7.203e-07	7.210e-07	-6.142	-6.142	0.000	1.80
NaSO4-	8.817e-08	8.240e-08	-7.055	-7.084	-0.029	14.01
NaF	1.900e-08	1.902e-08	-7.721	-7.721	0.000	7.26
NaCO3-	1.206e-10	1.125e-10	-9.919	-9.949	-0.030	-0.98
NaHPO4-	2.273e-12	2.125e-12	-11.643	-11.673	-0.029	33.74
NaOH	6.778e-23	6.785e-23	-22.169	-22.168	0.000	(0)
O(0)	0.000e+00					
O2	0.000e+00	0.000e+00	-65.049	-65.049	0.000	30.41
P	2.906e-07					
H2PO4-	2.811e-07	2.627e-07	-6.551	-6.581	-0.029	33.24
MgH2PO4+	3.409e-09	3.185e-09	-8.467	-8.497	-0.029	(0)
CaH2PO4+	2.717e-09	2.539e-09	-8.566	-8.595	-0.029	(0)
HPO4-2	2.144e-09	1.632e-09	-8.669	-8.787	-0.119	6.83
MgHPO4	4.497e-10	4.501e-10	-9.347	-9.347	0.000	(0)
H3PO4	3.867e-10	3.871e-10	-9.413	-9.412	0.000	47.41
CaHPO4	3.376e-10	3.379e-10	-9.472	-9.471	0.000	(0)
FeH2PO4+	5.312e-11	4.964e-11	-10.275	-10.304	-0.029	(0)
FeHPO4	2.447e-12	2.449e-12	-11.611	-11.611	0.000	(0)
NaHPO4-	2.273e-12	2.125e-12	-11.643	-11.673	-0.029	33.74
KHPO4-	3.653e-13	3.413e-13	-12.437	-12.467	-0.029	38.14
MgPO4-	1.138e-13	1.064e-13	-12.944	-12.973	-0.029	(0)
CaPO4-	8.565e-14	8.004e-14	-13.067	-13.097	-0.029	(0)
PO4-3	1.378e-16	7.364e-17	-15.861	-16.133	-0.272	-22.97
FeH2PO4+2	5.997e-21	4.574e-21	-20.222	-20.340	-0.118	(0)
FeHPO4+	3.047e-23	2.846e-23	-22.516	-22.546	-0.030	(0)
Pb	3.427e-09					

PbHCO3+	1.775e-09	1.656e-09	-8.751	-8.781	-0.030	(0)
Pb+2	1.433e-09	1.085e-09	-8.844	-8.964	-0.121	-15.44
PbCO3	1.699e-10	1.701e-10	-9.770	-9.769	0.000	(0)
PbCl+	2.018e-11	1.882e-11	-10.695	-10.725	-0.030	7.98
PbSO4	1.501e-11	1.502e-11	-10.824	-10.823	0.000	(0)
PbNO3+	1.095e-11	1.022e-11	-10.960	-10.991	-0.030	(0)
PbOH+	2.267e-12	2.114e-12	-11.645	-11.675	-0.030	(0)
PbF+	1.024e-12	9.551e-13	-11.990	-12.020	-0.030	(0)
PbBr+	3.598e-13	3.356e-13	-12.444	-12.474	-0.030	(0)
PbCl2	1.295e-14	1.296e-14	-13.888	-13.887	0.000	34.98
Pb(CO3)2-2	5.087e-15	3.853e-15	-14.294	-14.414	-0.121	(0)
Pb(SO4)2-2	2.561e-15	1.940e-15	-14.592	-14.712	-0.121	(0)
PbF2	9.642e-16	9.651e-16	-15.016	-15.015	0.000	(0)
Pb(OH)2	8.212e-17	8.219e-17	-16.086	-16.085	0.000	(0)
PbCl3-	4.804e-18	4.482e-18	-17.318	-17.349	-0.030	65.99
PbBr2	8.221e-19	8.229e-19	-18.085	-18.085	0.000	(0)
PbF3-	3.709e-19	3.460e-19	-18.431	-18.461	-0.030	(0)
Pb2OH+3	9.599e-20	5.137e-20	-19.018	-19.289	-0.271	(0)
PbCl4-2	1.233e-21	9.337e-22	-20.909	-21.030	-0.121	101.48
Pb(OH)3-	1.011e-22	9.429e-23	-21.995	-22.026	-0.030	(0)
PbF4-2	1.082e-23	8.196e-24	-22.966	-23.086	-0.121	(0)
Pb(OH)4-2	2.850e-29	2.158e-29	-28.545	-28.666	-0.121	(0)
Pb3(OH)4+2	2.238e-31	1.695e-31	-30.650	-30.771	-0.121	(0)
S(6)	3.644e-05					
SO4-2	3.235e-05	2.461e-05	-4.490	-4.609	-0.119	14.64
MgSO4	2.146e-06	2.148e-06	-5.668	-5.668	0.000	5.84
CaSO4	1.651e-06	1.652e-06	-5.782	-5.782	0.000	7.50
BaSO4	1.533e-07	1.534e-07	-6.815	-6.814	0.000	(0)
NaSO4-	8.817e-08	8.240e-08	-7.055	-7.084	-0.029	14.01
HSO4-	2.568e-08	2.396e-08	-7.590	-7.621	-0.030	40.31
KSO4-	1.987e-08	1.857e-08	-7.702	-7.731	-0.029	34.14
ZnSO4	6.600e-09	6.606e-09	-8.180	-8.180	0.000	21.71
FeSO4	1.650e-09	1.652e-09	-8.782	-8.782	0.000	18.91
MnSO4	6.278e-10	6.284e-10	-9.202	-9.202	0.000	22.52
CaHSO4+	1.165e-10	1.087e-10	-9.934	-9.964	-0.030	(0)
CdSO4	4.514e-11	4.518e-11	-10.345	-10.345	0.000	78.02
PbSO4	1.501e-11	1.502e-11	-10.824	-10.823	0.000	(0)
AlSO4+	3.675e-12	3.430e-12	-11.435	-11.465	-0.030	(0)
Zn(SO4)2-2	1.744e-12	1.321e-12	-11.758	-11.879	-0.121	-12.94
CuSO4	6.182e-13	6.188e-13	-12.209	-12.208	0.000	13.10
FeHSO4+	1.164e-13	1.086e-13	-12.934	-12.964	-0.030	(0)
Cd(SO4)2-2	1.609e-14	1.219e-14	-13.793	-13.914	-0.121	-105.51
Al(SO4)2-	2.861e-15	2.670e-15	-14.544	-14.573	-0.030	(0)
Pb(SO4)2-2	2.561e-15	1.940e-15	-14.592	-14.712	-0.121	(0)
AlHSO4+2	4.018e-18	3.043e-18	-17.396	-17.517	-0.121	(0)
FeSO4+	1.871e-20	1.748e-20	-19.728	-19.757	-0.030	(0)
Fe(SO4)2-	1.009e-23	9.413e-24	-22.996	-23.026	-0.030	(0)
FeHSO4+2	6.179e-25	4.680e-25	-24.209	-24.330	-0.121	(0)
Zn	1.812e-06					
Zn+2	1.504e-06	1.145e-06	-5.823	-5.941	-0.119	-25.26
ZnHCO3+	2.966e-07	2.767e-07	-6.528	-6.558	-0.030	(0)
ZnSO4	6.600e-09	6.606e-09	-8.180	-8.180	0.000	21.71
ZnCO3	2.057e-09	2.059e-09	-8.687	-8.686	0.000	(0)
ZnCl+	1.441e-09	1.344e-09	-8.841	-8.872	-0.030	-13.83
ZnF+	8.583e-10	8.007e-10	-9.066	-9.097	-0.030	(0)
ZnOH+	1.350e-10	1.260e-10	-9.870	-9.900	-0.030	(0)
Zn(SO4)2-2	1.744e-12	1.321e-12	-11.758	-11.879	-0.121	-12.94
ZnBr+	1.693e-12	1.580e-12	-11.771	-11.801	-0.030	(0)
ZnOHCl	1.646e-12	1.647e-12	-11.784	-11.783	0.000	(0)
ZnCl2	6.117e-13	6.123e-13	-12.213	-12.213	0.000	101.91
Zn(CO3)2-2	5.242e-13	3.971e-13	-12.280	-12.401	-0.121	(0)
Zn(OH)2	1.437e-13	1.438e-13	-12.843	-12.842	0.000	(0)
ZnCl3-	3.205e-16	2.990e-16	-15.494	-15.524	-0.030	16.99
ZnBr2	3.296e-18	3.299e-18	-17.482	-17.482	0.000	(0)
ZnCl4-2	8.569e-20	6.522e-20	-19.067	-19.186	-0.119	145.30
Zn(OH)3-	4.872e-20	4.545e-20	-19.312	-19.342	-0.030	(0)
Zn(OH)4-2	9.503e-28	7.198e-28	-27.022	-27.143	-0.121	(0)

-------------------------Distribution of alkalinity--------------------------

Total alkalinity (eq/kgw) = 2.064e-03

Species	Alkalinity	Molality	Alk/Mol
HCO3-	2.055e-03	2.055e-03	1.00
H+	-1.065e-05	1.065e-05	-1.00
CaHCO3+	9.896e-06	9.896e-06	1.00
MgHCO3+	8.957e-06	8.957e-06	1.00
HF	-7.423e-07	7.423e-07	-1.00
NaHCO3	7.203e-07	7.203e-07	1.00
ZnHCO3+	2.966e-07	2.966e-07	1.00
BaHCO3+	2.459e-07	2.459e-07	1.00
FeHCO3+	7.762e-08	7.762e-08	1.00
MnHCO3+	2.628e-08	2.628e-08	1.00
HSO4-	-2.568e-08	2.568e-08	-1.00
CO3-2	2.365e-08	1.182e-08	2.00
CaCO3	1.144e-08	5.718e-09	2.00
MgCO3	6.397e-09	3.199e-09	2.00
ZnCO3	4.115e-09	2.057e-09	2.00
HPO4-2	2.144e-09	2.144e-09	1.00
PbHCO3+	1.775e-09	1.775e-09	1.00
OH-	1.090e-09	1.090e-09	1.00
H2BO3-	7.794e-10	7.794e-10	1.00
MgHPO4	4.497e-10	4.497e-10	1.00
CdHCO3+	4.143e-10	4.143e-10	1.00
H3PO4	-3.867e-10	3.867e-10	-1.00
PbCO3	3.399e-10	1.699e-10	2.00
CaHPO4	3.376e-10	3.376e-10	1.00
NaCO3-	2.411e-10	1.206e-10	2.00
MnCO3	2.053e-10	1.026e-10	2.00
FeCO3	1.630e-10	8.149e-11	2.00
HF2-	-1.513e-10	1.513e-10	-1.00
MgOH+	1.449e-10	1.449e-10	1.00
ZnOH+	1.350e-10	1.350e-10	1.00
CuHCO3+	1.270e-10	1.270e-10	1.00
CaHSO4+	-1.165e-10	1.165e-10	-1.00
BaCO3	1.159e-10	5.796e-11	2.00
Al(OH)2+	7.394e-11	3.697e-11	2.00
AlOH+2	5.754e-11	5.754e-11	1.00
BF2(OH)2-	-1.416e-11	1.416e-11	-1.00
FeOH+	1.281e-11	1.281e-11	1.00
CuCO3	1.191e-11	5.956e-12	2.00
CaOH+	6.707e-12	6.707e-12	1.00
FeHPO4	2.447e-12	2.447e-12	1.00
NaHPO4-	2.273e-12	2.273e-12	1.00
PbOH+	2.267e-12	2.267e-12	1.00
Zn(CO3)2-2	2.097e-12	5.242e-13	4.00
ZnOHCl	1.646e-12	1.646e-12	1.00
Al(OH)3	1.531e-12	5.104e-13	3.00
Al(OH)4-	4.126e-13	1.032e-13	4.00
MnOH+	3.963e-13	3.963e-13	1.00
KHPO4-	3.653e-13	3.653e-13	1.00
Zn(OH)2	2.874e-13	1.437e-13	2.00
MgPO4-	2.276e-13	1.138e-13	2.00
CaPO4-	1.713e-13	8.565e-14	2.00
CuOH+	1.319e-13	1.319e-13	1.00
FeHSO4+	-1.164e-13	1.164e-13	-1.00
CdCO3	9.108e-14	4.554e-14	2.00
CdOH+	5.694e-14	5.694e-14	1.00
Cu(OH)2	5.131e-14	2.565e-14	2.00
BaOH+	4.508e-14	4.508e-14	1.00
Pb(CO3)2-2	2.035e-14	5.087e-15	4.00
BF3OH-	-1.536e-14	7.679e-15	-2.00
CdOHCl	1.092e-14	1.092e-14	1.00
Cu(CO3)2-2	3.574e-16	8.936e-17	4.00
PO4-3	2.755e-16	1.378e-16	2.00

Pb(OH)2	1.642e-16	8.212e-17	2.00
FeOH+2	-5.503e-17	5.503e-17	-1.00
BF4-	-4.648e-17	1.549e-17	-3.00
FeF2+	-2.144e-17	1.072e-17	-2.00
Fe(OH)2	2.044e-17	1.022e-17	2.00
Fe(OH)3	1.791e-17	1.791e-17	1.00
FeF+2	-1.335e-17	6.673e-18	-2.00
Cd(CO3)2-2	6.865e-18	1.716e-18	4.00
AlHSO4+2	-4.018e-18	4.018e-18	-1.00
FeF3	-1.570e-18	7.848e-19	-2.00
Cd(OH)2	5.670e-19	2.835e-19	2.00
Fe+3	-2.289e-19	1.145e-19	-2.00
Zn(OH)3-	1.462e-19	4.872e-20	3.00
Pb2OH+3	9.599e-20	9.599e-20	1.00
FeSO4+	-3.743e-20	1.871e-20	-2.00
Cu2(OH)2+2	1.758e-20	8.792e-21	2.00
FeH2PO4+2	-1.199e-20	5.997e-21	-2.00
Fe(OH)4-	3.504e-21	1.752e-21	2.00
Cd2OH+3	3.091e-21	3.091e-21	1.00
FeCl+2	-2.238e-21	1.119e-21	-2.00
Cu(OH)3-	4.971e-22	1.657e-22	3.00
Pb(OH)3-	3.032e-22	1.011e-22	3.00
Fe(OH)3-	1.221e-22	4.068e-23	3.00
NaOH	6.778e-23	6.778e-23	1.00
FeHPO4+	-3.047e-23	3.047e-23	-1.00
Fe(SO4)2-	-2.018e-23	1.009e-23	-2.00
FeCl2+	-3.536e-24	1.768e-24	-2.00
FeHSO4+2	-1.854e-24	6.179e-25	-3.00
Cd(OH)3-	1.023e-26	3.410e-27	3.00
Mn(OH)3-	7.283e-27	2.428e-27	3.00
Zn(OH)4-2	3.801e-27	9.503e-28	4.00
FeCl3	-1.436e-28	7.178e-29	-2.00
Pb(OH)4-2	1.140e-28	2.850e-29	4.00
Cu(OH)4-2	1.628e-29	4.069e-30	4.00
Pb3(OH)4+2	8.951e-31	2.238e-31	4.00
Fe2(OH)2+4	-2.861e-31	1.431e-31	-2.00
Cd(OH)4-2	1.496e-35	3.740e-36	4.00
Fe3(OH)4+5	-0.000e+00	0.000e+00	-2.00

-------------------------------Saturation indices-------------------------------

Phase	SI**	log IAP	log K(298 K, 1 atm)	
Al(OH)3(a)	-6.15	4.64	10.80	Al(OH)3
Alunite	-12.85	-14.26	-1.41	KAl3(SO4)2(OH)6
Anglesite	-5.78	-13.57	-7.79	PbSO4
Anhydrite	-3.75	-8.03	-4.28	CaSO4
Aragonite	-3.13	-11.47	-8.34	CaCO3
BaCl2	-13.86	-11.63	2.23	BaCl2
BaCl2:2H2O	-11.84	-11.63	0.21	BaCl2:2H2O
BaCl2:H2O	-12.45	-11.63	0.82	BaCl2:H2O
Barite	0.33	-9.51	-9.84	BaSO4
Calcite	-2.99	-11.47	-8.48	CaCO3
Cd(OH)2	-11.85	1.80	13.65	Cd(OH)2
CdSO4	-12.70	-12.81	-0.10	CdSO4
Cerussite	-3.88	-17.01	-13.13	PbCO3
CO2(g)	0.10	-1.36	-1.47	CO2
Dolomite	-5.85	-22.94	-17.09	CaMg(CO3)2
Fe(OH)3(a)	-9.08	-4.19	4.89	Fe(OH)3
Fluorite	-1.44	-12.03	-10.60	CaF2
Gibbsite	-3.46	4.64	8.11	Al(OH)3
Goethite	-3.19	-4.19	-1.00	FeOOH
Gypsum	-3.45	-8.03	-4.58	CaSO4:2H2O
H2(g)	-10.56	-13.66	-3.10	H2
H2O(g)	-1.50	-0.00	1.50	H2O
Halite	-8.11	-6.54	1.57	NaCl
Hausmannite	-41.04	19.97	61.02	Mn3O4
Hematite	-4.37	-8.38	-4.01	Fe2O3

Hydroxyapatite	-20.05	-23.48	-3.43	Ca5(PO4)3OH
Jarosite-K	-31.54	-40.76	-9.21	KFe3(SO4)2(OH)6
Manganite	-16.93	8.41	25.34	MnOOH
Melanterite	-8.83	-11.04	-2.21	FeSO4:7H2O
O2(g)	-62.16	-65.05	-2.89	O2
Otavite	-4.14	-16.24	-12.10	CdCO3
Pb(OH)2	-7.11	1.03	8.15	Pb(OH)2
Pyrochroite	-12.04	3.16	15.20	Mn(OH)2
Pyrolusite	-27.71	13.66	41.37	MnO2:H2O
Rhodochrosite	-3.76	-14.89	-11.13	MnCO3
Siderite	-3.58	-14.47	-10.89	FeCO3
Smithsonite	-3.99	-13.99	-10.00	ZnCO3
Sylvite	-8.23	-7.33	0.90	KCl
Vivianite	-15.54	-51.54	-36.00	Fe3(PO4)2:8H2O
Witherite	-4.39	-12.95	-8.56	BaCO3
Zn(OH)2(e)	-7.44	4.06	11.50	Zn(OH)2

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
For ideal gases, phi = 1.

Initial solution 29.

-----------------------------Solution composition-----------------------------

Elements	Molality	Moles
Al	3.148e-07	3.148e-07
Alkalinity	3.752e-03	3.752e-03
B	5.330e-06	5.330e-06
Ba	7.648e-06	7.648e-06
Br	4.758e-34	4.758e-34
Ca	1.597e-04	1.597e-04
Cd	6.497e-09	6.497e-09
Cl	1.044e-04	1.044e-04
Cu	8.674e-08	8.674e-08
F	1.474e-05	1.474e-05
Fe	1.970e-06	1.970e-06
K	6.140e-05	6.140e-05
Mg	3.580e-05	3.580e-05
Mn	1.639e-06	1.639e-06
N(-3)	4.285e-07	4.285e-07
N(3)	2.857e-07	2.857e-07
N(5)	3.642e-06	3.642e-06
Na	3.324e-03	3.324e-03
P	2.196e-06	2.196e-06
Pb	1.753e-08	1.753e-08
S(6)	8.330e-06	8.330e-06
Si	5.061e-04	5.061e-04
Zn	2.115e-06	2.115e-06

----------------------------Description of solution----------------------------

pH	= 8.000
pe	= -1.995
Specific Conductance (µS/cm, 25°C)	= 350
Density (g/cm³)	= 0.99732
Volume (L)	= 1.00306
Activity of water	= 1.000
Ionic strength (mol/kgw)	= 4.045e-03
Mass of water (kg)	= 1.000e+00
Total carbon (mol/kg)	= 3.788e-03
Total CO2 (mol/kg)	= 3.788e-03
Temperature (°C)	= 24.94
Electrical balance (eq)	= -8.873e-05
Percent error, 100*(Cat-|An|)/(Cat+|An|)	= -1.16
Iterations	= 11 (308 overall)
Total H	= 1.110182e+02
Total O	= 5.551960e+01

---------------------------------Redox couples---------------------------------

Redox couple	pe	Eh (volts)
N(-3)/N(3)	4.3958	0.2600
N(-3)/N(5)	5.0071	0.2961
N(3)/N(5)	6.8410	0.4046

----------------------------Distribution of species----------------------------

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma	mole V cm³/mol
OH-	1.080e-06	1.007e-06	-5.967	-5.997	-0.030	-4.08
H+	1.065e-08	1.000e-08	-7.973	-8.000	-0.027	0.00
H2O	5.551e+01	9.999e-01	1.744	-0.000	0.000	18.07
Al	3.148e-07					
Al(OH)4-	3.131e-07	2.924e-07	-6.504	-6.534	-0.030	(0)
Al(OH)3	1.552e-09	1.553e-09	-8.809	-8.809	0.000	(0)
Al(OH)2+	1.132e-10	1.059e-10	-9.946	-9.975	-0.029	(0)
AlOH+2	1.777e-13	1.358e-13	-12.750	-12.867	-0.117	-27.66
AlF2+	1.381e-13	1.291e-13	-12.860	-12.889	-0.029	(0)
AlF+2	2.460e-14	1.881e-14	-13.609	-13.726	-0.117	(0)
AlF3	2.226e-14	2.228e-14	-13.652	-13.652	0.000	(0)
Al+3	2.417e-16	1.373e-16	-15.617	-15.862	-0.246	-42.07
AlF4-	1.302e-16	1.216e-16	-15.886	-15.915	-0.030	(0)
AlSO4+	2.849e-18	2.661e-18	-17.545	-17.575	-0.030	(0)
Al(SO4)2-	5.526e-22	5.162e-22	-21.258	-21.287	-0.030	(0)
AlHSO4+2	3.106e-27	2.359e-27	-26.508	-26.627	-0.120	(0)
B	5.330e-06					
H3BO3	5.021e-06	5.025e-06	-5.299	-5.299	0.000	39.23
H2BO3-	3.094e-07	2.889e-07	-6.509	-6.539	-0.030	(0)
BF(OH)3-	2.935e-11	2.740e-11	-10.532	-10.562	-0.030	(0)
BF2(OH)2-	4.311e-16	4.025e-16	-15.365	-15.395	-0.030	(0)
BF3OH-	6.486e-23	6.055e-23	-22.188	-22.218	-0.030	(0)
BF4-	3.622e-29	3.381e-29	-28.441	-28.471	-0.030	(0)
Ba	7.648e-06					
Ba+2	7.385e-06	5.613e-06	-5.132	-5.251	-0.119	-12.64
BaHCO3+	1.973e-07	1.842e-07	-6.705	-6.735	-0.030	(0)
BaCO3	4.650e-08	4.654e-08	-7.333	-7.332	0.000	-10.70
BaSO4	1.724e-08	1.726e-08	-7.763	-7.763	0.000	(0)
BaCl+	1.809e-09	1.689e-09	-8.742	-8.772	-0.030	(0)
BaOH+	2.035e-11	1.902e-11	-10.691	-10.721	-0.029	(0)
BaNO3+	2.570e-12	2.399e-12	-11.590	-11.620	-0.030	(0)
Br	4.758e-34					
Br-	4.758e-34	4.435e-34	-33.323	-33.353	-0.031	24.59
CdBr+	3.112e-40	2.905e-40	-39.507	-39.537	-0.030	(0)
ZnBr+	0.000e+00	0.000e+00	-40.402	-40.432	-0.030	(0)
PbBr+	0.000e+00	0.000e+00	-41.787	-41.817	-0.030	(0)
CdBr2	0.000e+00	0.000e+00	-72.160	-72.160	0.000	(0)
ZnBr2	0.000e+00	0.000e+00	-74.186	-74.185	0.000	(0)
PbBr2	0.000e+00	0.000e+00	-75.500	-75.500	0.000	(0)
C(4)	3.788e-03					
HCO3-	3.669e-03	3.430e-03	-2.436	-2.465	-0.029	24.72
CO2	7.712e-05	7.720e-05	-4.113	-4.112	0.000	34.43
CO3-2	2.102e-05	1.607e-05	-4.677	-4.794	-0.117	-5.15
NaHCO3	5.971e-06	5.977e-06	-5.224	-5.224	0.000	1.80
CaHCO3+	5.392e-06	5.045e-06	-5.268	-5.297	-0.029	9.70
CaCO3	3.108e-06	3.111e-06	-5.508	-5.507	0.000	-14.60
MgHCO3+	1.126e-06	1.051e-06	-5.949	-5.979	-0.030	5.50
ZnCO3	1.015e-06	1.016e-06	-5.993	-5.993	0.000	(0)
NaCO3-	9.897e-07	9.239e-07	-6.004	-6.034	-0.030	-0.99
MnCO3	7.179e-07	7.186e-07	-6.144	-6.144	0.000	(0)
Zn(CO3)2-2	4.597e-07	3.491e-07	-6.338	-6.457	-0.120	(0)
MgCO3	4.007e-07	4.011e-07	-6.397	-6.397	0.000	-17.09
FeCO3	3.617e-07	3.621e-07	-6.442	-6.441	0.000	(0)
FeHCO3+	3.452e-07	3.222e-07	-6.462	-6.492	-0.030	(0)

BaHCO3+	1.973e-07	1.842e-07	-6.705	-6.735	-0.030	(0)
MnHCO3+	1.842e-07	1.721e-07	-6.735	-6.764	-0.029	(0)
ZnHCO3+	1.466e-07	1.369e-07	-6.834	-6.864	-0.030	(0)
BaCO3	4.650e-08	4.654e-08	-7.333	-7.332	0.000	-10.70
PbCO3	1.629e-08	1.630e-08	-7.788	-7.788	0.000	(0)
Pb(CO3)2-2	8.663e-10	6.579e-10	-9.062	-9.182	-0.120	(0)
CdHCO3+	5.144e-10	4.802e-10	-9.289	-9.319	-0.030	(0)
PbHCO3+	1.704e-10	1.591e-10	-9.769	-9.798	-0.030	(0)
CuCO3	1.332e-10	1.333e-10	-9.875	-9.875	0.000	(0)
(CO2)2	1.091e-10	1.092e-10	-9.962	-9.962	0.000	68.86
CdCO3	5.645e-11	5.650e-11	-10.248	-10.248	0.000	(0)
Cd(CO3)2-2	3.780e-12	2.871e-12	-11.422	-11.542	-0.120	(0)
Cu(CO3)2-2	3.552e-12	2.697e-12	-11.450	-11.569	-0.120	(0)
CuHCO3+	2.846e-12	2.657e-12	-11.546	-11.576	-0.030	(0)
Ca	1.597e-04					
Ca+2	1.510e-04	1.154e-04	-3.821	-3.938	-0.117	-18.04
CaHCO3+	5.392e-06	5.045e-06	-5.268	-5.297	-0.029	9.70
CaCO3	3.108e-06	3.111e-06	-5.508	-5.507	0.000	-14.60
CaSO4	1.257e-07	1.258e-07	-6.901	-6.900	0.000	7.50
CaHPO4	8.680e-08	8.688e-08	-7.062	-7.061	0.000	(0)
CaPO4-	2.196e-08	2.053e-08	-7.658	-7.688	-0.029	(0)
CaOH+	2.051e-09	1.915e-09	-8.688	-8.718	-0.030	(0)
CaH2PO4+	6.985e-10	6.532e-10	-9.156	-9.185	-0.029	(0)
CaHSO4+	8.852e-15	8.263e-15	-14.053	-14.083	-0.030	(0)
Cd	6.497e-09					
Cd+2	5.829e-09	4.427e-09	-8.234	-8.354	-0.120	-18.65
CdHCO3+	5.144e-10	4.802e-10	-9.289	-9.319	-0.030	(0)
CdCO3	5.645e-11	5.650e-11	-10.248	-10.248	0.000	(0)
CdCl+	4.335e-11	4.047e-11	-10.363	-10.393	-0.030	5.86
CdOH+	3.926e-11	3.665e-11	-10.406	-10.436	-0.030	(0)
CdSO4	7.822e-12	7.829e-12	-11.107	-11.106	0.000	78.08
Cd(CO3)2-2	3.780e-12	2.871e-12	-11.422	-11.542	-0.120	(0)
CdOHCl	1.668e-12	1.669e-12	-11.778	-11.777	0.000	(0)
CdF+	8.181e-13	7.637e-13	-12.087	-12.117	-0.030	(0)
Cd(OH)2	1.975e-13	1.977e-13	-12.704	-12.704	0.000	(0)
CdNO3+	4.051e-14	3.782e-14	-13.392	-13.422	-0.030	17.55
CdCl2	1.614e-14	1.615e-14	-13.792	-13.792	0.000	23.14
Cd(SO4)2-2	6.937e-16	5.268e-16	-15.159	-15.278	-0.120	-105.59
CdF2	2.627e-17	2.629e-17	-16.581	-16.580	0.000	(0)
Cd(OH)3-	2.376e-18	2.218e-18	-17.624	-17.654	-0.030	(0)
Cd2OH+3	1.477e-18	7.952e-19	-17.831	-18.100	-0.269	(0)
CdCl3-	1.044e-18	9.749e-19	-17.981	-18.011	-0.030	69.39
Cd(OH)4-2	2.602e-24	1.976e-24	-23.585	-23.704	-0.120	(0)
CdBr+	3.112e-40	2.905e-40	-39.507	-39.537	-0.030	(0)
CdBr2	0.000e+00	0.000e+00	-72.160	-72.160	0.000	(0)
Cl	1.044e-04					
Cl-	1.026e-04	9.575e-05	-3.989	-4.019	-0.030	18.10
NaCl	1.772e-06	1.774e-06	-5.751	-5.751	0.000	(0)
BaCl+	1.809e-09	1.689e-09	-8.742	-8.772	-0.030	(0)
CuCl2-	2.489e-10	2.324e-10	-9.604	-9.634	-0.030	(0)
MnCl+	2.350e-10	2.196e-10	-9.629	-9.658	-0.029	-3.08
FeCl+	1.330e-10	1.242e-10	-9.876	-9.906	-0.030	(0)
ZnOHCl	1.004e-10	1.005e-10	-9.998	-9.998	0.000	(0)
ZnCl+	8.729e-11	8.148e-11	-10.059	-10.089	-0.030	-13.95
CdCl+	4.335e-11	4.047e-11	-10.363	-10.393	-0.030	5.86
CdOHCl	1.668e-12	1.669e-12	-11.778	-11.777	0.000	(0)
PbCl+	2.380e-13	2.222e-13	-12.623	-12.653	-0.030	7.97
CuCl3-2	4.620e-14	3.525e-14	-13.335	-13.453	-0.117	(0)
CdCl2	1.614e-14	1.615e-14	-13.792	-13.792	0.000	23.14
MnCl2	9.171e-15	9.180e-15	-14.038	-14.037	0.000	85.96
ZnCl2	8.160e-15	8.168e-15	-14.088	-14.088	0.000	102.14
CuCl+	4.254e-16	3.971e-16	-15.371	-15.401	-0.030	0.68
PbCl2	3.373e-17	3.376e-17	-16.472	-16.472	0.000	34.97
CdCl3-	1.044e-18	9.749e-19	-17.981	-18.011	-0.030	69.39
ZnCl3-	9.398e-19	8.772e-19	-18.027	-18.057	-0.030	16.98
MnCl3-	2.590e-19	2.421e-19	-18.587	-18.616	-0.029	43.39
CuCl2	2.039e-20	2.041e-20	-19.691	-19.690	0.000	30.95
PbCl3-	2.750e-21	2.567e-21	-20.561	-20.591	-0.030	65.97

ZnCl4-2	5.515e-23	4.208e-23	-22.258	-22.376	-0.117	145.29
FeCl+2	3.421e-24	2.610e-24	-23.466	-23.583	-0.117	(0)
PbCl4-2	1.548e-25	1.176e-25	-24.810	-24.930	-0.120	101.46
CuCl3-	7.420e-27	6.926e-27	-26.130	-26.160	-0.030	(0)
FeCl2+	1.197e-27	1.119e-27	-26.922	-26.951	-0.029	(0)
FeCl3	1.070e-32	1.071e-32	-31.971	-31.970	0.000	(0)
CuCl4-2	4.350e-33	3.319e-33	-32.362	-32.479	-0.117	(0)
Cu(1)	8.627e-08					
Cu+	8.602e-08	8.013e-08	-7.065	-7.096	-0.031	(0)
CuCl2-	2.489e-10	2.324e-10	-9.604	-9.634	-0.030	(0)
CuCl3-2	4.620e-14	3.525e-14	-13.335	-13.453	-0.117	(0)
Cu(2)	4.658e-10					
Cu(OH)2	3.225e-10	3.228e-10	-9.492	-9.491	0.000	(0)
CuCO3	1.332e-10	1.333e-10	-9.875	-9.875	0.000	(0)
Cu(CO3)2-2	3.552e-12	2.697e-12	-11.450	-11.569	-0.120	(0)
CuHCO3+	2.846e-12	2.657e-12	-11.546	-11.576	-0.030	(0)
Cu+2	2.015e-12	1.545e-12	-11.696	-11.811	-0.115	-26.51
CuOH+	1.655e-12	1.545e-12	-11.781	-11.811	-0.030	(0)
Cu(OH)3-	2.083e-15	1.945e-15	-14.681	-14.711	-0.030	(0)
CuSO4	1.933e-15	1.935e-15	-14.714	-14.713	0.000	13.08
CuCl+	4.254e-16	3.971e-16	-15.371	-15.401	-0.030	0.68
CuF+	4.126e-16	3.852e-16	-15.384	-15.414	-0.030	(0)
Cu2(OH)2+2	1.367e-18	1.038e-18	-17.864	-17.984	-0.120	(0)
Cu(OH)4-2	5.109e-20	3.880e-20	-19.292	-19.411	-0.120	(0)
CuCl2	2.039e-20	2.041e-20	-19.691	-19.690	0.000	30.95
CuCl3-	7.420e-27	6.926e-27	-26.130	-26.160	-0.030	(0)
CuCl4-2	4.350e-33	3.319e-33	-32.362	-32.479	-0.117	(0)
F	1.474e-05					
F-	1.469e-05	1.370e-05	-4.833	-4.863	-0.030	-1.29
MgF+	2.535e-08	2.368e-08	-7.596	-7.626	-0.030	-10.55
NaF	2.440e-08	2.443e-08	-7.613	-7.612	0.000	7.26
HF	2.051e-10	2.053e-10	-9.688	-9.688	0.000	12.50
FeF+	1.379e-10	1.287e-10	-9.860	-9.890	-0.030	(0)
ZnF+	6.568e-11	6.132e-11	-10.183	-10.212	-0.030	(0)
MnF+	5.711e-11	5.338e-11	-10.243	-10.273	-0.029	(0)
BF(OH)3-	2.935e-11	2.740e-11	-10.532	-10.562	-0.030	(0)
CdF+	8.181e-13	7.637e-13	-12.087	-12.117	-0.030	(0)
AlF2+	1.381e-13	1.291e-13	-12.860	-12.889	-0.029	(0)
AlF+2	2.460e-14	1.881e-14	-13.609	-13.726	-0.117	(0)
AlF3	2.226e-14	2.228e-14	-13.652	-13.652	0.000	(0)
PbF+	1.524e-14	1.423e-14	-13.817	-13.847	-0.030	(0)
HF2-	1.156e-14	1.079e-14	-13.937	-13.967	-0.030	22.09
BF2(OH)2-	4.311e-16	4.025e-16	-15.365	-15.395	-0.030	(0)
CuF+	4.126e-16	3.852e-16	-15.384	-15.414	-0.030	(0)
AlF4-	1.302e-16	1.216e-16	-15.886	-15.915	-0.030	(0)
CdF2	2.627e-17	2.629e-17	-16.581	-16.580	0.000	(0)
PbF2	3.977e-18	3.981e-18	-17.400	-17.400	0.000	(0)
FeF+2	2.572e-20	1.963e-20	-19.590	-19.707	-0.117	(0)
FeF2+	1.145e-20	1.070e-20	-19.941	-19.971	-0.029	(0)
PbF3-	4.234e-22	3.952e-22	-21.373	-21.403	-0.030	(0)
FeF3	2.322e-22	2.324e-22	-21.634	-21.634	0.000	(0)
BF3OH-	6.486e-23	6.055e-23	-22.188	-22.218	-0.030	(0)
PbF4-2	3.414e-27	2.592e-27	-26.467	-26.586	-0.120	(0)
BF4-	3.622e-29	3.381e-29	-28.441	-28.471	-0.030	(0)
SiF6-2	6.594e-35	5.031e-35	-34.181	-34.298	-0.117	42.69
Fe(2)	1.970e-06					
Fe+2	1.225e-06	9.393e-07	-5.912	-6.027	-0.115	-22.04
FeCO3	3.617e-07	3.621e-07	-6.442	-6.441	0.000	(0)
FeHCO3+	3.452e-07	3.222e-07	-6.462	-6.492	-0.030	(0)
FeOH+	3.164e-08	2.957e-08	-7.500	-7.529	-0.029	(0)
FeHPO4	5.136e-09	5.141e-09	-8.289	-8.289	0.000	(0)
FeSO4	1.023e-09	1.024e-09	-8.990	-8.990	0.000	19.03
FeF+	1.379e-10	1.287e-10	-9.860	-9.890	-0.030	(0)
FeCl+	1.330e-10	1.242e-10	-9.876	-9.906	-0.030	(0)
FeH2PO4+	1.115e-10	1.043e-10	-9.953	-9.982	-0.029	(0)
Fe(OH)2	2.501e-11	2.503e-11	-10.602	-10.602	0.000	(0)
Fe(OH)3-	9.943e-14	9.293e-14	-13.002	-13.032	-0.029	(0)
FeHSO4+	7.206e-17	6.727e-17	-16.142	-16.172	-0.030	(0)

Fe(3)	2.913e-10					
Fe(OH)3	2.467e-10	2.469e-10	-9.608	-9.607	0.000	(0)
Fe(OH)4-	2.402e-11	2.246e-11	-10.619	-10.649	-0.029	(0)
Fe(OH)2+	2.055e-11	1.922e-11	-10.687	-10.716	-0.029	(0)
FeOH+2	7.625e-16	5.818e-16	-15.118	-15.235	-0.117	(0)
FeF+2	2.572e-20	1.963e-20	-19.590	-19.707	-0.117	(0)
FeF2+	1.145e-20	1.070e-20	-19.941	-19.971	-0.029	(0)
Fe+3	1.593e-21	9.044e-22	-20.798	-21.044	-0.246	(0)
FeHPO4+	3.574e-22	3.340e-22	-21.447	-21.476	-0.029	(0)
FeF3	2.322e-22	2.324e-22	-21.634	-21.634	0.000	(0)
FeH2PO4+2	7.053e-23	5.392e-23	-22.152	-22.268	-0.117	(0)
FeSO4+	6.501e-23	6.076e-23	-22.187	-22.216	-0.029	(0)
FeCl+2	3.421e-24	2.610e-24	-23.466	-23.583	-0.117	(0)
Fe(SO4)2-	8.733e-27	8.153e-27	-26.059	-26.089	-0.030	(0)
FeCl2+	1.197e-27	1.119e-27	-26.922	-26.951	-0.029	(0)
Fe2(OH)2+4	2.746e-29	9.134e-30	-28.561	-29.039	-0.478	(0)
FeHSO4+2	2.142e-30	1.627e-30	-29.669	-29.789	-0.120	(0)
FeCl3	1.070e-32	1.071e-32	-31.971	-31.970	0.000	(0)
Fe3(OH)4+5	2.059e-37	3.688e-38	-36.686	-37.433	-0.747	(0)
H(0)	1.383e-15					
H2	6.916e-16	6.922e-16	-15.160	-15.160	0.000	28.61
K	6.140e-05					
K+	6.139e-05	5.727e-05	-4.212	-4.242	-0.030	9.04
KSO4-	2.637e-09	2.466e-09	-8.579	-8.608	-0.029	34.13
KHPO4-	1.642e-10	1.535e-10	-9.785	-9.814	-0.029	38.15
Mg	3.580e-05					
Mg+2	3.416e-05	2.618e-05	-4.466	-4.582	-0.116	-21.72
MgHCO3+	1.126e-06	1.051e-06	-5.949	-5.979	-0.030	5.50
MgCO3	4.007e-07	4.011e-07	-6.397	-6.397	0.000	-17.09
MgSO4	3.756e-08	3.759e-08	-7.425	-7.425	0.000	5.83
MgHPO4	2.663e-08	2.665e-08	-7.575	-7.574	0.000	(0)
MgF+	2.535e-08	2.368e-08	-7.596	-7.626	-0.030	-10.55
MgOH+	1.010e-08	9.453e-09	-7.996	-8.024	-0.029	(0)
MgPO4-	6.720e-09	6.284e-09	-8.173	-8.202	-0.029	(0)
MgH2PO4+	2.018e-10	1.887e-10	-9.695	-9.724	-0.029	(0)
Mn(2)	1.639e-06					
Mn+2	7.342e-07	5.630e-07	-6.134	-6.249	-0.115	-20.37
MnCO3	7.179e-07	7.186e-07	-6.144	-6.144	0.000	(0)
MnHCO3+	1.842e-07	1.721e-07	-6.735	-6.764	-0.029	(0)
MnOH+	1.541e-09	1.440e-09	-8.812	-8.842	-0.029	(0)
MnSO4	6.129e-10	6.135e-10	-9.213	-9.212	0.000	22.57
MnCl+	2.350e-10	2.196e-10	-9.629	-9.658	-0.029	-3.08
MnF+	5.711e-11	5.338e-11	-10.243	-10.273	-0.029	(0)
MnCl2	9.171e-15	9.180e-15	-14.038	-14.037	0.000	85.96
Mn(NO3)2	2.581e-17	2.584e-17	-16.588	-16.588	0.000	41.05
Mn(OH)3-	9.543e-18	8.919e-18	-17.020	-17.050	-0.029	(0)
MnCl3-	2.590e-19	2.421e-19	-18.587	-18.616	-0.029	43.39
Mn(3)	3.072e-34					
Mn+3	3.072e-34	1.745e-34	-33.513	-33.758	-0.246	(0)
N(-3)	4.285e-07					
NH4+	4.070e-07	3.791e-07	-6.390	-6.421	-0.031	17.99
NH3	2.149e-08	2.151e-08	-7.668	-7.667	0.000	24.42
NH4SO4-	3.209e-11	2.996e-11	-10.494	-10.523	-0.030	37.63
N(3)	2.857e-07					
NO2-	2.857e-07	2.663e-07	-6.544	-6.575	-0.031	24.99
N(5)	3.642e-06					
NO3-	3.642e-06	3.395e-06	-5.439	-5.469	-0.031	29.51
BaNO3+	2.570e-12	2.399e-12	-11.590	-11.620	-0.030	(0)
CdNO3+	4.051e-14	3.782e-14	-13.392	-13.422	-0.030	17.55
PbNO3+	3.140e-15	2.931e-15	-14.503	-14.533	-0.030	(0)
Mn(NO3)2	2.581e-17	2.584e-17	-16.588	-16.588	0.000	41.05
Na	3.324e-03					
Na+	3.315e-03	3.097e-03	-2.479	-2.509	-0.030	-1.43
NaHCO3	5.971e-06	5.977e-06	-5.224	-5.224	0.000	1.80
NaCl	1.772e-06	1.774e-06	-5.751	-5.751	0.000	(0)
NaCO3-	9.897e-07	9.239e-07	-6.004	-6.034	-0.030	-0.99
NaSO4-	1.018e-07	9.519e-08	-6.992	-7.021	-0.029	14.01
NaF	2.440e-08	2.443e-08	-7.613	-7.612	0.000	7.26

NaHPO4-	8.879e-09	8.303e-09	-8.052	-8.081	-0.029	33.74
NaOH	3.117e-19	3.120e-19	-18.506	-18.506	0.000	(0)
O(0)	0.000e+00					
O2	0.000e+00	0.000e+00	-62.080	-62.080	0.000	30.40
P	2.196e-06					
HPO4-2	1.802e-06	1.375e-06	-5.744	-5.862	-0.117	6.83
H2PO4-	2.369e-07	2.215e-07	-6.625	-6.655	-0.029	33.24
CaHPO4	8.680e-08	8.688e-08	-7.062	-7.061	0.000	(0)
MgHPO4	2.663e-08	2.665e-08	-7.575	-7.574	0.000	(0)
CaPO4-	2.196e-08	2.053e-08	-7.658	-7.688	-0.029	(0)
NaHPO4-	8.879e-09	8.303e-09	-8.052	-8.081	-0.029	33.74
MgPO4-	6.720e-09	6.284e-09	-8.173	-8.202	-0.029	(0)
FeHPO4	5.136e-09	5.141e-09	-8.289	-8.289	0.000	(0)
CaH2PO4+	6.985e-10	6.532e-10	-9.156	-9.185	-0.029	(0)
MgH2PO4+	2.018e-10	1.887e-10	-9.695	-9.724	-0.029	(0)
KHPO4-	1.642e-10	1.535e-10	-9.785	-9.814	-0.029	38.15
PO4-3	1.151e-10	6.190e-11	-9.939	-10.208	-0.269	-22.97
FeH2PO4+	1.115e-10	1.043e-10	-9.953	-9.982	-0.029	(0)
H3PO4	3.256e-13	3.259e-13	-12.487	-12.487	0.000	47.41
FeHPO4+	3.574e-22	3.340e-22	-21.447	-21.476	-0.029	(0)
FeH2PO4+2	7.053e-23	5.392e-23	-22.152	-22.268	-0.117	(0)
Pb	1.753e-08					
PbCO3	1.629e-08	1.630e-08	-7.788	-7.788	0.000	(0)
Pb(CO3)2-2	8.663e-10	6.579e-10	-9.062	-9.182	-0.120	(0)
PbHCO3+	1.704e-10	1.591e-10	-9.769	-9.798	-0.030	(0)
PbOH+	1.219e-10	1.138e-10	-9.914	-9.944	-0.030	(0)
Pb+2	7.687e-11	5.838e-11	-10.114	-10.234	-0.120	-15.44
Pb(OH)2	4.423e-12	4.427e-12	-11.354	-11.354	0.000	(0)
PbCl+	2.380e-13	2.222e-13	-12.623	-12.653	-0.030	7.97
PbSO4	2.012e-13	2.014e-13	-12.696	-12.696	0.000	(0)
PbF+	1.524e-14	1.423e-14	-13.817	-13.847	-0.030	(0)
Pb(OH)3-	5.444e-15	5.082e-15	-14.264	-14.294	-0.030	(0)
PbNO3+	3.140e-15	2.931e-15	-14.503	-14.533	-0.030	(0)
PbCl2	3.373e-17	3.376e-17	-16.472	-16.472	0.000	34.97
Pb(SO4)2-2	8.538e-18	6.484e-18	-17.069	-17.188	-0.120	(0)
PbF2	3.977e-18	3.981e-18	-17.400	-17.400	0.000	(0)
Pb(OH)4-2	1.533e-18	1.164e-18	-17.814	-17.934	-0.120	(0)
Pb2OH+3	2.762e-19	1.487e-19	-18.559	-18.828	-0.269	(0)
PbCl3-	2.750e-21	2.567e-21	-20.561	-20.591	-0.030	65.97
PbF3-	4.234e-22	3.952e-22	-21.373	-21.403	-0.030	(0)
Pb3(OH)4+2	3.420e-23	2.597e-23	-22.466	-22.585	-0.120	(0)
PbCl4-2	1.548e-25	1.176e-25	-24.810	-24.930	-0.120	101.46
PbF4-2	3.414e-27	2.592e-27	-26.467	-26.586	-0.120	(0)
PbBr+	0.000e+00	0.000e+00	-41.787	-41.817	-0.030	(0)
PbBr2	0.000e+00	0.000e+00	-75.500	-75.500	0.000	(0)
S(6)	8.330e-06					
SO4-2	8.043e-06	6.135e-06	-5.095	-5.212	-0.118	14.63
CaSO4	1.257e-07	1.258e-07	-6.901	-6.900	0.000	7.50
NaSO4-	1.018e-07	9.519e-08	-6.992	-7.021	-0.029	14.01
MgSO4	3.756e-08	3.759e-08	-7.425	-7.425	0.000	5.83
BaSO4	1.724e-08	1.726e-08	-7.763	-7.763	0.000	(0)
KSO4-	2.637e-09	2.466e-09	-8.579	-8.608	-0.029	34.13
FeSO4	1.023e-09	1.024e-09	-8.990	-8.990	0.000	19.03
MnSO4	6.129e-10	6.135e-10	-9.213	-9.212	0.000	22.57
ZnSO4	4.552e-10	4.557e-10	-9.342	-9.341	0.000	21.72
NH4SO4-	3.209e-11	2.996e-11	-10.494	-10.523	-0.030	37.63
CdSO4	7.822e-12	7.829e-12	-11.107	-11.106	0.000	78.08
HSO4-	6.381e-12	5.957e-12	-11.195	-11.225	-0.030	40.30
PbSO4	2.012e-13	2.014e-13	-12.696	-12.696	0.000	(0)
Zn(SO4)2-2	2.993e-14	2.273e-14	-13.524	-13.643	-0.120	-13.04
CaHSO4+	8.852e-15	8.263e-15	-14.053	-14.083	-0.030	(0)
CuSO4	1.933e-15	1.935e-15	-14.714	-14.713	0.000	13.08
Cd(SO4)2-2	6.937e-16	5.268e-16	-15.159	-15.278	-0.120	-105.59
FeHSO4+	7.206e-17	6.727e-17	-16.142	-16.172	-0.030	(0)
Pb(SO4)2-2	8.538e-18	6.484e-18	-17.069	-17.188	-0.120	(0)
AlSO4+	2.849e-18	2.661e-18	-17.545	-17.575	-0.030	(0)
Al(SO4)2-	5.526e-22	5.162e-22	-21.258	-21.287	-0.030	(0)
FeSO4+	6.501e-23	6.076e-23	-22.187	-22.216	-0.029	(0)

Fe(SO4)2-	8.733e-27	8.153e-27	-26.059	-26.089	-0.030	(0)
AlHSO4+2	3.106e-27	2.359e-27	-26.508	-26.627	-0.120	(0)
FeHSO4+2	2.142e-30	1.627e-30	-29.669	-29.789	-0.120	(0)
Si	5.061e-04					
H4SiO4	4.983e-04	4.987e-04	-3.303	-3.302	0.000	52.08
H3SiO4-	7.862e-06	7.338e-06	-5.104	-5.134	-0.030	28.00
H2SiO4-2	6.503e-11	4.972e-11	-10.187	-10.303	-0.117	(0)
SiF6-2	6.594e-35	5.031e-35	-34.181	-34.298	-0.117	42.69
Zn	2.115e-06					
ZnCO3	1.015e-06	1.016e-06	-5.993	-5.993	0.000	(0)
Zn(CO3)2-2	4.597e-07	3.491e-07	-6.338	-6.457	-0.120	(0)
Zn+2	4.154e-07	3.170e-07	-6.381	-6.499	-0.117	-25.25
ZnHCO3+	1.466e-07	1.369e-07	-6.834	-6.864	-0.030	(0)
Zn(OH)2	3.986e-08	3.990e-08	-7.399	-7.399	0.000	(0)
ZnOH+	3.706e-08	3.459e-08	-7.431	-7.461	-0.030	(0)
ZnSO4	4.552e-10	4.557e-10	-9.342	-9.341	0.000	21.72
ZnOHCl	1.004e-10	1.005e-10	-9.998	-9.998	0.000	(0)
ZnCl+	8.729e-11	8.148e-11	-10.059	-10.089	-0.030	-13.95
ZnF+	6.568e-11	6.132e-11	-10.183	-10.212	-0.030	(0)
Zn(OH)3-	1.351e-11	1.261e-11	-10.869	-10.899	-0.030	(0)
Zn(SO4)2-2	2.993e-14	2.273e-14	-13.524	-13.643	-0.120	-13.04
ZnCl2	8.160e-15	8.168e-15	-14.088	-14.088	0.000	102.14
Zn(OH)4-2	2.632e-16	1.999e-16	-15.580	-15.699	-0.120	(0)
ZnCl3-	9.398e-19	8.772e-19	-18.027	-18.057	-0.030	16.98
ZnCl4-2	5.515e-23	4.208e-23	-22.258	-22.376	-0.117	145.29
ZnBr+	0.000e+00	0.000e+00	-40.402	-40.432	-0.030	(0)
ZnBr2	0.000e+00	0.000e+00	-74.186	-74.185	0.000	(0)

----------Distribution of alkalinity----------

Total alkalinity (eq/kgw) = 3.752e-03

Species	Alkalinity	Molality	Alk/Mol
HCO3-	3.669e-03	3.669e-03	1.00
CO3-2	4.203e-05	2.102e-05	2.00
H3SiO4-	7.862e-06	7.862e-06	1.00
CaCO3	6.216e-06	3.108e-06	2.00
NaHCO3	5.971e-06	5.971e-06	1.00
CaHCO3+	5.392e-06	5.392e-06	1.00
ZnCO3	2.031e-06	1.015e-06	2.00
NaCO3-	1.979e-06	9.897e-07	2.00
Zn(CO3)2-2	1.839e-06	4.597e-07	4.00
HPO4-2	1.802e-06	1.802e-06	1.00
MnCO3	1.436e-06	7.179e-07	2.00
Al(OH)4-	1.252e-06	3.131e-07	4.00
MgHCO3+	1.126e-06	1.126e-06	1.00
OH-	1.080e-06	1.080e-06	1.00
MgCO3	8.014e-07	4.007e-07	2.00
FeCO3	7.234e-07	3.617e-07	2.00
FeHCO3+	3.452e-07	3.452e-07	1.00
H2BO3-	3.094e-07	3.094e-07	1.00
BaHCO3+	1.973e-07	1.973e-07	1.00
MnHCO3+	1.842e-07	1.842e-07	1.00
ZnHCO3+	1.466e-07	1.466e-07	1.00
BaCO3	9.299e-08	4.650e-08	2.00
CaHPO4	8.680e-08	8.680e-08	1.00
Zn(OH)2	7.972e-08	3.986e-08	2.00
CaPO4-	4.391e-08	2.196e-08	2.00
ZnOH+	3.706e-08	3.706e-08	1.00
PbCO3	3.257e-08	1.629e-08	2.00
FeOH+	3.164e-08	3.164e-08	1.00
MgHPO4	2.663e-08	2.663e-08	1.00
NH3	2.149e-08	2.149e-08	1.00
MgPO4-	1.344e-08	6.720e-09	2.00
H+	-1.065e-08	1.065e-08	-1.00
MgOH+	1.010e-08	1.010e-08	1.00
NaHPO4-	8.879e-09	8.879e-09	1.00

FeHPO4	5.136e-09	5.136e-09	1.00
Al(OH)3	4.655e-09	1.552e-09	3.00
Pb(CO3)2-2	3.465e-09	8.663e-10	4.00
CaOH+	2.051e-09	2.051e-09	1.00
MnOH+	1.541e-09	1.541e-09	1.00
Cu(OH)2	6.450e-10	3.225e-10	2.00
CdHCO3+	5.144e-10	5.144e-10	1.00
CuCO3	2.664e-10	1.332e-10	2.00
Fe(OH)3	2.467e-10	2.467e-10	1.00
PO4-3	2.302e-10	1.151e-10	2.00
Al(OH)2+	2.265e-10	1.132e-10	2.00
HF	-2.051e-10	2.051e-10	-1.00
PbHCO3+	1.704e-10	1.704e-10	1.00
KHPO4-	1.642e-10	1.642e-10	1.00
H2SiO4-2	1.301e-10	6.503e-11	2.00
PbOH+	1.219e-10	1.219e-10	1.00
CdCO3	1.129e-10	5.645e-11	2.00
ZnOHCl	1.004e-10	1.004e-10	1.00
Fe(OH)2	5.002e-11	2.501e-11	2.00
Fe(OH)4-	4.804e-11	2.402e-11	2.00
Zn(OH)3-	4.054e-11	1.351e-11	3.00
CdOH+	3.926e-11	3.926e-11	1.00
BaOH+	2.035e-11	2.035e-11	1.00
Cd(CO3)2-2	1.512e-11	3.780e-12	4.00
Cu(CO3)2-2	1.421e-11	3.552e-12	4.00
Pb(OH)2	8.846e-12	4.423e-12	2.00
HSO4-	-6.381e-12	6.381e-12	-1.00
CuHCO3+	2.846e-12	2.846e-12	1.00
CdOHCl	1.668e-12	1.668e-12	1.00
CuOH+	1.655e-12	1.655e-12	1.00
Cd(OH)2	3.950e-13	1.975e-13	2.00
H3PO4	-3.256e-13	3.256e-13	-1.00
Fe(OH)3-	2.983e-13	9.943e-14	3.00
AlOH+2	1.777e-13	1.777e-13	1.00
Pb(OH)3-	1.633e-14	5.444e-15	3.00
HF2-	-1.156e-14	1.156e-14	-1.00
CaHSO4+	-8.852e-15	8.852e-15	-1.00
Cu(OH)3-	6.249e-15	2.083e-15	3.00
Zn(OH)4-2	1.053e-15	2.632e-16	4.00
FeOH+2	-7.625e-16	7.625e-16	-1.00
BF2(OH)2-	-4.311e-16	4.311e-16	-1.00
FeHSO4+	-7.206e-17	7.206e-17	-1.00
Mn(OH)3-	2.863e-17	9.543e-18	3.00
Cd(OH)3-	7.127e-18	2.376e-18	3.00
Pb(OH)4-2	6.131e-18	1.533e-18	4.00
Cu2(OH)2+2	2.735e-18	1.367e-18	2.00
Cd2OH+3	1.477e-18	1.477e-18	1.00
NaOH	3.117e-19	3.117e-19	1.00
Pb2OH+3	2.762e-19	2.762e-19	1.00
Cu(OH)4-2	2.043e-19	5.109e-20	4.00
FeF+2	-5.145e-20	2.572e-20	-2.00
FeF2+	-2.290e-20	1.145e-20	-2.00
Fe+3	-3.185e-21	1.593e-21	-2.00
FeF3	-4.643e-22	2.322e-22	-2.00
FeHPO4+	-3.574e-22	3.574e-22	-1.00
FeH2PO4+2	-1.411e-22	7.053e-23	-2.00
Pb3(OH)4+2	1.368e-22	3.420e-23	4.00
FeSO4+	-1.300e-22	6.501e-23	-2.00
BF3OH-	-1.297e-22	6.486e-23	-2.00
Cd(OH)4-2	1.041e-23	2.602e-24	4.00
FeCl+2	-6.842e-24	3.421e-24	-2.00
Fe(SO4)2-	-1.747e-26	8.733e-27	-2.00
AlHSO4+2	-3.106e-27	3.106e-27	-1.00
FeCl2+	-2.394e-27	1.197e-27	-2.00
BF4-	-1.087e-28	3.622e-29	-3.00
Fe2(OH)2+4	-5.492e-29	2.746e-29	-2.00
FeHSO4+2	-6.427e-30	2.142e-30	-3.00
FeCl3	-2.140e-32	1.070e-32	-2.00

SiF6-2	-2.638e-34	6.594e-35	-4.00
Fe3(OH)4+5	-4.119e-37	2.059e-37	-2.00

----------Saturation indices----------

Phase	SI**	log IAP	log K(298 K, 1 atm)	
Al(OH)3(a)	-2.67	8.14	10.80	Al(OH)3
Albite	-0.94	-18.95	-18.01	NaAlSi3O8
Alunite	-12.86	-14.25	-1.39	KAl3(SO4)2(OH)6
Anglesite	-7.66	-15.45	-7.79	PbSO4
Anhydrite	-4.87	-9.15	-4.28	CaSO4
Anorthite	-3.89	-23.61	-19.72	CaAl2Si2O8
Aragonite	-0.40	-8.73	-8.34	CaCO3
BaCl2	-15.52	-13.29	2.23	BaCl2
BaCl2:2H2O	-13.50	-13.29	0.21	BaCl2:2H2O
BaCl2:H2O	-14.11	-13.29	0.82	BaCl2:H2O
Barite	-0.62	-10.46	-9.84	BaSO4
Ca-Montmorillonite	1.04	-43.99	-45.04	Ca0.165Al2.33Si3.67O10(OH)2
Calcite	-0.25	-8.73	-8.48	CaCO3
Cd(OH)2	-6.00	7.65	13.65	Cd(OH)2
CdSiO3	-4.72	4.34	9.06	CdSiO3
CdSO4	-13.47	-13.57	-0.10	CdSO4
Cerussite	-1.90	-15.03	-13.13	PbCO3
Chalcedony	0.25	-3.30	-3.55	SiO2
Chlorite(14A)	-4.94	63.46	68.40	Mg5Al2Si3O10(OH)8
Chrysotile	-4.56	27.65	32.21	Mg3Si2O5(OH)4
CO2(g)	-2.64	-4.11	-1.47	CO2
Dolomite	-1.02	-18.11	-17.09	CaMg(CO3)2
Fe(OH)3(a)	-1.93	2.96	4.89	Fe(OH)3
Fluorite	-3.06	-13.66	-10.60	CaF2
Gibbsite	0.02	8.14	8.11	Al(OH)3
Goethite	3.95	2.96	-1.00	FeOOH
Gypsum	-4.57	-9.15	-4.58	CaSO4:2H2O
H2(g)	-12.06	-15.16	-3.10	H2
H2O(g)	-1.50	-0.00	1.50	H2O
Halite	-8.10	-6.53	1.57	NaCl
Hausmannite	-19.78	41.26	61.04	Mn3O4
Hematite	9.92	5.91	-4.00	Fe2O3
Hydroxyapatite	-1.86	-5.27	-3.42	Ca5(PO4)3OH
Illite	0.40	-39.88	-40.28	K0.6Mg0.25Al2.3Si3.5O10(OH)2
Jarosite-K	-20.59	-29.80	-9.21	KFe3(SO4)2(OH)6
K-feldspar	-0.10	-20.68	-20.58	KAlSi3O8
K-mica	5.55	18.26	12.71	KAl3Si3O10(OH)2
Kaolinite	2.23	9.67	7.44	Al2Si2O5(OH)4
Manganite	-9.58	15.76	25.34	MnOOH
Melanterite	-9.03	-11.24	-2.21	FeSO4:7H2O
NH3(g)	-9.46	-7.67	1.80	NH3
O2(g)	-59.19	-62.08	-2.89	O2
Otavite	-1.05	-13.15	-12.10	CdCO3
Pb(OH)2	-2.39	5.77	8.15	Pb(OH)2
Pyrochroite	-5.45	9.75	15.20	Mn(OH)2
Pyrolusite	-19.63	21.76	41.39	MnO2:H2O
Quartz	0.68	-3.30	-3.98	SiO2
Rhodochrosite	0.09	-11.04	-11.13	MnCO3
Sepiolite	-2.83	12.93	15.76	Mg2Si3O7.5OH:3H2O
Sepiolite(d)	-5.73	12.93	18.66	Mg2Si3O7.5OH:3H2O
Siderite	0.07	-10.82	-10.89	FeCO3
SiO2(a)	-0.59	-3.30	-2.71	SiO2
Smithsonite	-1.29	-11.29	-10.00	ZnCO3
Sylvite	-9.16	-8.26	0.90	KCl
Talc	-0.36	21.05	21.41	Mg3Si4O10(OH)2
Vivianite	-2.50	-38.50	-36.00	Fe3(PO4)2:8H2O
Willemite	0.37	15.70	15.33	Zn2SiO4
Witherite	-1.48	-10.04	-8.56	BaCO3
Zn(OH)2(e)	-2.00	9.50	11.50	Zn(OH)2

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.

For ideal gases, phi = 1.

Initial solution 30.

----------Solution composition----------

Elements	Molality	Moles
Al	2.491e-07	2.491e-07
Alkalinity	2.572e-03	2.572e-03
B	2.128e-06	2.128e-06
Ba	2.695e-06	2.695e-06
Br	2.624e-34	2.624e-34
Ca	1.398e-04	1.398e-04
Cd	5.874e-09	5.874e-09
Cu	1.464e-08	1.464e-08
F	1.106e-05	1.106e-05
Fe	1.308e-05	1.308e-05
K	1.074e-04	1.074e-04
Mg	5.020e-05	5.020e-05
Mn	2.549e-06	2.549e-06
N(-3)	7.141e-07	7.141e-07
N(3)	3.571e-07	3.571e-07
N(5)	5.927e-06	5.927e-06
Na	2.106e-03	2.106e-03
P	1.431e-05	1.431e-05
Pb	7.097e-09	7.097e-09
S(6)	2.083e-04	2.083e-04
Si	1.195e-03	1.195e-03
Zn	1.576e-06	1.576e-06

----------Description of solution----------

pH	= 6.000
pe	= -2.317
Specific Conductance (µS/cm, 25°C)	= 267
Density (g/cm³)	= 0.99737
Volume (L)	= 1.00323
Activity of water	= 1.000
Ionic strength (mol/kgw)	= 3.206e-03
Mass of water (kg)	= 1.000e+00
Total carbon (mol/kg)	= 8.004e-03
Total CO2 (mol/kg)	= 8.004e-03
Temperature (°C)	= 24.81
Electrical balance (eq)	= -3.858e-04
Percent error, 100*(Cat-|An|)/(Cat+|An|)	= -6.87
Iterations	= 12 (320 overall)
Total H	= 1.110198e+02
Total O	= 5.553049e+01

----------Redox couples----------

Redox couple	pe	Eh (volts)
N(-3)/N(3)	7.0457	0.4165
N(-3)/N(5)	7.5106	0.4440
N(3)/N(5)	8.9053	0.5265

----------Distribution of species----------

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma	mole V cm³/mol
H+	1.059e-06	1.000e-06	-5.975	-6.000	-0.025	0.00
OH-	1.062e-08	9.974e-09	-7.974	-8.001	-0.027	-4.09
H2O	5.551e+01	9.998e-01	1.744	-0.000	0.000	18.07
Al	2.491e-07					
AlF2+	1.555e-07	1.464e-07	-6.808	-6.834	-0.026	(0)

AlF+2	3.740e-08	2.937e-08	-7.427	-7.532	-0.105	(0)
Al(OH)2+	2.371e-08	2.232e-08	-7.625	-7.651	-0.026	(0)
AlF3	1.834e-08	1.835e-08	-7.737	-7.736	0.000	(0)
Al(OH)4-	6.480e-09	6.094e-09	-8.188	-8.215	-0.027	(0)
AlOH+2	3.688e-09	2.896e-09	-8.433	-8.538	-0.105	-27.67
Al(OH)3	3.240e-09	3.243e-09	-8.489	-8.489	0.000	(0)
Al+3	4.929e-10	2.953e-10	-9.307	-9.530	-0.223	-42.11
AlSO4+	1.565e-10	1.472e-10	-9.805	-9.832	-0.027	(0)
AlF4-	7.736e-11	7.276e-11	-10.111	-10.138	-0.027	(0)
Al(SO4)2-	7.818e-13	7.353e-13	-12.107	-12.134	-0.027	(0)
AlHSO4+2	1.669e-17	1.303e-17	-16.778	-16.885	-0.107	(0)
B	2.128e-06					
H3BO3	2.127e-06	2.129e-06	-5.672	-5.672	0.000	39.22
H2BO3-	1.298e-09	1.221e-09	-8.887	-8.913	-0.027	(0)
BF(OH)3-	8.958e-12	8.421e-12	-11.048	-11.075	-0.027	(0)
BF2(OH)2-	9.563e-15	8.990e-15	-14.019	-14.046	-0.027	(0)
BF3OH-	1.048e-19	9.852e-20	-18.980	-19.006	-0.027	(0)
BF4-	4.253e-24	3.999e-24	-23.371	-23.398	-0.027	(0)
Ba	2.695e-06					
Ba+2	2.493e-06	1.948e-06	-5.603	-5.710	-0.107	-12.67
BaSO4	1.543e-07	1.544e-07	-6.812	-6.811	0.000	(0)
BaHCO3+	4.762e-08	4.477e-08	-7.322	-7.349	-0.027	(0)
BaCO3	1.129e-10	1.130e-10	-9.947	-9.947	0.000	-10.70
BaNO3+	1.452e-12	1.365e-12	-11.838	-11.865	-0.027	(0)
BaOH+	7.015e-14	6.601e-14	-13.154	-13.180	-0.026	(0)
Br	2.624e-34					
Br-	2.624e-34	2.464e-34	-33.581	-33.608	-0.027	24.57
CdBr+	1.619e-40	1.522e-40	-39.791	-39.817	-0.027	(0)
ZnBr+	0.000e+00	0.000e+00	-40.184	-40.211	-0.027	(0)
PbBr+	0.000e+00	0.000e+00	-40.693	-40.720	-0.027	(0)
CdBr2	0.000e+00	0.000e+00	-72.697	-72.696	0.000	(0)
ZnBr2	0.000e+00	0.000e+00	-74.219	-74.219	0.000	(0)
PbBr2	0.000e+00	0.000e+00	-74.657	-74.657	0.000	(0)
C(4)	8.004e-03					
CO2	5.431e-03	5.435e-03	-2.265	-2.265	0.000	34.42
HCO3-	2.561e-03	2.411e-03	-2.592	-2.618	-0.026	24.70
CaHCO3+	3.408e-06	3.210e-06	-5.467	-5.493	-0.026	9.69
NaHCO3	2.681e-06	2.683e-06	-5.572	-5.571	0.000	1.80
FeHCO3+	2.139e-06	2.011e-06	-5.670	-5.697	-0.027	(0)
MgHCO3+	1.124e-06	1.056e-06	-5.949	-5.976	-0.027	5.49
(CO2)2	5.384e-07	5.388e-07	-6.269	-6.269	0.000	68.85
MnHCO3+	3.791e-07	3.567e-07	-6.421	-6.448	-0.026	(0)
ZnHCO3+	3.067e-07	2.883e-07	-6.513	-6.540	-0.027	(0)
CO3-2	1.434e-07	1.126e-07	-6.843	-6.948	-0.105	-5.19
BaHCO3+	4.762e-08	4.477e-08	-7.322	-7.349	-0.027	(0)
FeCO3	2.252e-08	2.254e-08	-7.647	-7.647	0.000	(0)
ZnCO3	2.133e-08	2.135e-08	-7.671	-7.671	0.000	(0)
CaCO3	1.971e-08	1.973e-08	-7.705	-7.705	0.000	-14.60
MnCO3	1.484e-08	1.485e-08	-7.829	-7.828	0.000	(0)
NaCO3-	4.369e-09	4.107e-09	-8.360	-8.386	-0.027	-1.01
MgCO3	4.013e-09	4.016e-09	-8.397	-8.396	0.000	-17.09
PbHCO3+	2.685e-09	2.524e-09	-8.571	-8.598	-0.027	(0)
PbCO3	2.578e-09	2.580e-09	-8.589	-8.588	0.000	(0)
CdHCO3+	3.385e-10	3.182e-10	-9.470	-9.497	-0.027	(0)
BaCO3	1.129e-10	1.130e-10	-9.947	-9.947	0.000	-10.70
Zn(CO3)2-2	6.583e-11	5.142e-11	-10.182	-10.289	-0.107	(0)
Pb(CO3)2-2	9.347e-13	7.301e-13	-12.029	-12.137	-0.107	(0)
CdCO3	3.731e-13	3.734e-13	-12.428	-12.428	0.000	(0)
CuHCO3+	1.625e-13	1.527e-13	-12.789	-12.816	-0.027	(0)
CuCO3	7.640e-14	7.645e-14	-13.117	-13.117	0.000	(0)
Cd(CO3)2-2	1.703e-16	1.330e-16	-15.769	-15.876	-0.107	(0)
Cu(CO3)2-2	1.388e-17	1.084e-17	-16.858	-16.965	-0.107	(0)
Ca	1.398e-04					
Ca+2	1.333e-04	1.047e-04	-3.875	-3.980	-0.105	-18.06
CaHCO3+	3.408e-06	3.210e-06	-5.467	-5.493	-0.026	9.69
CaSO4	2.935e-06	2.938e-06	-5.532	-5.532	0.000	7.49
CaHPO4	4.379e-08	4.382e-08	-7.359	-7.358	0.000	(0)
CaH2PO4+	3.502e-08	3.297e-08	-7.456	-7.482	-0.026	(0)

CaCO3	1.971e-08	1.973e-08	-7.705	-7.705	0.000	-14.60
CaPO4-	1.097e-10	1.033e-10	-9.960	-9.986	-0.026	(0)
CaHSO4+	2.048e-11	1.926e-11	-10.689	-10.715	-0.027	(0)
CaOH+	1.847e-11	1.736e-11	-10.733	-10.760	-0.027	(0)
Cd	5.874e-09					
Cd+2	5.343e-09	4.173e-09	-8.272	-8.380	-0.107	-18.68
CdHCO3+	3.385e-10	3.182e-10	-9.470	-9.497	-0.027	(0)
CdSO4	1.899e-10	1.900e-10	-9.721	-9.721	0.000	78.14
CdF+	5.565e-13	5.232e-13	-12.255	-12.281	-0.027	(0)
Cd(SO4)2-2	4.222e-13	3.298e-13	-12.374	-12.482	-0.107	-105.69
CdCO3	3.731e-13	3.734e-13	-12.428	-12.428	0.000	(0)
CdOH+	3.640e-13	3.422e-13	-12.439	-12.466	-0.027	(0)
CdNO3+	6.241e-14	5.867e-14	-13.205	-13.232	-0.027	17.55
Cd(CO3)2-2	1.703e-16	1.330e-16	-15.769	-15.876	-0.107	(0)
Cd(OH)2	1.862e-17	1.863e-17	-16.730	-16.730	0.000	(0)
CdF2	1.308e-17	1.309e-17	-16.883	-16.883	0.000	(0)
Cd2OH+3	1.223e-20	7.011e-21	-19.913	-20.154	-0.241	(0)
Cd(OH)3-	2.224e-24	2.090e-24	-23.653	-23.680	-0.027	(0)
Cd(OH)4-2	2.385e-32	1.863e-32	-31.623	-31.730	-0.107	(0)
CdBr+	1.619e-40	1.522e-40	-39.791	-39.817	-0.027	(0)
CdBr2	0.000e+00	0.000e+00	-72.697	-72.696	0.000	(0)
Cu(1)	1.464e-08					
Cu+	1.464e-08	1.374e-08	-7.834	-7.862	-0.028	(0)
Cu(2)	4.075e-13					
CuHCO3+	1.625e-13	1.527e-13	-12.789	-12.816	-0.027	(0)
Cu+2	1.605e-13	1.264e-13	-12.794	-12.898	-0.104	-26.53
CuCO3	7.640e-14	7.645e-14	-13.117	-13.117	0.000	(0)
CuSO4	4.071e-15	4.074e-15	-14.390	-14.390	0.000	13.07
Cu(OH)2	2.638e-15	2.639e-15	-14.579	-14.578	0.000	(0)
CuOH+	1.344e-15	1.264e-15	-14.872	-14.898	-0.027	(0)
CuF+	2.432e-17	2.286e-17	-16.614	-16.641	-0.027	(0)
Cu(CO3)2-2	1.388e-17	1.084e-17	-16.858	-16.965	-0.107	(0)
Cu(OH)3-	1.691e-22	1.590e-22	-21.772	-21.799	-0.027	(0)
Cu2(OH)2+2	8.778e-25	6.856e-25	-24.057	-24.164	-0.107	(0)
Cu(OH)4-2	4.061e-29	3.172e-29	-28.391	-28.499	-0.107	(0)
F	1.106e-05					
F-	1.060e-05	9.958e-06	-4.975	-5.002	-0.027	-1.29
AlF2+	1.555e-07	1.464e-07	-6.808	-6.834	-0.026	(0)
AlF+2	3.740e-08	2.937e-08	-7.427	-7.532	-0.105	(0)
MgF+	2.612e-08	2.457e-08	-7.583	-7.610	-0.027	-10.55
AlF3	1.834e-08	1.835e-08	-7.737	-7.736	0.000	(0)
HF	1.487e-08	1.488e-08	-7.828	-7.827	0.000	12.49
NaF	1.132e-08	1.133e-08	-7.946	-7.946	0.000	7.25
FeF+	8.836e-10	8.306e-10	-9.054	-9.081	-0.027	(0)
ZnF+	1.418e-10	1.333e-10	-9.848	-9.875	-0.027	(0)
MnF+	1.215e-10	1.144e-10	-9.915	-9.942	-0.026	(0)
AlF4-	7.736e-11	7.276e-11	-10.111	-10.138	-0.027	(0)
BF(OH)3-	8.958e-12	8.421e-12	-11.048	-11.075	-0.027	(0)
HF2-	6.040e-13	5.678e-13	-12.219	-12.246	-0.027	22.08
CdF+	5.565e-13	5.232e-13	-12.255	-12.281	-0.027	(0)
PbF+	2.483e-13	2.334e-13	-12.605	-12.632	-0.027	(0)
BF2(OH)2-	9.563e-15	8.990e-15	-14.019	-14.046	-0.027	(0)
PbF2	4.742e-17	4.745e-17	-16.324	-16.324	0.000	(0)
CuF+	2.432e-17	2.286e-17	-16.614	-16.641	-0.027	(0)
CdF2	1.308e-17	1.309e-17	-16.883	-16.883	0.000	(0)
BF3OH-	1.048e-19	9.852e-20	-18.980	-19.006	-0.027	(0)
FeF+2	7.626e-20	5.979e-20	-19.118	-19.223	-0.106	(0)
FeF2+	2.513e-20	2.365e-20	-19.600	-19.626	-0.026	(0)
PbF3-	3.642e-21	3.423e-21	-20.439	-20.466	-0.027	(0)
FeF3	3.727e-22	3.730e-22	-21.429	-21.428	0.000	(0)
BF4-	4.253e-24	3.999e-24	-23.371	-23.398	-0.027	(0)
PbF4-2	2.089e-26	1.632e-26	-25.680	-25.787	-0.107	(0)
SiF6-2	2.293e-27	1.798e-27	-26.640	-26.745	-0.106	42.65
Fe(2)	1.308e-05					
Fe+2	1.060e-05	8.341e-06	-4.975	-5.079	-0.104	-22.07
FeHCO3+	2.139e-06	2.011e-06	-5.670	-5.697	-0.027	(0)
FeSO4	2.335e-07	2.337e-07	-6.632	-6.631	0.000	19.17
FeH2PO4+	5.488e-08	5.166e-08	-7.261	-7.287	-0.026	(0)

FeHPO4	2.543e-08	2.545e-08	-7.595	-7.594	0.000	(0)
FeCO3	2.252e-08	2.254e-08	-7.647	-7.647	0.000	(0)
FeOH+	2.763e-09	2.600e-09	-8.559	-8.585	-0.026	(0)
FeF+	8.836e-10	8.306e-10	-9.054	-9.081	-0.027	(0)
FeHSO4+	1.633e-12	1.535e-12	-11.787	-11.814	-0.027	(0)
Fe(OH)2	2.175e-14	2.176e-14	-13.663	-13.662	0.000	(0)
Fe(OH)3-	8.575e-19	8.069e-19	-18.067	-18.093	-0.026	(0)
Fe(3)	9.518e-15					
Fe(OH)2+	8.468e-15	7.972e-15	-14.072	-14.098	-0.026	(0)
Fe(OH)3	1.018e-15	1.018e-15	-14.992	-14.992	0.000	(0)
FeOH+2	3.093e-17	2.425e-17	-16.510	-16.615	-0.106	(0)
Fe(OH)4-	9.788e-19	9.214e-19	-18.009	-18.036	-0.026	(0)
FeF+2	7.626e-20	5.979e-20	-19.118	-19.223	-0.106	(0)
FeF2+	2.513e-20	2.365e-20	-19.600	-19.626	-0.026	(0)
FeH2PO4+2	1.609e-20	1.264e-20	-19.793	-19.898	-0.105	(0)
FeSO4+	6.969e-21	6.558e-21	-20.157	-20.183	-0.026	(0)
Fe+3	6.343e-21	3.799e-21	-20.198	-20.420	-0.223	(0)
FeHPO4+	8.278e-22	7.789e-22	-21.082	-21.108	-0.026	(0)
FeF3	3.727e-22	3.730e-22	-21.429	-21.428	0.000	(0)
Fe(SO4)2-	2.411e-23	2.266e-23	-22.618	-22.645	-0.027	(0)
FeHSO4+2	2.248e-26	1.756e-26	-25.648	-25.755	-0.107	(0)
Fe2(OH)2+4	4.288e-32	1.596e-32	-31.368	-31.797	-0.429	(0)
Fe3(OH)4+5	0.000e+00	0.000e+00	-42.897	-43.568	-0.671	(0)
H(0)	6.103e-11					
H2	3.051e-11	3.054e-11	-10.515	-10.515	0.000	28.61
K	1.074e-04					
K+	1.073e-04	1.008e-04	-3.969	-3.996	-0.027	9.02
KSO4-	1.186e-07	1.116e-07	-6.926	-6.952	-0.026	34.12
KHPO4-	1.601e-10	1.507e-10	-9.796	-9.822	-0.026	38.15
Mg	5.020e-05					
Mg+2	4.762e-05	3.747e-05	-4.322	-4.426	-0.104	-21.73
MgSO4	1.381e-06	1.382e-06	-5.860	-5.860	0.000	5.83
MgHCO3+	1.124e-06	1.056e-06	-5.949	-5.976	-0.027	5.49
MgF+	2.612e-08	2.457e-08	-7.583	-7.610	-0.027	-10.55
MgHPO4	2.120e-08	2.121e-08	-7.674	-7.673	0.000	(0)
MgH2PO4+	1.597e-08	1.503e-08	-7.797	-7.823	-0.026	(0)
MgCO3	4.013e-09	4.016e-09	-8.397	-8.396	0.000	-17.09
MgOH+	1.419e-10	1.337e-10	-9.848	-9.874	-0.026	(0)
MgPO4-	5.300e-11	4.990e-11	-10.276	-10.302	-0.026	(0)
Mn(2)	2.549e-06					
Mn+2	2.108e-06	1.660e-06	-5.676	-5.780	-0.104	-20.49
MnHCO3+	3.791e-07	3.567e-07	-6.421	-6.448	-0.026	(0)
MnSO4	4.646e-08	4.649e-08	-7.333	-7.333	0.000	22.63
MnCO3	1.484e-08	1.485e-08	-7.829	-7.828	0.000	(0)
MnF+	1.215e-10	1.144e-10	-9.915	-9.942	-0.026	(0)
MnOH+	4.464e-11	4.200e-11	-10.350	-10.377	-0.026	(0)
Mn(NO3)2	2.046e-16	2.048e-16	-15.689	-15.689	0.000	41.09
Mn(OH)3-	2.794e-23	2.629e-23	-22.554	-22.580	-0.026	(0)
Mn(3)	4.014e-34					
Mn+3	4.014e-34	2.405e-34	-33.396	-33.619	-0.223	(0)
N(-3)	7.141e-07					
NH4+	7.123e-07	6.685e-07	-6.147	-6.175	-0.028	17.98
NH4SO4-	1.448e-09	1.361e-09	-8.839	-8.866	-0.027	37.59
NH3	3.756e-10	3.759e-10	-9.425	-9.425	0.000	24.41
N(3)	3.571e-07					
NO2-	3.571e-07	3.353e-07	-6.447	-6.475	-0.027	24.98
N(5)	5.927e-06					
NO3-	5.927e-06	5.566e-06	-5.227	-5.254	-0.027	29.49
BaNO3+	1.452e-12	1.365e-12	-11.838	-11.865	-0.027	(0)
PbNO3+	1.154e-13	1.085e-13	-12.938	-12.965	-0.027	(0)
CdNO3+	6.241e-14	5.867e-14	-13.205	-13.232	-0.027	17.55
Mn(NO3)2	2.046e-16	2.048e-16	-15.689	-15.689	0.000	41.09
Na	2.106e-03					
Na+	2.102e-03	1.977e-03	-2.677	-2.704	-0.027	-1.45
NaHCO3	2.681e-06	2.683e-06	-5.572	-5.571	0.000	1.80
NaSO4-	1.662e-06	1.564e-06	-5.779	-5.806	-0.026	13.95
NaF	1.132e-08	1.133e-08	-7.946	-7.946	0.000	7.25
NaCO3-	4.369e-09	4.107e-09	-8.360	-8.386	-0.027	-1.01

NaHPO4-	3.138e-09	2.954e-09	-8.503	-8.530	-0.026	33.67
NaOH	1.970e-21	1.972e-21	-20.705	-20.705	0.000	(0)
O(0)	0.000e+00					
O2	0.000e+00	0.000e+00	-71.411	-71.411	0.000	30.39
P	1.431e-05					
H2PO4-	1.313e-05	1.236e-05	-4.882	-4.908	-0.026	33.24
HPO4-2	9.775e-07	7.664e-07	-6.010	-6.116	-0.106	6.81
FeH2PO4+	5.488e-08	5.166e-08	-7.261	-7.287	-0.026	(0)
CaHPO4	4.379e-08	4.382e-08	-7.359	-7.358	0.000	(0)
CaH2PO4+	3.502e-08	3.297e-08	-7.456	-7.482	-0.026	(0)
FeHPO4	2.543e-08	2.545e-08	-7.595	-7.594	0.000	(0)
MgHPO4	2.120e-08	2.121e-08	-7.674	-7.673	0.000	(0)
MgH2PO4+	1.597e-08	1.503e-08	-7.797	-7.823	-0.026	(0)
NaHPO4-	3.138e-09	2.954e-09	-8.503	-8.530	-0.026	33.67
H3PO4	1.814e-09	1.815e-09	-8.741	-8.741	0.000	47.40
KHPO4-	1.601e-10	1.507e-10	-9.796	-9.822	-0.026	38.15
CaPO4-	1.097e-10	1.033e-10	-9.960	-9.986	-0.026	(0)
MgPO4-	5.300e-11	4.990e-11	-10.276	-10.302	-0.026	(0)
PO4-3	6.007e-13	3.442e-13	-12.221	-12.463	-0.242	-23.01
FeH2PO4+2	1.609e-20	1.264e-20	-19.793	-19.898	-0.105	(0)
FeHPO4+	8.278e-22	7.789e-22	-21.082	-21.108	-0.026	(0)
Pb	7.097e-09					
PbHCO3+	2.685e-09	2.524e-09	-8.571	-8.598	-0.027	(0)
PbCO3	2.578e-09	2.580e-09	-8.589	-8.588	0.000	(0)
Pb+2	1.688e-09	1.318e-09	-8.773	-8.880	-0.107	-15.46
PbSO4	1.171e-10	1.172e-10	-9.932	-9.931	0.000	(0)
PbOH+	2.733e-11	2.569e-11	-10.563	-10.590	-0.027	(0)
Pb(CO3)2-2	9.347e-13	7.301e-13	-12.029	-12.137	-0.107	(0)
PbF+	2.483e-13	2.334e-13	-12.605	-12.632	-0.027	(0)
Pb(SO4)2-2	1.244e-13	9.719e-14	-12.905	-13.012	-0.107	(0)
PbNO3+	1.154e-13	1.085e-13	-12.938	-12.965	-0.027	(0)
Pb(OH)2	9.987e-15	9.994e-15	-14.001	-14.000	0.000	(0)
PbF2	4.742e-17	4.745e-17	-16.324	-16.324	0.000	(0)
Pb2OH+3	1.322e-18	7.582e-19	-17.879	-18.120	-0.241	(0)
Pb(OH)3-	1.220e-19	1.147e-19	-18.914	-18.940	-0.027	(0)
PbF3-	3.642e-21	3.423e-21	-20.439	-20.466	-0.027	(0)
Pb(OH)4-2	3.364e-25	2.628e-25	-24.473	-24.580	-0.107	(0)
PbF4-2	2.089e-26	1.632e-26	-25.680	-25.787	-0.107	(0)
Pb3(OH)4+2	3.753e-27	2.931e-27	-26.426	-26.533	-0.107	(0)
PbBr+	0.000e+00	0.000e+00	-40.693	-40.720	-0.027	(0)
PbBr2	0.000e+00	0.000e+00	-74.657	-74.657	0.000	(0)
S(6)	2.083e-04					
SO4-2	2.017e-04	1.581e-04	-3.695	-3.801	-0.106	14.58
CaSO4	2.935e-06	2.938e-06	-5.532	-5.532	0.000	7.49
NaSO4-	1.662e-06	1.564e-06	-5.779	-5.806	-0.026	13.95
MgSO4	1.381e-06	1.382e-06	-5.860	-5.860	0.000	5.83
FeSO4	2.335e-07	2.337e-07	-6.632	-6.631	0.000	19.17
BaSO4	1.543e-07	1.544e-07	-6.812	-6.811	0.000	(0)
KSO4-	1.186e-07	1.116e-07	-6.926	-6.952	-0.026	34.12
MnSO4	4.646e-08	4.649e-08	-7.333	-7.333	0.000	22.63
ZnSO4	3.512e-08	3.515e-08	-7.454	-7.454	0.000	21.75
HSO4-	1.628e-08	1.530e-08	-7.788	-7.815	-0.027	40.29
NH4SO4-	1.448e-09	1.361e-09	-8.839	-8.866	-0.027	37.59
CdSO4	1.899e-10	1.900e-10	-9.721	-9.721	0.000	78.14
AlSO4+	1.565e-10	1.472e-10	-9.805	-9.832	-0.027	(0)
PbSO4	1.171e-10	1.172e-10	-9.932	-9.931	0.000	(0)
Zn(SO4)2-2	5.791e-11	4.523e-11	-10.237	-10.345	-0.107	-13.19
CaHSO4+	2.048e-11	1.926e-11	-10.689	-10.715	-0.027	(0)
FeHSO4+	1.633e-12	1.535e-12	-11.787	-11.814	-0.027	(0)
Al(SO4)2-	7.818e-13	7.353e-13	-12.107	-12.134	-0.027	(0)
Cd(SO4)2-2	4.222e-13	3.298e-13	-12.374	-12.482	-0.107	-105.69
Pb(SO4)2-2	1.244e-13	9.719e-14	-12.905	-13.012	-0.107	(0)
CuSO4	4.071e-15	4.074e-15	-14.390	-14.390	0.000	13.07
AlHSO4+2	1.669e-17	1.303e-17	-16.778	-16.885	-0.107	(0)
FeSO4+	6.969e-21	6.558e-21	-20.157	-20.183	-0.026	(0)
Fe(SO4)2-	2.411e-23	2.266e-23	-22.618	-22.645	-0.027	(0)
FeHSO4+2	2.248e-26	1.756e-26	-25.648	-25.755	-0.107	(0)
Si	1.195e-03					

H4SiO4	1.195e-03	1.196e-03	-2.923	-2.922	0.000	52.09
H3SiO4-	1.864e-07	1.752e-07	-6.730	-6.756	-0.027	27.99
H2SiO4-2	1.499e-14	1.177e-14	-13.824	-13.929	-0.105	(0)
SiF6-2	2.293e-27	1.798e-27	-26.640	-26.745	-0.106	42.65
Zn	1.576e-06					
Zn+2	1.212e-06	9.499e-07	-5.917	-6.022	-0.106	-25.27
ZnHCO3+	3.067e-07	2.883e-07	-6.513	-6.540	-0.027	(0)
ZnSO4	3.512e-08	3.515e-08	-7.454	-7.454	0.000	21.75
ZnCO3	2.133e-08	2.135e-08	-7.671	-7.671	0.000	(0)
ZnOH+	1.092e-09	1.026e-09	-8.962	-8.989	-0.027	(0)
ZnF+	1.418e-10	1.333e-10	-9.848	-9.875	-0.027	(0)
Zn(CO3)2-2	6.583e-11	5.142e-11	-10.182	-10.289	-0.107	(0)
Zn(SO4)2-2	5.791e-11	4.523e-11	-10.237	-10.345	-0.107	-13.19
Zn(OH)2	1.195e-11	1.195e-11	-10.923	-10.922	0.000	(0)
Zn(OH)3-	4.020e-17	3.779e-17	-16.396	-16.423	-0.027	(0)
Zn(OH)4-2	7.668e-24	5.989e-24	-23.115	-23.223	-0.107	(0)
ZnBr+	0.000e+00	0.000e+00	-40.184	-40.211	-0.027	(0)
ZnBr2	0.000e+00	0.000e+00	-74.219	-74.219	0.000	(0)

----------Distribution of alkalinity----------

Total alkalinity (eq/kgw) = 2.572e-03

Species	Alkalinity	Molality	Alk/Mol
HCO3-	2.561e-03	2.561e-03	1.00
CaHCO3+	3.408e-06	3.408e-06	1.00
NaHCO3	2.681e-06	2.681e-06	1.00
FeHCO3+	2.139e-06	2.139e-06	1.00
MgHCO3+	1.124e-06	1.124e-06	1.00
H+	-1.059e-06	1.059e-06	-1.00
HPO4-2	9.775e-07	9.775e-07	1.00
MnHCO3+	3.791e-07	3.791e-07	1.00
ZnHCO3+	3.067e-07	3.067e-07	1.00
CO3-2	2.869e-07	1.434e-07	2.00
H3SiO4-	1.864e-07	1.864e-07	1.00
BaHCO3+	4.762e-08	4.762e-08	1.00
Al(OH)2+	4.742e-08	2.371e-08	2.00
FeCO3	4.505e-08	2.252e-08	2.00
CaHPO4	4.379e-08	4.379e-08	1.00
ZnCO3	4.267e-08	2.133e-08	2.00
CaCO3	3.943e-08	1.971e-08	2.00
MnCO3	2.968e-08	1.484e-08	2.00
Al(OH)4-	2.592e-08	6.480e-09	4.00
FeHPO4	2.543e-08	2.543e-08	1.00
MgHPO4	2.120e-08	2.120e-08	1.00
HSO4-	-1.628e-08	1.628e-08	-1.00
HF	-1.487e-08	1.487e-08	-1.00
OH-	1.062e-08	1.062e-08	1.00
Al(OH)3	9.720e-09	3.240e-09	3.00
NaCO3-	8.737e-09	4.369e-09	2.00
MgCO3	8.026e-09	4.013e-09	2.00
PbCO3	5.156e-09	2.578e-09	2.00
AlOH+2	3.688e-09	3.688e-09	1.00
NaHPO4-	3.138e-09	3.138e-09	1.00
FeOH+	2.763e-09	2.763e-09	1.00
PbHCO3+	2.685e-09	2.685e-09	1.00
H3PO4	-1.814e-09	1.814e-09	-1.00
H2BO3-	1.298e-09	1.298e-09	1.00
ZnOH+	1.092e-09	1.092e-09	1.00
NH3	3.756e-10	3.756e-10	1.00
CdHCO3+	3.385e-10	3.385e-10	1.00
Zn(CO3)2-2	2.633e-10	6.583e-11	4.00
BaCO3	2.258e-10	1.129e-10	2.00
CaPO4-	2.195e-10	1.097e-10	2.00
KHPO4-	1.601e-10	1.601e-10	1.00
MgOH+	1.419e-10	1.419e-10	1.00
MgPO4-	1.060e-10	5.300e-11	2.00

MnOH+	4.464e-11	4.464e-11	1.00
PbOH+	2.733e-11	2.733e-11	1.00
Zn(OH)2	2.389e-11	1.195e-11	2.00
CaHSO4+	-2.048e-11	2.048e-11	-1.00
CaOH+	1.847e-11	1.847e-11	1.00
Pb(CO3)2-2	3.739e-12	9.347e-13	4.00
FeHSO4+	-1.633e-12	1.633e-12	-1.00
PO4-3	1.201e-12	6.007e-13	2.00
CdCO3	7.463e-13	3.731e-13	2.00
HF2-	-6.040e-13	6.040e-13	-1.00
CdOH+	3.640e-13	3.640e-13	1.00
CuHCO3+	1.625e-13	1.625e-13	1.00
CuCO3	1.528e-13	7.640e-14	2.00
BaOH+	7.015e-14	7.015e-14	1.00
Fe(OH)2	4.349e-14	2.175e-14	2.00
H2SiO4-2	2.997e-14	1.499e-14	2.00
Pb(OH)2	1.997e-14	9.987e-15	2.00
BF2(OH)2-	-9.563e-15	9.563e-15	-1.00
Cu(OH)2	5.275e-15	2.638e-15	2.00
CuOH+	1.344e-15	1.344e-15	1.00
Fe(OH)3	1.018e-15	1.018e-15	1.00
Cd(CO3)2-2	6.812e-16	1.703e-16	4.00
Zn(OH)3-	1.206e-16	4.020e-17	3.00
Cu(CO3)2-2	5.553e-17	1.388e-17	4.00
Cd(OH)2	3.724e-17	1.862e-17	2.00
FeOH+2	-3.093e-17	3.093e-17	-1.00
AlHSO4+2	-1.669e-17	1.669e-17	-1.00
Fe(OH)3-	2.572e-18	8.575e-19	3.00
Fe(OH)4-	1.958e-18	9.788e-19	2.00
Pb2OH+3	1.322e-18	1.322e-18	1.00
Pb(OH)3-	3.661e-19	1.220e-19	3.00
BF3OH-	-2.096e-19	1.048e-19	-2.00
FeF+2	-1.525e-19	7.626e-20	-2.00
FeF2+	-5.027e-20	2.513e-20	-2.00
FeH2PO4+2	-3.218e-20	1.609e-20	-2.00
FeSO4+	-1.394e-20	6.969e-21	-2.00
Fe+3	-1.269e-20	6.343e-21	-2.00
Cd2OH+3	1.223e-20	1.223e-20	1.00
NaOH	1.970e-21	1.970e-21	1.00
FeHPO4+	-8.278e-22	8.278e-22	-1.00
FeF3	-7.455e-22	3.727e-22	-2.00
Cu(OH)3-	5.074e-22	1.691e-22	3.00
Mn(OH)3-	8.382e-23	2.794e-23	3.00
Fe(SO4)2-	-4.821e-23	2.411e-23	-2.00
Zn(OH)4-2	3.067e-23	7.668e-24	4.00
BF4-	-1.276e-23	4.253e-24	-3.00
Cd(OH)3-	6.671e-24	2.224e-24	3.00
Cu2(OH)2+2	1.756e-24	8.778e-25	2.00
Pb(OH)4-2	1.346e-24	3.364e-25	4.00
FeHSO4+2	-6.745e-26	2.248e-26	-3.00
Pb3(OH)4+2	1.501e-26	3.753e-27	4.00
SiF6-2	-9.172e-27	2.293e-27	-4.00
Cu(OH)4-2	1.625e-28	4.061e-29	4.00
Cd(OH)4-2	9.539e-32	2.385e-32	4.00
Fe2(OH)2+4	-8.576e-32	4.288e-32	-2.00
Fe3(OH)4+5	-0.000e+00	0.000e+00	-2.00

-------------------------------Saturation indices-------------------------------

Phase	SI**	log IAP	log K(297 K, 1 atm)	
Al(OH)3(a)	-2.34	8.47	10.81	Al(OH)3
Albite	-1.67	-19.69	-18.01	NaAlSi3O8
Alunite	-2.81	-4.19	-1.38	KAl3(SO4)2(OH)6
Anglesite	-4.89	-12.68	-7.79	PbSO4
Anhydrite	-3.51	-7.78	-4.28	CaSO4
Anorthite	-6.53	-26.25	-19.72	CaAl2Si2O8
Aragonite	-2.59	-10.93	-8.33	CaCO3

Barite	0.33	-9.51	-9.85	BaSO4
Ca-Montmorillonite	2.53	-42.52	-45.05	Ca0.165Al2.33Si3.67O10(OH)2
Calcite	-2.45	-10.93	-8.48	CaCO3
Cd(OH)2	-10.03	3.62	13.65	Cd(OH)2
CdSiO3	-8.37	0.70	9.07	CdSiO3
CdSO4	-12.09	-12.18	-0.09	CdSO4
Cerussite	-2.70	-15.83	-13.13	PbCO3
Chalcedony	0.63	-2.92	-3.55	SiO2
Chlorite(14A)	-22.41	46.04	68.45	Mg5Al2Si3O10(OH)8
Chrysotile	-15.35	16.88	32.22	Mg3Si2O5(OH)4
CO2(g)	-0.80	-2.26	-1.47	CO2
Dolomite	-5.22	-22.30	-17.09	CaMg(CO3)2
Fe(OH)3(a)	-7.31	-2.42	4.89	Fe(OH)3
Fluorite	-3.38	-13.98	-10.60	CaF2
Gibbsite	0.35	8.47	8.12	Al(OH)3
Goethite	-1.43	-2.42	-0.99	FeOOH
Gypsum	-3.20	-7.78	-4.58	CaSO4:2H2O
H2(g)	-7.41	-10.52	-3.10	H2
H2O(g)	-1.51	-0.00	1.51	H2O
Hausmannite	-35.05	26.03	61.08	Mn3O4
Hematite	-0.85	-4.84	-3.99	Fe2O3
Hydroxyapatite	-10.84	-14.25	-3.40	Ca5(PO4)3OH
Illite	0.47	-39.83	-40.29	K0.6Mg0.25Al2.3Si3.5O10(OH)2
Jarosite-K	-27.66	-36.86	-9.20	KFe3(SO4)2(OH)6
K-feldspar	-0.39	-20.98	-20.59	KAlSi3O8
K-mica	5.92	18.65	12.73	KAl3Si3O10(OH)2
Kaolinite	3.64	11.10	7.45	Al2Si2O5(OH)4
Manganite	-15.44	9.90	25.34	MnOOH
Melanterite	-6.67	-8.88	-2.21	FeSO4:7H2O
NH3(g)	-11.23	-9.42	1.80	NH3
O2(g)	-68.52	-71.41	-2.89	O2
Otavite	-3.23	-15.33	-12.10	CdCO3
Pb(OH)2	-5.04	3.12	8.16	Pb(OH)2
Pyrochroite	-8.98	6.22	15.20	Mn(OH)2
Pyrolusite	-27.82	13.59	41.41	MnO2:H2O
Quartz	1.06	-2.92	-3.98	SiO2
Rhodochrosite	-1.60	-12.73	-11.13	MnCO3
Sepiolite	-9.38	6.38	15.77	Mg2Si3O7.5OH:3H2O
Sepiolite(d)	-12.28	6.38	18.66	Mg2Si3O7.5OH:3H2O
Siderite	-1.14	-12.03	-10.89	FeCO3
SiO2(a)	-0.21	-2.92	-2.71	SiO2
Smithsonite	-2.97	-12.97	-10.00	ZnCO3
Talc	-10.39	11.03	21.42	Mg3Si4O10(OH)2
Vivianite	-4.16	-40.16	-36.00	Fe3(PO4)2:8H2O
Willemite	-6.31	9.03	15.35	Zn2SiO4
Witherite	-4.10	-12.66	-8.56	BaCO3
Zn(OH)2(e)	-5.52	5.98	11.50	Zn(OH)2

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
For ideal gases, phi = 1.

Initial solution 31.

-----------------------------Solution composition--------------------------------

Elements	Molality	Moles
Al	5.603e-08	5.603e-08
Alkalinity	2.886e-03	2.886e-03
B	2.241e-06	2.241e-06
Ba	1.283e-05	1.283e-05
Br	5.399e-34	5.399e-34
Ca	4.522e-03	4.522e-03
Cd	6.146e-09	6.146e-09
Cl	1.768e-02	1.768e-02
Cu	2.600e-07	2.600e-07
Fe	4.224e-04	4.224e-04
K	4.814e-04	4.814e-04

Mg	7.837e-04	7.837e-04
Mn	8.274e-05	8.274e-05
N(-3)	5.433e-06	5.433e-06
N(3)	1.072e-06	1.072e-06
N(5)	4.146e-06	4.146e-06
Na	6.271e-03	6.271e-03
P	2.101e-06	2.101e-06
Pb	1.174e-08	1.174e-08
Si	1.166e-03	1.166e-03
Zn	1.473e-06	1.473e-06

----------Description of solution----------

pH	= 7.000
pe	= -2.047
Specific Conductance (µS/cm, 25°C)	= 2100
Density (g/cm³)	= 0.99809
Volume (L)	= 1.00325
Activity of water	= 0.999
Ionic strength (mol/kgw)	= 2.448e-02
Mass of water (kg)	= 1.000e+00
Total carbon (mol/kg)	= 3.387e-03
Total CO2 (mol/kg)	= 3.387e-03
Temperature (°C)	= 24.74
Electrical balance (eq)	= -2.164e-03
Percent error, 100*(Cat-|An|)/(Cat+|An|)	= -5.74
Iterations	= 11 (331 overall)
Total H	= 1.110200e+02
Total O	= 5.552055e+01

----------Redox couples----------

Redox couple	pe	Eh (volts)
N(-3)/N(3)	5.6497	0.3339
N(-3)/N(5)	6.1355	0.3626
N(3)/N(5)	7.5928	0.4488

----------Distribution of species----------

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma	mole V cm³/mol
OH-	1.159e-07	9.917e-08	-6.936	-7.004	-0.068	-3.97
H+	1.134e-07	1.000e-07	-6.945	-7.000	-0.055	0.00
H2O	5.551e+01	9.994e-01	1.744	-0.000	0.000	18.07
Al	5.603e-08					
Al(OH)4-	5.174e-08	4.457e-08	-7.286	-7.351	-0.065	(0)
Al(OH)3	2.361e-09	2.374e-09	-8.627	-8.624	0.002	(0)
Al(OH)2+	1.898e-09	1.644e-09	-8.722	-8.784	-0.062	(0)
AlOH+2	3.815e-11	2.146e-11	-10.419	-10.668	-0.250	-27.40
Al+3	6.809e-13	2.199e-13	-12.167	-12.658	-0.491	-41.60
B	2.241e-06					
H3BO3	2.227e-06	2.239e-06	-5.652	-5.650	0.002	39.21
H2BO3-	1.490e-08	1.282e-08	-7.827	-7.892	-0.065	(0)
Ba	1.283e-05					
Ba+2	1.229e-05	6.740e-06	-4.910	-5.171	-0.261	-12.39
BaCl+	3.626e-07	3.120e-07	-6.441	-6.506	-0.065	(0)
BaHCO3+	1.729e-07	1.488e-07	-6.762	-6.827	-0.065	(0)
BaCO3	3.731e-09	3.752e-09	-8.428	-8.426	0.002	-10.70
BaNO3+	3.487e-12	3.001e-12	-11.458	-11.523	-0.065	(0)
BaOH+	2.642e-12	2.283e-12	-11.578	-11.642	-0.063	(0)
Br	5.399e-34					
Br-	5.399e-34	4.605e-34	-33.268	-33.337	-0.069	24.66
CdBr+	1.337e-40	1.151e-40	-39.874	-39.939	-0.065	(0)
ZnBr+	0.000e+00	0.000e+00	-40.068	-40.133	-0.065	(0)
PbBr+	0.000e+00	0.000e+00	-40.808	-40.874	-0.065	(0)
CdBr2	0.000e+00	0.000e+00	-72.549	-72.546	0.002	(0)

ZnBr2	0.000e+00	0.000e+00	-73.872	-73.870	0.002	(0)
PbBr2	0.000e+00	0.000e+00	-74.541	-74.539	0.002	(0)
C(4)	3.387e-03					
HCO3-	2.681e-03	2.322e-03	-2.572	-2.634	-0.062	24.84
CO2	5.211e-04	5.240e-04	-3.283	-3.281	0.002	34.42
CaHCO3+	8.465e-05	7.357e-05	-4.072	-4.133	-0.061	9.75
FeHCO3+	5.485e-05	4.720e-05	-4.261	-4.326	-0.065	(0)
MgHCO3+	1.387e-05	1.191e-05	-4.858	-4.924	-0.066	5.56
MnHCO3+	9.222e-06	7.968e-06	-5.035	-5.099	-0.063	(0)
NaHCO3	6.536e-06	6.573e-06	-5.185	-5.182	0.002	1.80
FeCO3	5.252e-06	5.282e-06	-5.280	-5.277	0.002	(0)
CaCO3	4.488e-06	4.513e-06	-5.348	-5.345	0.002	-14.60
MnCO3	3.294e-06	3.313e-06	-5.482	-5.480	0.002	(0)
CO3-2	1.925e-06	1.083e-06	-5.716	-5.965	-0.250	-4.81
MgCO3	4.491e-07	4.517e-07	-6.348	-6.345	0.002	-17.09
ZnHCO3+	2.066e-07	1.778e-07	-6.685	-6.750	-0.065	(0)
BaHCO3+	1.729e-07	1.488e-07	-6.762	-6.827	-0.065	(0)
ZnCO3	1.307e-07	1.314e-07	-6.884	-6.881	0.002	(0)
NaCO3-	1.163e-07	1.001e-07	-6.935	-7.000	-0.065	-0.83
PbCO3	9.275e-09	9.327e-09	-8.033	-8.030	0.002	(0)
Zn(CO3)2-2	5.550e-09	3.044e-09	-8.256	-8.517	-0.261	(0)
(CO2)2	4.969e-09	4.997e-09	-8.304	-8.301	0.002	68.84
BaCO3	3.731e-09	3.752e-09	-8.428	-8.426	0.002	-10.70
PbHCO3+	1.062e-09	9.139e-10	-8.974	-9.039	-0.065	(0)
CdHCO3+	1.440e-10	1.239e-10	-9.842	-9.907	-0.065	(0)
Pb(CO3)2-2	4.628e-11	2.538e-11	-10.335	-10.596	-0.261	(0)
CdCO3	1.444e-12	1.452e-12	-11.840	-11.838	0.002	(0)
CuCO3	3.051e-13	3.068e-13	-12.516	-12.513	0.002	(0)
CuHCO3+	7.132e-14	6.138e-14	-13.147	-13.212	-0.065	(0)
Cd(CO3)2-2	9.070e-15	4.974e-15	-14.042	-14.303	-0.261	(0)
Cu(CO3)2-2	7.629e-16	4.184e-16	-15.118	-15.378	-0.261	(0)
Ca	4.522e-03					
Ca+2	4.432e-03	2.493e-03	-2.353	-2.603	-0.250	-17.78
CaHCO3+	8.465e-05	7.357e-05	-4.072	-4.133	-0.061	9.75
CaCO3	4.488e-06	4.513e-06	-5.348	-5.345	0.002	-14.60
CaHPO4	4.354e-07	4.379e-07	-6.361	-6.359	0.002	(0)
CaH2PO4+	3.805e-08	3.295e-08	-7.420	-7.482	-0.062	(0)
CaPO4-	1.190e-08	1.031e-08	-7.924	-7.987	-0.062	(0)
CaOH+	4.806e-09	4.136e-09	-8.318	-8.383	-0.065	(0)
Cd	6.146e-09					
Cd+2	3.078e-09	1.688e-09	-8.512	-8.773	-0.261	-18.41
CdCl+	2.765e-09	2.379e-09	-8.558	-8.624	-0.065	6.03
CdCl2	1.455e-10	1.464e-10	-9.837	-9.835	0.002	23.14
CdHCO3+	1.440e-10	1.239e-10	-9.842	-9.907	-0.065	(0)
CdOHCl	9.712e-12	9.767e-12	-11.013	-11.010	0.002	(0)
CdOH+	1.599e-12	1.376e-12	-11.796	-11.861	-0.065	(0)
CdCl3-	1.579e-12	1.359e-12	-11.802	-11.867	-0.065	69.62
CdCO3	1.444e-12	1.452e-12	-11.840	-11.838	0.002	(0)
CdNO3+	1.755e-14	1.511e-14	-13.756	-13.821	-0.065	17.64
Cd(CO3)2-2	9.070e-15	4.974e-15	-14.042	-14.303	-0.261	(0)
Cd(OH)2	7.488e-16	7.530e-16	-15.126	-15.123	0.002	(0)
Cd2OH+3	4.411e-20	1.141e-20	-19.356	-19.943	-0.587	(0)
Cd(OH)3-	9.813e-22	8.444e-22	-21.008	-21.073	-0.065	(0)
Cd(OH)4-2	1.372e-28	7.522e-29	-27.863	-28.124	-0.261	(0)
CdBr+	1.337e-40	1.151e-40	-39.874	-39.939	-0.065	(0)
CdBr2	0.000e+00	0.000e+00	-72.549	-72.546	0.002	(0)
Cl	1.768e-02					
Cl-	1.723e-02	1.477e-02	-1.764	-1.831	-0.067	18.18
NaCl	4.410e-04	4.435e-04	-3.356	-3.353	0.002	(0)
FeCl+	4.817e-06	4.145e-06	-5.317	-5.382	-0.065	(0)
MnCl+	2.682e-06	2.317e-06	-5.572	-5.635	-0.063	-3.07
BaCl+	3.626e-07	3.120e-07	-6.441	-6.506	-0.065	(0)
CuCl2-	2.474e-07	2.125e-07	-6.607	-6.673	-0.066	(0)
ZnCl+	2.784e-08	2.391e-08	-7.555	-7.622	-0.066	-14.15
MnCl2	1.486e-08	1.494e-08	-7.828	-7.826	0.002	86.21
CuCl3-2	8.916e-09	4.970e-09	-8.050	-8.304	-0.254	(0)
ZnOHCl	2.957e-09	2.973e-09	-8.529	-8.527	0.002	(0)
CdCl+	2.765e-09	2.379e-09	-8.558	-8.624	-0.065	6.03

ZnCl2	3.673e-10	3.694e-10	-9.435	-9.432	0.002	102.54
PbCl+	3.365e-10	2.896e-10	-9.473	-9.538	-0.065	8.03
CdCl2	1.455e-10	1.464e-10	-9.837	-9.835	0.002	23.14
MnCl3-	7.037e-11	6.080e-11	-10.153	-10.216	-0.063	43.53
CdOHCl	9.712e-12	9.767e-12	-11.013	-11.010	0.002	(0)
ZnCl3-	7.120e-12	6.114e-12	-11.148	-11.214	-0.066	16.89
PbCl2	6.774e-12	6.812e-12	-11.169	-11.167	0.002	34.95
CdCl3-	1.579e-12	1.359e-12	-11.802	-11.867	-0.065	69.62
PbCl3-	9.275e-14	7.981e-14	-13.033	-13.098	-0.065	66.04
ZnCl4-2	8.104e-14	4.517e-14	-13.091	-13.345	-0.254	145.68
CuCl+	2.411e-15	2.071e-15	-14.618	-14.684	-0.066	0.82
PbCl4-2	1.027e-15	5.632e-16	-14.988	-15.249	-0.261	101.78
CuCl2	1.629e-17	1.638e-17	-16.788	-16.786	0.002	30.71
FeCl+2	1.363e-19	7.599e-20	-18.865	-19.119	-0.254	(0)
FeCl2+	5.852e-21	5.056e-21	-20.233	-20.296	-0.063	(0)
CuCl3-	9.953e-22	8.547e-22	-21.002	-21.068	-0.066	(0)
FeCl3	7.427e-24	7.469e-24	-23.129	-23.127	0.002	(0)
CuCl4-2	1.128e-25	6.290e-26	-24.948	-25.201	-0.254	(0)
Cu(1)	2.600e-07					
CuCl2-	2.474e-07	2.125e-07	-6.607	-6.673	-0.066	(0)
CuCl3-2	8.916e-09	4.970e-09	-8.050	-8.304	-0.254	(0)
Cu+	3.621e-09	3.077e-09	-8.441	-8.512	-0.071	(0)
Cu(2)	5.877e-13					
CuCO3	3.051e-13	3.068e-13	-12.516	-12.513	0.002	(0)
Cu(OH)2	1.094e-13	1.101e-13	-12.961	-12.958	0.002	(0)
Cu+2	9.248e-14	5.274e-14	-13.034	-13.278	-0.244	-26.26
CuHCO3+	7.132e-14	6.138e-14	-13.147	-13.212	-0.065	(0)
CuOH+	6.139e-15	5.271e-15	-14.212	-14.278	-0.066	(0)
CuCl+	2.411e-15	2.071e-15	-14.618	-14.684	-0.066	0.82
Cu(CO3)2-2	7.629e-16	4.184e-16	-15.118	-15.378	-0.261	(0)
CuCl2	1.629e-17	1.638e-17	-16.788	-16.786	0.002	30.71
Cu(OH)3-	7.703e-20	6.628e-20	-19.113	-19.179	-0.065	(0)
CuCl3-	9.953e-22	8.547e-22	-21.002	-21.068	-0.066	(0)
Cu2(OH)2+2	2.161e-23	1.185e-23	-22.665	-22.926	-0.261	(0)
Cu(OH)4-2	2.410e-25	1.322e-25	-24.618	-24.879	-0.261	(0)
CuCl4-2	1.128e-25	6.290e-26	-24.948	-25.201	-0.254	(0)
Fe(2)	4.224e-04					
Fe+2	3.564e-04	2.033e-04	-3.448	-3.692	-0.244	-21.80
FeHCO3+	5.485e-05	4.720e-05	-4.261	-4.326	-0.065	(0)
FeCO3	5.252e-06	5.282e-06	-5.280	-5.277	0.002	(0)
FeCl+	4.817e-06	4.145e-06	-5.317	-5.382	-0.065	(0)
FeOH+	7.292e-07	6.301e-07	-6.137	-6.201	-0.063	(0)
FeHPO4	2.590e-07	2.605e-07	-6.587	-6.584	0.002	(0)
FeH2PO4+	6.107e-08	5.289e-08	-7.214	-7.277	-0.062	(0)
Fe(OH)2	5.210e-11	5.240e-11	-10.283	-10.281	0.002	(0)
Fe(OH)3-	2.246e-14	1.941e-14	-13.649	-13.712	-0.063	(0)
Fe(3)	8.706e-11					
Fe(OH)3	4.527e-11	4.553e-11	-10.344	-10.342	0.002	(0)
Fe(OH)2+	4.129e-11	3.576e-11	-10.384	-10.447	-0.062	(0)
Fe(OH)4-	4.742e-13	4.107e-13	-12.324	-12.387	-0.062	(0)
FeOH+2	1.958e-14	1.091e-14	-13.708	-13.962	-0.254	(0)
Fe+3	5.318e-19	1.718e-19	-18.274	-18.765	-0.491	(0)
FeCl+2	1.363e-19	7.599e-20	-18.865	-19.119	-0.254	(0)
FeH2PO4+2	4.265e-20	2.400e-20	-19.370	-19.620	-0.250	(0)
FeHPO4+	1.707e-20	1.475e-20	-19.768	-19.831	-0.063	(0)
FeCl2+	5.852e-21	5.056e-21	-20.233	-20.296	-0.063	(0)
FeCl3	7.427e-24	7.469e-24	-23.129	-23.127	0.002	(0)
Fe2(OH)2+4	3.584e-26	3.241e-27	-25.446	-26.489	-1.044	(0)
Fe3(OH)4+5	1.060e-33	2.481e-35	-32.975	-34.605	-1.631	(0)
H(0)	1.753e-13					
H2	8.763e-14	8.813e-14	-13.057	-13.055	0.002	28.61
K	4.814e-04					
K+	4.814e-04	4.123e-04	-3.318	-3.385	-0.067	9.11
KHPO4-	2.988e-10	2.588e-10	-9.525	-9.587	-0.062	38.27
Mg	7.837e-04					
Mg+2	7.693e-04	4.387e-04	-3.114	-3.358	-0.244	-21.46
MgHCO3+	1.387e-05	1.191e-05	-4.858	-4.924	-0.066	5.56
MgCO3	4.491e-07	4.517e-07	-6.348	-6.345	0.002	-17.09

MgHPO4	1.036e-07	1.042e-07	-6.985	-6.982	0.002	(0)
MgOH+	1.785e-08	1.555e-08	-7.748	-7.808	-0.060	(0)
MgH2PO4+	8.526e-09	7.385e-09	-8.069	-8.132	-0.062	(0)
MgPO4-	2.825e-09	2.447e-09	-8.549	-8.611	-0.062	(0)
Mn(2)	8.274e-05					
Mn+2	6.752e-05	3.851e-05	-4.171	-4.414	-0.244	-19.26
MnHCO3+	9.222e-06	7.968e-06	-5.035	-5.099	-0.063	(0)
MnCO3	3.294e-06	3.313e-06	-5.482	-5.480	0.002	(0)
MnCl+	2.682e-06	2.317e-06	-5.572	-5.635	-0.063	-3.07
MnCl2	1.486e-08	1.494e-08	-7.828	-7.826	0.002	86.21
MnOH+	1.121e-08	9.684e-09	-7.950	-8.014	-0.063	(0)
MnCl3-	7.037e-11	6.080e-11	-10.153	-10.216	-0.063	43.53
Mn(NO3)2	1.907e-15	1.918e-15	-14.720	-14.717	0.002	41.11
Mn(OH)3-	7.051e-19	6.092e-19	-18.152	-18.215	-0.063	(0)
Mn(3)	3.183e-32					
Mn+3	3.183e-32	1.028e-32	-31.497	-31.988	-0.491	(0)
N(-3)	5.433e-06					
NH4+	5.407e-06	4.595e-06	-5.267	-5.338	-0.071	18.06
NH3	2.556e-08	2.571e-08	-7.592	-7.590	0.002	24.41
N(3)	1.072e-06					
NO2-	1.072e-06	9.145e-07	-5.970	-6.039	-0.069	25.07
N(5)	4.146e-06					
NO3-	4.146e-06	3.536e-06	-5.382	-5.451	-0.069	29.58
BaNO3+	3.487e-12	3.001e-12	-11.458	-11.523	-0.065	(0)
PbNO3+	3.012e-14	2.592e-14	-13.521	-13.586	-0.065	(0)
CdNO3+	1.755e-14	1.511e-14	-13.756	-13.821	-0.065	17.64
Mn(NO3)2	1.907e-15	1.918e-15	-14.720	-14.717	0.002	41.11
Na	6.271e-03					
Na+	5.824e-03	5.026e-03	-2.235	-2.299	-0.064	-1.31
NaCl	4.410e-04	4.435e-04	-3.356	-3.353	0.002	(0)
NaHCO3	6.536e-06	6.573e-06	-5.185	-5.182	0.002	1.80
NaCO3-	1.163e-07	1.001e-07	-6.935	-7.000	-0.065	-0.83
NaHPO4-	3.642e-09	3.154e-09	-8.439	-8.501	-0.062	35.26
NaOH	4.957e-20	4.985e-20	-19.305	-19.302	0.002	(0)
O(0)	0.000e+00					
O2	0.000e+00	0.000e+00	-66.357	-66.355	0.002	30.38
P	2.101e-06					
H2PO4-	5.994e-07	5.191e-07	-6.222	-6.285	-0.062	33.36
HPO4-2	5.774e-07	3.218e-07	-6.239	-6.492	-0.254	7.19
CaHPO4	4.354e-07	4.379e-07	-6.361	-6.359	0.002	(0)
FeHPO4	2.590e-07	2.605e-07	-6.587	-6.584	0.002	(0)
MgHPO4	1.036e-07	1.042e-07	-6.985	-6.982	0.002	(0)
FeH2PO4+	6.107e-08	5.289e-08	-7.214	-7.277	-0.062	(0)
CaH2PO4+	3.805e-08	3.295e-08	-7.420	-7.482	-0.062	(0)
CaPO4-	1.190e-08	1.031e-08	-7.924	-7.987	-0.062	(0)
MgH2PO4+	8.526e-09	7.385e-09	-8.069	-8.132	-0.062	(0)
NaHPO4-	3.642e-09	3.154e-09	-8.439	-8.501	-0.062	35.26
MgPO4-	2.825e-09	2.447e-09	-8.549	-8.611	-0.062	(0)
KHPO4-	2.988e-10	2.588e-10	-9.525	-9.587	-0.062	38.27
H3PO4	7.577e-12	7.620e-12	-11.121	-11.118	0.002	47.39
PO4-3	5.687e-12	1.443e-12	-11.245	-11.841	-0.595	-22.18
FeH2PO4+2	4.265e-20	2.400e-20	-19.370	-19.620	-0.250	(0)
FeHPO4+	1.707e-20	1.475e-20	-19.768	-19.831	-0.063	(0)
Pb	1.174e-08					
PbCO3	9.275e-09	9.327e-09	-8.033	-8.030	0.002	(0)
PbHCO3+	1.062e-09	9.139e-10	-8.974	-9.039	-0.065	(0)
Pb+2	9.036e-10	4.955e-10	-9.044	-9.305	-0.261	-15.18
PbCl+	3.365e-10	2.896e-10	-9.473	-9.538	-0.065	8.03
PbOH+	1.122e-10	9.656e-11	-9.950	-10.015	-0.065	(0)
Pb(CO3)2-2	4.628e-11	2.538e-11	-10.335	-10.596	-0.261	(0)
PbCl2	6.774e-12	6.812e-12	-11.169	-11.167	0.002	34.95
Pb(OH)2	3.733e-13	3.755e-13	-12.428	-12.425	0.002	(0)
PbCl3-	9.275e-14	7.981e-14	-13.033	-13.098	-0.065	66.04
PbNO3+	3.012e-14	2.592e-14	-13.521	-13.586	-0.065	(0)
PbCl4-2	1.027e-15	5.632e-16	-14.988	-15.249	-0.261	101.78
Pb(OH)3-	5.007e-17	4.308e-17	-16.300	-16.366	-0.065	(0)
Pb2OH+3	4.140e-18	1.071e-18	-17.383	-17.970	-0.587	(0)
Pb(OH)4-2	1.799e-21	9.864e-22	-20.745	-21.006	-0.261	(0)

Pb3(OH)4+2	2.807e-24	1.539e-24	-23.552	-23.813	-0.261	(0)
PbBr+	0.000e+00	0.000e+00	-40.808	-40.874	-0.065	(0)
PbBr2	0.000e+00	0.000e+00	-74.541	-74.539	0.002	(0)
Si	1.166e-03					
H4SiO4	1.164e-03	1.171e-03	-2.934	-2.931	0.002	52.10
H3SiO4-	1.993e-06	1.711e-06	-5.701	-5.767	-0.066	28.09
H2SiO4-2	2.034e-12	1.144e-12	-11.692	-11.941	-0.250	(0)
Zn	1.473e-06					
Zn+2	1.091e-06	6.082e-07	-5.962	-6.216	-0.254	-24.99
ZnHCO3+	2.066e-07	1.778e-07	-6.685	-6.750	-0.065	(0)
ZnCO3	1.307e-07	1.314e-07	-6.884	-6.881	0.002	(0)
ZnCl+	2.784e-08	2.391e-08	-7.555	-7.622	-0.066	-14.15
ZnOH+	7.593e-09	6.534e-09	-8.120	-8.185	-0.065	(0)
Zn(CO3)2-2	5.550e-09	3.044e-09	-8.256	-8.517	-0.261	(0)
ZnOHCl	2.957e-09	2.973e-09	-8.529	-8.527	0.002	(0)
Zn(OH)2	7.604e-10	7.647e-10	-9.119	-9.116	0.002	(0)
ZnCl2	3.673e-10	3.694e-10	-9.435	-9.432	0.002	102.54
ZnCl3-	7.120e-12	6.114e-12	-11.148	-11.214	-0.066	16.89
ZnCl4-2	8.104e-14	4.517e-14	-13.091	-13.345	-0.254	145.68
Zn(OH)3-	2.809e-14	2.417e-14	-13.552	-13.617	-0.065	(0)
Zn(OH)4-2	6.981e-20	3.828e-20	-19.156	-19.417	-0.261	(0)
ZnBr+	0.000e+00	0.000e+00	-40.068	-40.133	-0.065	(0)
ZnBr2	0.000e+00	0.000e+00	-73.872	-73.870	0.002	(0)

----------Distribution of alkalinity----------

Total alkalinity (eq/kgw) = 2.886e-03

Species	Alkalinity	Molality	Alk/Mol
HCO3-	2.681e-03	2.681e-03	1.00
CaHCO3+	8.465e-05	8.465e-05	1.00
FeHCO3+	5.485e-05	5.485e-05	1.00
MgHCO3+	1.387e-05	1.387e-05	1.00
FeCO3	1.050e-05	5.252e-06	2.00
MnHCO3+	9.222e-06	9.222e-06	1.00
CaCO3	8.976e-06	4.488e-06	2.00
MnCO3	6.589e-06	3.294e-06	2.00
NaHCO3	6.536e-06	6.536e-06	1.00
CO3-2	3.850e-06	1.925e-06	2.00
H3SiO4-	1.993e-06	1.993e-06	1.00
MgCO3	8.983e-07	4.491e-07	2.00
FeOH+	7.292e-07	7.292e-07	1.00
HPO4-2	5.774e-07	5.774e-07	1.00
CaHPO4	4.354e-07	4.354e-07	1.00
ZnCO3	2.614e-07	1.307e-07	2.00
FeHPO4	2.590e-07	2.590e-07	1.00
NaCO3-	2.325e-07	1.163e-07	2.00
Al(OH)4-	2.069e-07	5.174e-08	4.00
ZnHCO3+	2.066e-07	2.066e-07	1.00
BaHCO3+	1.729e-07	1.729e-07	1.00
OH-	1.159e-07	1.159e-07	1.00
H+	-1.134e-07	1.134e-07	-1.00
MgHPO4	1.036e-07	1.036e-07	1.00
NH3	2.556e-08	2.556e-08	1.00
CaPO4-	2.381e-08	1.190e-08	2.00
Zn(CO3)2-2	2.220e-08	5.550e-09	4.00
PbCO3	1.855e-08	9.275e-09	2.00
MgOH+	1.785e-08	1.785e-08	1.00
H2BO3-	1.490e-08	1.490e-08	1.00
MnOH+	1.121e-08	1.121e-08	1.00
ZnOH+	7.593e-09	7.593e-09	1.00
BaCO3	7.462e-09	3.731e-09	2.00
Al(OH)3	7.083e-09	2.361e-09	3.00
MgPO4-	5.651e-09	2.825e-09	2.00
CaOH+	4.806e-09	4.806e-09	1.00
Al(OH)2+	3.795e-09	1.898e-09	2.00
NaHPO4-	3.642e-09	3.642e-09	1.00

ZnOHCl	2.957e-09	2.957e-09	1.00
Zn(OH)2	1.521e-09	7.604e-10	2.00
PbHCO3+	1.062e-09	1.062e-09	1.00
KHPO4-	2.988e-10	2.988e-10	1.00
Pb(CO3)2-2	1.851e-10	4.628e-11	4.00
CdHCO3+	1.440e-10	1.440e-10	1.00
PbOH+	1.122e-10	1.122e-10	1.00
Fe(OH)2	1.042e-10	5.210e-11	2.00
Fe(OH)3	4.527e-11	4.527e-11	1.00
AlOH+2	3.815e-11	3.815e-11	1.00
PO4-3	1.137e-11	5.687e-12	2.00
CdOHCl	9.712e-12	9.712e-12	1.00
H3PO4	-7.577e-12	7.577e-12	-1.00
H2SiO4-2	4.068e-12	2.034e-12	2.00
CdCO3	2.888e-12	1.444e-12	2.00
BaOH+	2.642e-12	2.642e-12	1.00
CdOH+	1.599e-12	1.599e-12	1.00
Fe(OH)4-	9.483e-13	4.742e-13	2.00
Pb(OH)2	7.467e-13	3.733e-13	2.00
CuCO3	6.101e-13	3.051e-13	2.00
Cu(OH)2	2.189e-13	1.094e-13	2.00
Zn(OH)3-	8.426e-14	2.809e-14	3.00
CuHCO3+	7.132e-14	7.132e-14	1.00
Fe(OH)3-	6.738e-14	2.246e-14	3.00
Cd(CO3)2-2	3.628e-14	9.070e-15	4.00
FeOH+2	-1.958e-14	1.958e-14	-1.00
CuOH+	6.139e-15	6.139e-15	1.00
Cu(CO3)2-2	3.052e-15	7.629e-16	4.00
Cd(OH)2	1.498e-15	7.488e-16	2.00
Pb(OH)3-	1.502e-16	5.007e-17	3.00
Pb2OH+3	4.140e-18	4.140e-18	1.00
Mn(OH)3-	2.115e-18	7.051e-19	3.00
Fe+3	-1.064e-18	5.318e-19	-2.00
Zn(OH)4-2	2.792e-19	6.981e-20	4.00
FeCl+2	-2.727e-19	1.363e-19	-2.00
Cu(OH)3-	2.311e-19	7.703e-20	3.00
FeH2PO4+2	-8.530e-20	4.265e-20	-2.00
NaOH	4.957e-20	4.957e-20	1.00
Cd2OH+3	4.411e-20	4.411e-20	1.00
FeHPO4+	-1.707e-20	1.707e-20	-1.00
FeCl2+	-1.170e-20	5.852e-21	-2.00
Pb(OH)4-2	7.195e-21	1.799e-21	4.00
Cd(OH)3-	2.944e-21	9.813e-22	3.00
Cu2(OH)2+2	4.321e-23	2.161e-23	2.00
FeCl3	-1.485e-23	7.427e-24	-2.00
Pb3(OH)4+2	1.123e-23	2.807e-24	4.00
Cu(OH)4-2	9.641e-25	2.410e-25	4.00
Fe2(OH)2+4	-7.168e-26	3.584e-26	-2.00
Cd(OH)4-2	5.486e-28	1.372e-28	4.00
Fe3(OH)4+5	-2.120e-33	1.060e-33	-2.00

-------------------------------Saturation indices--------------------------------

Phase	SI**	log IAP	log K(297 K, 1 atm)	
Al(OH)3(a)	-2.48	8.34	10.82	Al(OH)3
Albite	-0.42	-18.44	-18.02	NaAlSi3O8
Anorthite	-3.44	-23.17	-19.72	CaAl2Si2O8
Aragonite	-0.23	-8.57	-8.33	CaCO3
BaCl2	-11.06	-8.83	2.23	BaCl2
BaCl2:2H2O	-9.04	-8.83	0.21	BaCl2:2H2O
BaCl2:H2O	-9.66	-8.83	0.82	BaCl2:H2O
Ca-Montmorillonite	2.75	-42.31	-45.06	Ca0.165Al2.33Si3.67O10(OH)2
Calcite	-0.09	-8.57	-8.48	CaCO3
Cd(OH)2	-8.42	5.23	13.65	Cd(OH)2
CdSiO3	-6.77	2.30	9.07	CdSiO3
Cerussite	-2.14	-15.27	-13.13	PbCO3
Chalcedony	0.62	-2.93	-3.55	SiO2

Chlorite(14A)	-7.38	61.10	68.48	Mg5Al2Si3O10(OH)8
Chrysotile	-6.17	26.06	32.23	Mg3Si2O5(OH)4
CO2(g)	-1.82	-3.28	-1.47	CO2
Dolomite	-0.81	-17.89	-17.08	CaMg(CO3)2
Fe(OH)3(a)	-2.66	2.23	4.89	Fe(OH)3
Gibbsite	0.22	8.34	8.12	Al(OH)3
Goethite	3.23	2.23	-0.99	FeOOH
H2(g)	-9.95	-13.05	-3.10	H2
H2O(g)	-1.51	-0.00	1.51	H2O
Halite	-5.70	-4.13	1.57	NaCl
Hausmannite	-22.43	38.66	61.09	Mn3O4
Hematite	8.46	4.47	-3.99	Fe2O3
Hydroxyapatite	-1.10	-4.49	-3.40	Ca5(PO4)3OH
Illite	1.87	-38.43	-40.30	K0.6Mg0.25Al2.3Si3.5O10(OH)2
K-feldspar	1.06	-19.53	-20.59	KAlSi3O8
K-mica	7.11	19.85	12.74	KAl3Si3O10(OH)2
Kaolinite	3.36	10.82	7.46	Al2Si2O5(OH)4
Manganite	-10.80	14.54	25.34	MnOOH
NH3(g)	-9.39	-7.59	1.80	NH3
O2(g)	-63.46	-66.35	-2.89	O2
Otavite	-2.64	-14.74	-12.10	CdCO3
Pb(OH)2	-3.46	4.69	8.16	Pb(OH)2
Pyrochroite	-5.61	9.59	15.20	Mn(OH)2
Pyrolusite	-21.93	19.49	41.42	MnO2:H2O
Quartz	1.05	-2.93	-3.98	SiO2
Rhodochrosite	0.75	-10.38	-11.13	MnCO3
Sepiolite	-3.28	12.49	15.77	Mg2Si3O7.5OH:3H2O
Sepiolite(d)	-6.17	12.49	18.66	Mg2Si3O7.5OH:3H2O
Siderite	1.23	-9.66	-10.89	FeCO3
SiO2(a)	-0.22	-2.93	-2.71	SiO2
Smithsonite	-2.18	-12.18	-10.00	ZnCO3
Sylvite	-6.11	-5.22	0.90	KCl
Talc	-1.23	20.20	21.43	Mg3Si4O10(OH)2
Vivianite	1.24	-34.76	-36.00	Fe3(PO4)2:8H2O
Willemite	-2.71	12.64	15.35	Zn2SiO4
Witherite	-2.57	-11.14	-8.56	BaCO3
Zn(OH)2(e)	-3.72	7.78	11.50	Zn(OH)2

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
For ideal gases, phi = 1.

Initial solution 32.

-----------------------------Solution composition------------------------------

Elements	Molality	Moles
Al	1.883e-07	1.883e-07
Alkalinity	2.982e-03	2.982e-03
B	2.054e-06	2.054e-06
Ba	4.224e-06	4.224e-06
Br	4.705e-34	4.705e-34
Ca	9.508e-04	9.508e-04
Cd	6.051e-09	6.051e-09
Cl	1.608e-04	1.608e-04
Cu	1.143e-06	1.143e-06
F	2.106e-05	2.106e-05
Fe	3.582e-07	3.582e-07
K	1.509e-04	1.509e-04
Mg	1.530e-04	1.530e-04
Mn	3.641e-07	3.641e-07
N(-3)	2.142e-07	2.142e-07
N(3)	3.571e-07	3.571e-07
N(5)	3.856e-06	3.856e-06
Na	3.959e-04	3.959e-04
P	1.776e-06	1.776e-06
Pb	9.028e-09	9.028e-09
S(6)	4.165e-05	4.165e-05

Si	4.678e-04	4.678e-04
Zn	1.507e-06	1.507e-06

----------Description of solution----------

pH	= 7.200
pe	= 1.113
Specific Conductance (µS/cm, 26°C)	= 286
Density (g/cm³)	= 0.99706
Volume (L)	= 1.00327
Activity of water	= 1.000
Ionic strength (mol/kgw)	= 4.075e-03
Mass of water (kg)	= 1.000e+00
Total carbon (mol/kg)	= 3.357e-03
Total CO2 (mol/kg)	= 3.357e-03
Temperature (°C)	= 25.78
Electrical balance (eq)	= -4.830e-04
Percent error, 100*(Cat-|An|)/(Cat+|An|)	= -8.15
Iterations	= 11 (342 overall)
Total H	= 1.110173e+02
Total O	= 5.551797e+01

----------Redox couples----------

Redox couple	pe	Eh (volts)
N(-3)/N(3)	5.4765	0.3248
N(-3)/N(5)	5.9974	0.3557
N(3)/N(5)	7.5599	0.4484

----------Distribution of species----------

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma	mole V cm³/mol
OH-	1.825e-07	1.702e-07	-6.739	-6.769	-0.030	-4.04
H+	6.721e-08	6.310e-08	-7.173	-7.200	-0.027	0.00
H2O	5.551e+01	9.999e-01	1.744	-0.000	0.000	18.07
Al	1.883e-07					
Al(OH)4-	1.800e-07	1.681e-07	-6.745	-6.774	-0.030	(0)
Al(OH)3	5.563e-09	5.568e-09	-8.255	-8.254	0.000	(0)
Al(OH)2+	2.409e-09	2.252e-09	-8.618	-8.647	-0.029	(0)
AlF2+	2.101e-10	1.964e-10	-9.678	-9.707	-0.029	(0)
AlF3	4.816e-11	4.821e-11	-10.317	-10.317	0.000	(0)
AlF+2	2.623e-11	2.003e-11	-10.581	-10.698	-0.117	(0)
AlOH+2	2.219e-11	1.695e-11	-10.654	-10.771	-0.117	-27.69
AlF4-	4.005e-13	3.740e-13	-12.397	-12.427	-0.030	(0)
Al+3	1.807e-13	1.023e-13	-12.743	-12.990	-0.247	-42.13
AlSO4+	9.920e-15	9.262e-15	-14.003	-14.033	-0.030	(0)
Al(SO4)2-	8.921e-18	8.329e-18	-17.050	-17.079	-0.030	(0)
AlHSO4+2	6.880e-23	5.218e-23	-22.162	-22.282	-0.120	(0)
B	2.054e-06					
H3BO3	2.034e-06	2.036e-06	-5.692	-5.691	0.000	39.29
H2BO3-	2.018e-08	1.883e-08	-7.695	-7.725	-0.030	(0)
BF(OH)3-	1.706e-11	1.592e-11	-10.768	-10.798	-0.030	(0)
BF2(OH)2-	2.245e-15	2.095e-15	-14.649	-14.679	-0.030	(0)
BF3OH-	2.984e-21	2.784e-21	-20.525	-20.555	-0.030	(0)
BF4-	1.493e-26	1.393e-26	-25.826	-25.856	-0.030	(0)
Ba	4.224e-06					
Ba+2	4.086e-06	3.101e-06	-5.389	-5.508	-0.120	-12.60
BaHCO3+	8.957e-08	8.358e-08	-7.048	-7.078	-0.030	(0)
BaSO4	4.400e-08	4.404e-08	-7.357	-7.356	0.000	(0)
BaCO3	3.368e-09	3.371e-09	-8.473	-8.472	0.000	-10.69
BaCl+	1.583e-09	1.478e-09	-8.800	-8.830	-0.030	(0)
BaOH+	1.783e-12	1.665e-12	-11.749	-11.778	-0.030	(0)
BaNO3+	1.503e-12	1.403e-12	-11.823	-11.853	-0.030	(0)
Br	4.705e-34					
Br-	4.705e-34	4.384e-34	-33.327	-33.358	-0.031	24.62

CdBr+	2.912e-40	2.718e-40	-39.536	-39.566	-0.030	(0)
ZnBr+	0.000e+00	0.000e+00	-40.062	-40.092	-0.030	(0)
PbBr+	0.000e+00	0.000e+00	-41.201	-41.231	-0.030	(0)
CdBr2	0.000e+00	0.000e+00	-72.193	-72.192	0.000	(0)
ZnBr2	0.000e+00	0.000e+00	-73.851	-73.851	0.000	(0)
PbBr2	0.000e+00	0.000e+00	-74.925	-74.925	0.000	(0)
C(4)	3.357e-03					
HCO3-	2.935e-03	2.743e-03	-2.532	-2.562	-0.029	24.78
CO2	3.852e-04	3.856e-04	-3.414	-3.414	0.000	34.47
CaHCO3+	2.652e-05	2.481e-05	-4.576	-4.605	-0.029	9.73
MgHCO3+	3.909e-06	3.647e-06	-5.408	-5.438	-0.030	5.52
CO3-2	2.712e-06	2.071e-06	-5.567	-5.684	-0.117	-5.09
CaCO3	2.474e-06	2.477e-06	-5.607	-5.606	0.000	-14.60
NaHCO3	5.660e-07	5.665e-07	-6.247	-6.247	0.000	1.80
ZnCO3	2.894e-07	2.897e-07	-6.538	-6.538	0.000	(0)
ZnHCO3+	2.595e-07	2.421e-07	-6.586	-6.616	-0.030	(0)
MgCO3	2.262e-07	2.265e-07	-6.645	-6.645	0.000	-17.09
CuCO3	2.002e-07	2.004e-07	-6.699	-6.698	0.000	(0)
BaHCO3+	8.957e-08	8.358e-08	-7.048	-7.078	-0.030	(0)
FeHCO3+	6.322e-08	5.900e-08	-7.199	-7.229	-0.030	(0)
MnHCO3+	5.483e-08	5.122e-08	-7.261	-7.291	-0.030	(0)
MnCO3	3.443e-08	3.447e-08	-7.463	-7.463	0.000	(0)
CuHCO3+	2.655e-08	2.477e-08	-7.576	-7.606	-0.030	(0)
Zn(CO3)2-2	1.691e-08	1.283e-08	-7.772	-7.892	-0.120	(0)
NaCO3-	1.585e-08	1.479e-08	-7.800	-7.830	-0.030	-0.92
FeCO3	1.067e-08	1.068e-08	-7.972	-7.971	0.000	(0)
PbCO3	8.072e-09	8.080e-09	-8.093	-8.093	0.000	(0)
BaCO3	3.368e-09	3.371e-09	-8.473	-8.472	0.000	-10.69
(CO2)2	2.797e-09	2.799e-09	-8.553	-8.553	0.000	68.94
Cu(CO3)2-2	6.889e-10	5.225e-10	-9.162	-9.282	-0.120	(0)
PbHCO3+	5.242e-10	4.892e-10	-9.280	-9.311	-0.030	(0)
CdHCO3+	3.910e-10	3.649e-10	-9.408	-9.438	-0.030	(0)
Pb(CO3)2-2	5.542e-11	4.203e-11	-10.256	-10.376	-0.120	(0)
CdCO3	6.913e-12	6.920e-12	-11.160	-11.160	0.000	(0)
Cd(CO3)2-2	5.975e-14	4.532e-14	-13.224	-13.344	-0.120	(0)
Ca	9.508e-04					
Ca+2	9.180e-04	7.007e-04	-3.037	-3.154	-0.117	-18.03
CaHCO3+	2.652e-05	2.481e-05	-4.576	-4.605	-0.029	9.73
CaSO4	3.548e-06	3.551e-06	-5.450	-5.450	0.000	7.53
CaCO3	2.474e-06	2.477e-06	-5.607	-5.606	0.000	-14.60
CaHPO4	2.373e-07	2.375e-07	-6.625	-6.624	0.000	(0)
CaH2PO4+	1.200e-08	1.122e-08	-7.921	-7.950	-0.029	(0)
CaPO4-	9.670e-09	9.039e-09	-8.015	-8.044	-0.029	(0)
CaOH+	1.975e-09	1.843e-09	-8.705	-8.735	-0.030	(0)
CaHSO4+	1.596e-12	1.489e-12	-11.797	-11.827	-0.030	(0)
Cd	6.051e-09					
Cd+2	5.546e-09	4.206e-09	-8.256	-8.376	-0.120	-18.61
CdHCO3+	3.910e-10	3.649e-10	-9.408	-9.438	-0.030	(0)
CdCl+	6.460e-11	6.029e-11	-10.190	-10.220	-0.030	6.08
CdSO4	3.451e-11	3.454e-11	-10.462	-10.462	0.000	77.67
CdCO3	6.913e-12	6.920e-12	-11.160	-11.160	0.000	(0)
CdOH+	6.294e-12	5.874e-12	-11.201	-11.231	-0.030	(0)
CdF+	1.106e-12	1.032e-12	-11.956	-11.986	-0.030	(0)
CdOHCl	4.008e-13	4.012e-13	-12.397	-12.397	0.000	(0)
Cd(CO3)2-2	5.975e-14	4.532e-14	-13.224	-13.344	-0.120	(0)
CdNO3+	3.976e-14	3.711e-14	-13.401	-13.431	-0.030	17.53
CdCl2	3.769e-14	3.773e-14	-13.424	-13.423	0.000	23.14
Cd(SO4)2-2	1.408e-14	1.068e-14	-13.851	-13.971	-0.120	-105.06
Cd(OH)2	4.714e-15	4.719e-15	-14.327	-14.326	0.000	(0)
CdF2	5.045e-17	5.049e-17	-16.297	-16.297	0.000	(0)
CdCl3-	3.863e-18	3.605e-18	-17.413	-17.443	-0.030	68.80
Cd2OH+3	2.233e-19	1.199e-19	-18.651	-18.921	-0.270	(0)
Cd(OH)3-	8.991e-21	8.391e-21	-20.046	-20.076	-0.030	(0)
Cd(OH)4-2	1.563e-27	1.185e-27	-26.806	-26.926	-0.120	(0)
CdBr+	2.912e-40	2.718e-40	-39.536	-39.566	-0.030	(0)
CdBr2	0.000e+00	0.000e+00	-72.193	-72.192	0.000	(0)
Cl	1.608e-04					
Cl-	1.605e-04	1.497e-04	-3.795	-3.825	-0.030	18.13

NaCl	3.319e-07	3.322e-07	-6.479	-6.479	0.000	(0)
CuCl2-	5.565e-09	5.193e-09	-8.255	-8.285	-0.030	(0)
BaCl+	1.583e-09	1.478e-09	-8.800	-8.830	-0.030	(0)
ZnCl+	3.133e-10	2.923e-10	-9.504	-9.534	-0.030	-13.13
MnCl+	1.367e-10	1.278e-10	-9.864	-9.894	-0.030	-2.88
CdCl+	6.460e-11	6.029e-11	-10.190	-10.220	-0.030	6.08
ZnOHCl	5.502e-11	5.507e-11	-10.259	-10.259	0.000	(0)
FeCl+	4.762e-11	4.444e-11	-10.322	-10.352	-0.030	(0)
CuCl+	8.082e-12	7.541e-12	-11.092	-11.123	-0.030	0.46
CuCl3-2	1.621e-12	1.236e-12	-11.790	-11.908	-0.118	(0)
PbCl+	1.461e-12	1.364e-12	-11.835	-11.865	-0.030	8.01
CdOHCl	4.008e-13	4.012e-13	-12.397	-12.397	0.000	(0)
ZnCl2	4.592e-14	4.596e-14	-13.338	-13.338	0.000	100.52
CdCl2	3.769e-14	3.773e-14	-13.424	-13.423	0.000	23.14
MnCl2	8.339e-15	8.347e-15	-14.079	-14.078	0.000	84.94
CuCl2	6.107e-16	6.113e-16	-15.214	-15.214	0.000	31.91
PbCl2	3.186e-16	3.189e-16	-15.497	-15.496	0.000	35.03
ZnCl3-	8.311e-18	7.755e-18	-17.080	-17.110	-0.030	17.06
CdCl3-	3.863e-18	3.605e-18	-17.413	-17.443	-0.030	68.80
MnCl3-	3.683e-19	3.441e-19	-18.434	-18.463	-0.030	43.36
PbCl3-	4.082e-20	3.810e-20	-19.389	-19.419	-0.030	66.07
FeCl+2	1.690e-21	1.288e-21	-20.772	-20.890	-0.118	(0)
ZnCl4-2	7.682e-22	5.854e-22	-21.115	-21.233	-0.118	145.40
CuCl3-	3.528e-22	3.292e-22	-21.453	-21.483	-0.030	(0)
PbCl4-2	3.620e-24	2.746e-24	-23.441	-23.561	-0.120	101.59
FeCl2+	8.993e-25	8.403e-25	-24.046	-24.076	-0.030	(0)
CuCl4-2	3.299e-28	2.514e-28	-27.482	-27.600	-0.118	(0)
FeCl3	1.257e-29	1.258e-29	-28.901	-28.900	0.000	(0)
Cu(1)	7.941e-07					
Cu+	7.886e-07	7.343e-07	-6.103	-6.134	-0.031	(0)
CuCl2-	5.565e-09	5.193e-09	-8.255	-8.285	-0.030	(0)
CuCl3-2	1.621e-12	1.236e-12	-11.790	-11.908	-0.118	(0)
Cu(2)	3.486e-07					
CuCO3	2.002e-07	2.004e-07	-6.699	-6.698	0.000	(0)
Cu(OH)2	9.445e-08	9.454e-08	-7.025	-7.024	0.000	(0)
CuHCO3+	2.655e-08	2.477e-08	-7.576	-7.606	-0.030	(0)
Cu+2	2.353e-08	1.802e-08	-7.628	-7.744	-0.116	-26.51
CuOH+	3.060e-09	2.855e-09	-8.514	-8.544	-0.030	(0)
Cu(CO3)2-2	6.889e-10	5.225e-10	-9.162	-9.282	-0.120	(0)
CuSO4	1.047e-10	1.048e-10	-9.980	-9.980	0.000	13.19
CuCl+	8.082e-12	7.541e-12	-11.092	-11.123	-0.030	0.46
CuF+	6.894e-12	6.434e-12	-11.162	-11.192	-0.030	(0)
Cu2(OH)2+2	5.082e-12	3.854e-12	-11.294	-11.414	-0.120	(0)
Cu(OH)3-	9.674e-14	9.028e-14	-13.014	-13.044	-0.030	(0)
CuCl2	6.107e-16	6.113e-16	-15.214	-15.214	0.000	31.91
Cu(OH)4-2	3.764e-19	2.855e-19	-18.424	-18.544	-0.120	(0)
CuCl3-	3.528e-22	3.292e-22	-21.453	-21.483	-0.030	(0)
CuCl4-2	3.299e-28	2.514e-28	-27.482	-27.600	-0.118	(0)
F	2.106e-05					
F-	2.089e-05	1.948e-05	-4.680	-4.710	-0.030	-1.28
MgF+	1.583e-07	1.478e-07	-6.800	-6.830	-0.030	-10.55
NaF	4.131e-09	4.135e-09	-8.384	-8.383	0.000	7.29
HF	1.868e-09	1.870e-09	-8.729	-8.728	0.000	12.54
AlF2+	2.101e-10	1.964e-10	-9.678	-9.707	-0.029	(0)
ZnF+	2.088e-10	1.948e-10	-9.680	-9.710	-0.030	(0)
AlF3	4.816e-11	4.821e-11	-10.317	-10.317	0.000	(0)
FeF+	4.490e-11	4.190e-11	-10.348	-10.378	-0.030	(0)
MnF+	3.022e-11	2.824e-11	-10.520	-10.549	-0.030	(0)
AlF+2	2.623e-11	2.003e-11	-10.581	-10.698	-0.117	(0)
BF(OH)3-	1.706e-11	1.592e-11	-10.768	-10.798	-0.030	(0)
CuF+	6.894e-12	6.434e-12	-11.162	-11.192	-0.030	(0)
CdF+	1.106e-12	1.032e-12	-11.956	-11.986	-0.030	(0)
AlF4-	4.005e-13	3.740e-13	-12.397	-12.427	-0.030	(0)
HF2-	1.507e-13	1.406e-13	-12.822	-12.852	-0.030	22.13
PbF+	8.335e-14	7.778e-14	-13.079	-13.109	-0.030	(0)
BF2(OH)2-	2.245e-15	2.095e-15	-14.649	-14.679	-0.030	(0)
CdF2	5.045e-17	5.049e-17	-16.297	-16.297	0.000	(0)
PbF2	3.091e-17	3.094e-17	-16.510	-16.509	0.000	(0)

FeF+2	1.140e-17	8.687e-18	-16.943	-17.061	-0.118	(0)
FeF2+	7.279e-18	6.801e-18	-17.138	-17.167	-0.030	(0)
FeF3	2.104e-19	2.106e-19	-18.677	-18.677	0.000	(0)
PbF3-	4.680e-21	4.367e-21	-20.330	-20.360	-0.030	(0)
BF3OH-	2.984e-21	2.784e-21	-20.525	-20.555	-0.030	(0)
PbF4-2	5.369e-26	4.072e-26	-25.270	-25.390	-0.120	(0)
BF4-	1.493e-26	1.393e-26	-25.826	-25.856	-0.030	(0)
SiF6-2	7.488e-31	5.706e-31	-30.126	-30.244	-0.118	42.74
Fe(2)	3.577e-07					
Fe+2	2.808e-07	2.151e-07	-6.552	-6.667	-0.116	-21.99
FeHCO3+	6.322e-08	5.900e-08	-7.199	-7.229	-0.030	(0)
FeCO3	1.067e-08	1.068e-08	-7.972	-7.971	0.000	(0)
FeOH+	1.223e-09	1.142e-09	-8.913	-8.942	-0.030	(0)
FeSO4	1.098e-09	1.099e-09	-8.959	-8.959	0.000	18.16
FeHPO4	5.213e-10	5.218e-10	-9.283	-9.283	0.000	(0)
FeH2PO4+	7.110e-11	6.647e-11	-10.148	-10.177	-0.029	(0)
FeCl+	4.762e-11	4.444e-11	-10.322	-10.352	-0.030	(0)
FeF+	4.490e-11	4.190e-11	-10.348	-10.378	-0.030	(0)
Fe(OH)2	1.647e-13	1.649e-13	-12.783	-12.783	0.000	(0)
FeHSO4+	4.899e-16	4.572e-16	-15.310	-15.340	-0.030	(0)
Fe(OH)3-	1.047e-16	9.781e-17	-15.980	-16.010	-0.030	(0)
Fe(3)	5.172e-10					
Fe(OH)3	3.396e-10	3.399e-10	-9.469	-9.469	0.000	(0)
Fe(OH)2+	1.722e-10	1.610e-10	-9.764	-9.793	-0.029	(0)
Fe(OH)4-	5.422e-12	5.069e-12	-11.266	-11.295	-0.029	(0)
FeOH+2	3.908e-14	2.978e-14	-13.408	-13.526	-0.118	(0)
FeF+2	1.140e-17	8.687e-18	-16.943	-17.061	-0.118	(0)
FeF2+	7.279e-18	6.801e-18	-17.138	-17.167	-0.030	(0)
Fe+3	4.908e-19	2.780e-19	-18.309	-18.556	-0.247	(0)
FeF3	2.104e-19	2.106e-19	-18.677	-18.677	0.000	(0)
FeSO4+	9.405e-20	8.788e-20	-19.027	-19.056	-0.030	(0)
FeH2PO4+2	6.043e-20	4.614e-20	-19.219	-19.336	-0.117	(0)
FeHPO4+	5.006e-20	4.678e-20	-19.300	-19.330	-0.030	(0)
FeCl+2	1.690e-21	1.288e-21	-20.772	-20.890	-0.118	(0)
Fe(SO4)2-	5.855e-23	5.464e-23	-22.232	-22.262	-0.030	(0)
FeCl2+	8.993e-25	8.403e-25	-24.046	-24.076	-0.030	(0)
Fe2(OH)2+4	6.986e-26	2.311e-26	-25.156	-25.636	-0.480	(0)
FeHSO4+2	1.957e-26	1.485e-26	-25.708	-25.828	-0.120	(0)
FeCl3	1.257e-29	1.258e-29	-28.901	-28.900	0.000	(0)
Fe3(OH)4+5	4.073e-33	7.234e-34	-32.390	-33.141	-0.751	(0)
H(0)	3.321e-20					
H2	1.660e-20	1.662e-20	-19.780	-19.779	0.000	28.61
K	1.509e-04					
K+	1.509e-04	1.407e-04	-3.821	-3.852	-0.030	9.06
KSO4-	3.038e-08	2.840e-08	-7.517	-7.547	-0.029	34.15
KHPO4-	1.789e-10	1.672e-10	-9.747	-9.777	-0.029	38.09
Mg	1.530e-04					
Mg+2	1.479e-04	1.132e-04	-3.830	-3.946	-0.116	-21.75
MgHCO3+	3.909e-06	3.647e-06	-5.408	-5.438	-0.030	5.52
MgSO4	7.666e-07	7.673e-07	-6.115	-6.115	0.000	5.87
MgCO3	2.262e-07	2.265e-07	-6.645	-6.645	0.000	-17.09
MgF+	1.583e-07	1.478e-07	-6.800	-6.830	-0.030	-10.55
MgHPO4	5.185e-08	5.190e-08	-7.285	-7.285	0.000	(0)
MgOH+	7.466e-09	6.989e-09	-8.127	-8.156	-0.029	(0)
MgH2PO4+	2.470e-09	2.309e-09	-8.607	-8.637	-0.029	(0)
MgPO4-	2.108e-09	1.970e-09	-8.676	-8.705	-0.029	(0)
Mn(2)	3.641e-07					
Mn+2	2.735e-07	2.095e-07	-6.563	-6.679	-0.116	-20.35
MnHCO3+	5.483e-08	5.122e-08	-7.261	-7.291	-0.030	(0)
MnCO3	3.443e-08	3.447e-08	-7.463	-7.463	0.000	(0)
MnSO4	1.070e-09	1.071e-09	-8.970	-8.970	0.000	22.20
MnCl+	1.367e-10	1.278e-10	-9.864	-9.894	-0.030	-2.88
MnOH+	9.732e-11	9.093e-11	-10.012	-10.041	-0.030	(0)
MnF+	3.022e-11	2.824e-11	-10.520	-10.549	-0.030	(0)
MnCl2	8.339e-15	8.347e-15	-14.079	-14.078	0.000	84.94
Mn(NO3)2	1.074e-17	1.075e-17	-16.969	-16.969	0.000	40.83
MnCl3-	3.683e-19	3.441e-19	-18.434	-18.463	-0.030	43.36
Mn(OH)3-	1.414e-20	1.322e-20	-19.849	-19.879	-0.030	(0)

Mn(3)	1.661e-31					
Mn+3	1.661e-31	9.409e-32	-30.780	-31.026	-0.247	(0)
N(-3)	2.142e-07					
NH4+	2.123e-07	1.977e-07	-6.673	-6.704	-0.031	18.01
NH3	1.884e-09	1.886e-09	-8.725	-8.724	0.000	24.45
NH4SO4-	7.731e-11	7.215e-11	-10.112	-10.142	-0.030	37.88
N(3)	3.571e-07					
NO2-	3.571e-07	3.327e-07	-6.447	-6.478	-0.031	25.04
N(5)	3.856e-06					
NO3-	3.856e-06	3.593e-06	-5.414	-5.445	-0.031	29.59
BaNO3+	1.503e-12	1.403e-12	-11.823	-11.853	-0.030	(0)
CdNO3+	3.976e-14	3.711e-14	-13.401	-13.431	-0.030	17.53
PbNO3+	1.279e-14	1.193e-14	-13.893	-13.923	-0.030	(0)
Mn(NO3)2	1.074e-17	1.075e-17	-16.969	-16.969	0.000	40.83
Na	3.959e-04					
Na+	3.950e-04	3.688e-04	-3.403	-3.433	-0.030	-1.39
NaHCO3	5.660e-07	5.665e-07	-6.247	-6.247	0.000	1.80
NaCl	3.319e-07	3.322e-07	-6.479	-6.479	0.000	(0)
NaSO4-	5.631e-08	5.264e-08	-7.249	-7.279	-0.029	13.98
NaCO3-	1.585e-08	1.479e-08	-7.800	-7.830	-0.030	-0.92
NaF	4.131e-09	4.135e-09	-8.384	-8.383	0.000	7.29
NaHPO4-	4.689e-10	4.383e-10	-9.329	-9.358	-0.029	33.72
NaOH	6.272e-21	6.277e-21	-20.203	-20.202	0.000	(0)
O(0)	0.000e+00					
O2	0.000e+00	0.000e+00	-52.571	-52.570	0.000	30.46
P	1.776e-06					
HPO4-2	7.998e-07	6.095e-07	-6.097	-6.215	-0.118	6.81
H2PO4-	6.597e-07	6.167e-07	-6.181	-6.210	-0.029	33.22
CaHPO4	2.373e-07	2.375e-07	-6.625	-6.624	0.000	(0)
MgHPO4	5.185e-08	5.190e-08	-7.285	-7.285	0.000	(0)
CaH2PO4+	1.200e-08	1.122e-08	-7.921	-7.950	-0.029	(0)
CaPO4-	9.670e-09	9.039e-09	-8.015	-8.044	-0.029	(0)
MgH2PO4+	2.470e-09	2.309e-09	-8.607	-8.637	-0.029	(0)
MgPO4-	2.108e-09	1.970e-09	-8.676	-8.705	-0.029	(0)
FeHPO4	5.213e-10	5.218e-10	-9.283	-9.283	0.000	(0)
NaHPO4-	4.689e-10	4.383e-10	-9.329	-9.358	-0.029	33.72
KHPO4-	1.789e-10	1.672e-10	-9.747	-9.777	-0.029	38.09
FeH2PO4+	7.110e-11	6.647e-11	-10.148	-10.177	-0.029	(0)
PO4-3	8.249e-12	4.423e-12	-11.084	-11.354	-0.271	-23.04
H3PO4	5.777e-12	5.782e-12	-11.238	-11.238	0.000	47.45
FeH2PO4+2	6.043e-20	4.614e-20	-19.219	-19.336	-0.117	(0)
FeHPO4+	5.006e-20	4.678e-20	-19.300	-19.330	-0.030	(0)
Pb	9.028e-09					
PbCO3	8.072e-09	8.080e-09	-8.093	-8.093	0.000	(0)
PbHCO3+	5.242e-10	4.892e-10	-9.280	-9.311	-0.030	(0)
Pb+2	2.960e-10	2.245e-10	-9.529	-9.649	-0.120	-15.45
PbOH+	7.434e-11	6.937e-11	-10.129	-10.159	-0.030	(0)
Pb(CO3)2-2	5.542e-11	4.203e-11	-10.256	-10.376	-0.120	(0)
PbSO4	3.574e-12	3.577e-12	-11.447	-11.446	0.000	(0)
PbCl+	1.461e-12	1.364e-12	-11.835	-11.865	-0.030	8.01
Pb(OH)2	4.273e-13	4.277e-13	-12.369	-12.369	0.000	(0)
PbF+	8.335e-14	7.778e-14	-13.079	-13.109	-0.030	(0)
PbNO3+	1.279e-14	1.193e-14	-13.893	-13.923	-0.030	(0)
Pb(SO4)2-2	7.013e-16	5.319e-16	-15.154	-15.274	-0.120	(0)
PbCl2	3.186e-16	3.189e-16	-15.497	-15.496	0.000	35.03
Pb(OH)3-	8.339e-17	7.782e-17	-16.079	-16.109	-0.030	(0)
PbF2	3.091e-17	3.094e-17	-16.510	-16.509	0.000	(0)
Pb2OH+3	6.495e-19	3.487e-19	-18.187	-18.458	-0.270	(0)
PbCl3-	4.082e-20	3.810e-20	-19.389	-19.419	-0.030	66.07
PbF3-	4.680e-21	4.367e-21	-20.330	-20.360	-0.030	(0)
Pb(OH)4-2	3.725e-21	2.825e-21	-20.429	-20.549	-0.120	(0)
PbCl4-2	3.620e-24	2.746e-24	-23.441	-23.561	-0.120	101.59
Pb3(OH)4+2	1.394e-24	1.057e-24	-23.856	-23.976	-0.120	(0)
PbF4-2	5.369e-26	4.072e-26	-25.270	-25.390	-0.120	(0)
PbBr+	0.000e+00	0.000e+00	-41.201	-41.231	-0.030	(0)
PbBr2	0.000e+00	0.000e+00	-74.925	-74.925	0.000	(0)
S(6)	4.165e-05					
SO4-2	3.720e-05	2.833e-05	-4.429	-4.548	-0.118	14.73

CaSO4	3.548e-06	3.551e-06	-5.450	-5.450	0.000	7.53
MgSO4	7.666e-07	7.673e-07	-6.115	-6.115	0.000	5.87
NaSO4-	5.631e-08	5.264e-08	-7.249	-7.279	-0.029	13.98
BaSO4	4.400e-08	4.404e-08	-7.357	-7.356	0.000	(0)
KSO4-	3.038e-08	2.840e-08	-7.517	-7.547	-0.029	34.15
ZnSO4	4.681e-09	4.685e-09	-8.330	-8.329	0.000	21.59
FeSO4	1.098e-09	1.099e-09	-8.959	-8.959	0.000	18.16
MnSO4	1.070e-09	1.071e-09	-8.970	-8.970	0.000	22.20
HSO4-	1.895e-10	1.768e-10	-9.722	-9.752	-0.030	40.36
CuSO4	1.047e-10	1.048e-10	-9.980	-9.980	0.000	13.19
NH4SO4-	7.731e-11	7.215e-11	-10.112	-10.142	-0.030	37.88
CdSO4	3.451e-11	3.454e-11	-10.462	-10.462	0.000	77.67
PbSO4	3.574e-12	3.577e-12	-11.447	-11.446	0.000	(0)
CaHSO4+	1.596e-12	1.489e-12	-11.797	-11.827	-0.030	(0)
Zn(SO4)2-2	1.414e-12	1.073e-12	-11.850	-11.970	-0.120	-12.34
Cd(SO4)2-2	1.408e-14	1.068e-14	-13.851	-13.971	-0.120	-105.06
AlSO4+	9.920e-15	9.262e-15	-14.003	-14.033	-0.030	(0)
Pb(SO4)2-2	7.013e-16	5.319e-16	-15.154	-15.274	-0.120	(0)
FeHSO4+	4.899e-16	4.572e-16	-15.310	-15.340	-0.030	(0)
Al(SO4)2-	8.921e-18	8.329e-18	-17.050	-17.079	-0.030	(0)
FeSO4+	9.405e-20	8.788e-20	-19.027	-19.056	-0.030	(0)
AlHSO4+2	6.880e-23	5.218e-23	-22.162	-22.282	-0.120	(0)
Fe(SO4)2-	5.855e-23	5.464e-23	-22.232	-22.262	-0.030	(0)
FeHSO4+2	1.957e-26	1.485e-26	-25.708	-25.828	-0.120	(0)
Si	4.678e-04					
H4SiO4	4.666e-04	4.670e-04	-3.331	-3.331	0.000	52.01
H3SiO4-	1.202e-06	1.121e-06	-5.920	-5.950	-0.030	28.02
H2SiO4-2	1.665e-12	1.272e-12	-11.779	-11.896	-0.117	(0)
SiF6-2	7.488e-31	5.706e-31	-30.126	-30.244	-0.118	42.74
Zn	1.507e-06					
Zn+2	9.200e-07	7.011e-07	-6.036	-6.154	-0.118	-25.31
ZnCO3	2.894e-07	2.897e-07	-6.538	-6.538	0.000	(0)
ZnHCO3+	2.595e-07	2.421e-07	-6.586	-6.616	-0.030	(0)
Zn(CO3)2-2	1.691e-08	1.283e-08	-7.772	-7.892	-0.120	(0)
ZnOH+	1.385e-08	1.292e-08	-7.859	-7.889	-0.030	(0)
ZnSO4	4.681e-09	4.685e-09	-8.330	-8.329	0.000	21.59
Zn(OH)2	2.215e-09	2.217e-09	-8.655	-8.654	0.000	(0)
ZnCl+	3.133e-10	2.923e-10	-9.504	-9.534	-0.030	-13.13
ZnF+	2.088e-10	1.948e-10	-9.680	-9.710	-0.030	(0)
ZnOHCl	5.502e-11	5.507e-11	-10.259	-10.259	0.000	(0)
Zn(SO4)2-2	1.414e-12	1.073e-12	-11.850	-11.970	-0.120	-12.34
Zn(OH)3-	1.190e-13	1.111e-13	-12.924	-12.954	-0.030	(0)
ZnCl2	4.592e-14	4.596e-14	-13.338	-13.338	0.000	100.52
ZnCl3-	8.311e-18	7.755e-18	-17.080	-17.110	-0.030	17.06
Zn(OH)4-2	3.679e-19	2.790e-19	-18.434	-18.554	-0.120	(0)
ZnCl4-2	7.682e-22	5.854e-22	-21.115	-21.233	-0.118	145.40
ZnBr+	0.000e+00	0.000e+00	-40.062	-40.092	-0.030	(0)
ZnBr2	0.000e+00	0.000e+00	-73.851	-73.851	0.000	(0)

----------Distribution of alkalinity----------

Total alkalinity (eq/kgw) = 2.982e-03

Species	Alkalinity	Molality	Alk/Mol
HCO3-	2.935e-03	2.935e-03	1.00
CaHCO3+	2.652e-05	2.652e-05	1.00
CO3-2	5.424e-06	2.712e-06	2.00
CaCO3	4.949e-06	2.474e-06	2.00
MgHCO3+	3.909e-06	3.909e-06	1.00
H3SiO4-	1.202e-06	1.202e-06	1.00
HPO4-2	7.998e-07	7.998e-07	1.00
Al(OH)4-	7.202e-07	1.800e-07	4.00
ZnCO3	5.789e-07	2.894e-07	2.00
NaHCO3	5.660e-07	5.660e-07	1.00
MgCO3	4.525e-07	2.262e-07	2.00
CuCO3	4.004e-07	2.002e-07	2.00
ZnHCO3+	2.595e-07	2.595e-07	1.00

CaHPO4	2.373e-07	2.373e-07	1.00
Cu(OH)2	1.889e-07	9.445e-08	2.00
OH-	1.825e-07	1.825e-07	1.00
BaHCO3+	8.957e-08	8.957e-08	1.00
MnCO3	6.887e-08	3.443e-08	2.00
Zn(CO3)2-2	6.765e-08	1.691e-08	4.00
H+	-6.721e-08	6.721e-08	-1.00
FeHCO3+	6.322e-08	6.322e-08	1.00
MnHCO3+	5.483e-08	5.483e-08	1.00
MgHPO4	5.185e-08	5.185e-08	1.00
NaCO3-	3.170e-08	1.585e-08	2.00
CuHCO3+	2.655e-08	2.655e-08	1.00
FeCO3	2.135e-08	1.067e-08	2.00
H2BO3-	2.018e-08	2.018e-08	1.00
CaPO4-	1.934e-08	9.670e-09	2.00
Al(OH)3	1.669e-08	5.563e-09	3.00
PbCO3	1.614e-08	8.072e-09	2.00
ZnOH+	1.385e-08	1.385e-08	1.00
MgOH+	7.466e-09	7.466e-09	1.00
BaCO3	6.735e-09	3.368e-09	2.00
Al(OH)2+	4.819e-09	2.409e-09	2.00
Zn(OH)2	4.429e-09	2.215e-09	2.00
MgPO4-	4.216e-09	2.108e-09	2.00
CuOH+	3.060e-09	3.060e-09	1.00
Cu(CO3)2-2	2.756e-09	6.889e-10	4.00
CaOH+	1.975e-09	1.975e-09	1.00
NH3	1.884e-09	1.884e-09	1.00
HF	-1.868e-09	1.868e-09	-1.00
FeOH+	1.223e-09	1.223e-09	1.00
PbHCO3+	5.242e-10	5.242e-10	1.00
FeHPO4	5.213e-10	5.213e-10	1.00
NaHPO4-	4.689e-10	4.689e-10	1.00
CdHCO3+	3.910e-10	3.910e-10	1.00
Fe(OH)3	3.396e-10	3.396e-10	1.00
Pb(CO3)2-2	2.217e-10	5.542e-11	4.00
HSO4-	-1.895e-10	1.895e-10	-1.00
KHPO4-	1.789e-10	1.789e-10	1.00
MnOH+	9.732e-11	9.732e-11	1.00
PbOH+	7.434e-11	7.434e-11	1.00
ZnOHCl	5.502e-11	5.502e-11	1.00
AlOH+2	2.219e-11	2.219e-11	1.00
PO4-3	1.650e-11	8.249e-12	2.00
CdCO3	1.383e-11	6.913e-12	2.00
Fe(OH)4-	1.084e-11	5.422e-12	2.00
Cu2(OH)2+2	1.016e-11	5.082e-12	2.00
CdOH+	6.294e-12	6.294e-12	1.00
H3PO4	-5.777e-12	5.777e-12	-1.00
H2SiO4-2	3.330e-12	1.665e-12	2.00
BaOH+	1.783e-12	1.783e-12	1.00
CaHSO4+	-1.596e-12	1.596e-12	-1.00
Pb(OH)2	8.546e-13	4.273e-13	2.00
CdOHCl	4.008e-13	4.008e-13	1.00
Zn(OH)3-	3.571e-13	1.190e-13	3.00
Fe(OH)2	3.294e-13	1.647e-13	2.00
Cu(OH)3-	2.902e-13	9.674e-14	3.00
Cd(CO3)2-2	2.390e-13	5.975e-14	4.00
HF2-	-1.507e-13	1.507e-13	-1.00
FeOH+2	-3.908e-14	3.908e-14	-1.00
Cd(OH)2	9.429e-15	4.714e-15	2.00
BF2(OH)2-	-2.245e-15	2.245e-15	-1.00
FeHSO4+	-4.899e-16	4.899e-16	-1.00
Fe(OH)3-	3.141e-16	1.047e-16	3.00
Pb(OH)3-	2.502e-16	8.339e-17	3.00
FeF+2	-2.280e-17	1.140e-17	-2.00
FeF2+	-1.456e-17	7.279e-18	-2.00
Cu(OH)4-2	1.506e-18	3.764e-19	4.00
Zn(OH)4-2	1.471e-18	3.679e-19	4.00
Fe+3	-9.816e-19	4.908e-19	-2.00

Pb2OH+3	6.495e-19	6.495e-19	1.00
FeF3	-4.207e-19	2.104e-19	-2.00
Cd2OH+3	2.233e-19	2.233e-19	1.00
FeSO4+	-1.881e-19	9.405e-20	-2.00
FeH2PO4+2	-1.209e-19	6.043e-20	-2.00
FeHPO4+	-5.006e-20	5.006e-20	-1.00
Mn(OH)3-	4.243e-20	1.414e-20	3.00
Cd(OH)3-	2.697e-20	8.991e-21	3.00
Pb(OH)4-2	1.490e-20	3.725e-21	4.00
NaOH	6.272e-21	6.272e-21	1.00
BF3OH-	-5.967e-21	2.984e-21	-2.00
FeCl+2	-3.381e-21	1.690e-21	-2.00
Fe(SO4)2-	-1.171e-22	5.855e-23	-2.00
AlHSO4+2	-6.880e-23	6.880e-23	-1.00
Pb3(OH)4+2	5.576e-24	1.394e-24	4.00
FeCl2+	-1.799e-24	8.993e-25	-2.00
Fe2(OH)2+4	-1.397e-25	6.986e-26	-2.00
FeHSO4+2	-5.872e-26	1.957e-26	-3.00
BF4-	-4.478e-26	1.493e-26	-3.00
Cd(OH)4-2	6.250e-27	1.563e-27	4.00
FeCl3	-2.513e-29	1.257e-29	-2.00
SiF6-2	-2.995e-30	7.488e-31	-4.00
Fe3(OH)4+5	-8.146e-33	4.073e-33	-2.00

----------Saturation indices----------

Phase	SI**	log IAP	log K(298 K, 1 atm)	
Al(OH)3(a)	-2.14	8.61	10.75	Al(OH)3
Albite	-2.25	-20.20	-17.95	NaAlSi3O8
Alunite	-7.22	-8.72	-1.50	KAl3(SO4)2(OH)6
Anglesite	-6.41	-14.20	-7.79	PbSO4
Anhydrite	-3.42	-7.70	-4.29	CaSO4
Anorthite	-3.67	-23.36	-19.69	CaAl2Si2O8
Aragonite	-0.50	-8.84	-8.34	CaCO3
BaCl2	-15.38	-13.16	2.22	BaCl2
BaCl2:2H2O	-13.37	-13.16	0.21	BaCl2:2H2O
BaCl2:H2O	-13.98	-13.16	0.83	BaCl2:H2O
Barite	-0.22	-10.06	-9.84	BaSO4
Ca-Montmorillonite	1.99	-42.93	-44.92	Ca0.165Al2.33Si3.67O10(OH)2
Calcite	-0.35	-8.84	-8.48	CaCO3
Cd(OH)2	-7.63	6.02	13.65	Cd(OH)2
CdSiO3	-6.33	2.69	9.03	CdSiO3
CdSO4	-12.80	-12.92	-0.13	CdSO4
Cerussite	-2.21	-15.33	-13.12	PbCO3
Chalcedony	0.21	-3.33	-3.54	SiO2
Chlorite(14A)	-8.59	59.50	68.09	Mg5Al2Si3O10(OH)8
Chrysotile	-7.40	24.70	32.10	Mg3Si2O5(OH)4
CO2(g)	-1.94	-3.41	-1.48	CO2
Dolomite	-1.36	-18.47	-17.11	CaMg(CO3)2
Fe(OH)3(a)	-1.85	3.04	4.89	Fe(OH)3
Fluorite	-1.98	-12.58	-10.59	CaF2
Gibbsite	0.54	8.61	8.07	Al(OH)3
Goethite	4.07	3.04	-1.03	FeOOH
Gypsum	-3.12	-7.70	-4.58	CaSO4:2H2O
H2(g)	-16.68	-19.78	-3.10	H2
H2O(g)	-1.48	-0.00	1.48	H2O
Halite	-8.83	-7.26	1.57	NaCl
Hausmannite	-21.05	39.79	60.84	Mn3O4
Hematite	10.16	6.09	-4.07	Fe2O3
Hydroxyapatite	-2.13	-5.62	-3.49	Ca5(PO4)3OH
Illite	0.99	-39.18	-40.16	K0.6Mg0.25Al2.3Si3.5O10(OH)2
Jarosite-K	-16.15	-25.42	-9.27	KFe3(SO4)2(OH)6
K-feldspar	-0.10	-20.62	-20.51	KAlSi3O8
K-mica	6.60	19.19	12.59	KAl3Si3O10(OH)2
Kaolinite	3.19	10.56	7.37	Al2Si2O5(OH)4
Manganite	-9.31	16.03	25.34	MnOOH
Melanterite	-9.02	-11.22	-2.20	FeSO4:7H2O

NH3(g)	-10.50	-8.72	1.78	NH3
O2(g)	-49.67	-52.57	-2.90	O2
Otavite	-1.96	-14.06	-12.10	CdCO3
Pb(OH)2	-3.37	4.75	8.12	Pb(OH)2
Pyrochroite	-7.48	7.72	15.20	Mn(OH)2
Pyrolusite	-16.91	24.35	41.26	MnO2:H2O
Quartz	0.64	-3.33	-3.97	SiO2
Rhodochrosite	-1.23	-12.36	-11.13	MnCO3
Sepiolite	-4.82	10.92	15.74	Mg2Si3O7.5OH:3H2O
Sepiolite(d)	-7.74	10.92	18.66	Mg2Si3O7.5OH:3H2O
Siderite	-1.46	-12.35	-10.89	FeCO3
SiO2(a)	-0.63	-3.33	-2.71	SiO2
Smithsonite	-1.83	-11.84	-10.01	ZnCO3
Sylvite	-8.58	-7.68	0.90	KCl
Talc	-3.27	18.04	21.31	Mg3Si4O10(OH)2
Vivianite	-6.71	-42.71	-36.00	Fe3(PO4)2:8H2O
Willemite	-2.11	13.16	15.27	Zn2SiO4
Witherite	-2.63	-11.19	-8.56	BaCO3
Zn(OH)2(e)	-3.25	8.25	11.50	Zn(OH)2

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
For ideal gases, phi = 1.

Initial solution 33.

-----------------------------Solution composition-----------------------------

Elements	Molality	Moles
Al	4.107e-07	4.107e-07
Alkalinity	4.914e-04	4.914e-04
B	7.216e-07	7.216e-07
Ba	5.825e-07	5.825e-07
Br	7.144e-35	7.144e-35
Ca	1.297e-04	1.297e-04
Cd	7.029e-09	7.029e-09
Cl	1.918e-04	1.918e-04
Cu	1.717e-07	1.717e-07
F	4.737e-06	4.737e-06
Fe	3.581e-07	3.581e-07
K	5.627e-05	5.627e-05
Mg	5.553e-05	5.553e-05
Mn	1.092e-06	1.092e-06
N(-3)	4.998e-07	4.998e-07
N(3)	3.570e-07	3.570e-07
N(5)	2.349e-05	2.349e-05
Na	1.827e-04	1.827e-04
P	5.166e-07	5.166e-07
Pb	2.993e-08	2.993e-08
Si	1.565e-04	1.565e-04
Zn	5.615e-07	5.615e-07

----------------------------Description of solution----------------------------

pH	=	6.000
pe	=	1.803
Specific Conductance (µS/cm, 26°C)	=	72
Density (g/cm³)	=	0.99685
Volume (L)	=	1.00327
Activity of water	=	1.000
Ionic strength (mol/kgw)	=	8.503e-04
Mass of water (kg)	=	1.000e+00
Total carbon (mol/kg)	=	1.547e-03
Total CO2 (mol/kg)	=	1.547e-03
Temperature (°C)	=	25.95
Electrical balance (eq)	=	-9.558e-05
Percent error, 100*(Cat-|An|)/(Cat+|An|)	=	-7.20
Iterations	=	13 (355 overall)

Total H = 1.110136e+02
Total O = 5.551050e+01

----------Redox couples----------

Redox couple	pe	Eh (volts)
N(-3)/N(3)	7.0046	0.4157
N(-3)/N(5)	7.5392	0.4474
N(3)/N(5)	9.1432	0.5426

----------Distribution of species----------

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma	mole V cm³/mol
H+	1.032e-06	1.000e-06	-5.986	-6.000	-0.014	0.00
OH-	1.124e-08	1.088e-08	-7.949	-7.963	-0.014	-4.08
H2O	5.551e+01	1.000e+00	1.744	-0.000	0.000	18.07
Al	4.107e-07					
AlF2+	1.300e-07	1.259e-07	-6.886	-6.900	-0.014	(0)
Al(OH)2+	1.292e-07	1.251e-07	-6.889	-6.903	-0.014	(0)
AlF+2	6.737e-08	5.913e-08	-7.172	-7.228	-0.057	(0)
Al(OH)4-	3.899e-08	3.772e-08	-7.409	-7.423	-0.014	(0)
Al(OH)3	1.975e-08	1.975e-08	-7.704	-7.704	0.000	(0)
AlOH+2	1.675e-08	1.470e-08	-7.776	-7.833	-0.057	-27.81
AlF3	6.701e-09	6.703e-09	-8.174	-8.174	0.000	(0)
Al+3	1.848e-09	1.391e-09	-8.733	-8.857	-0.123	-42.37
AlF4-	1.166e-11	1.128e-11	-10.933	-10.948	-0.014	(0)
B	7.216e-07					
H3BO3	7.212e-07	7.213e-07	-6.142	-6.142	0.000	39.30
H2BO3-	4.365e-10	4.223e-10	-9.360	-9.374	-0.014	(0)
BF(OH)3-	1.267e-12	1.226e-12	-11.897	-11.912	-0.014	(0)
BF2(OH)2-	5.730e-16	5.543e-16	-15.242	-15.256	-0.014	(0)
BF3OH-	2.610e-21	2.525e-21	-20.583	-20.598	-0.014	(0)
BF4-	4.487e-26	4.341e-26	-25.348	-25.362	-0.014	(0)
Ba	5.825e-07					
Ba+2	5.797e-07	5.081e-07	-6.237	-6.294	-0.057	-12.71
BaHCO3+	2.463e-09	2.383e-09	-8.608	-8.623	-0.014	(0)
BaCl+	3.106e-10	3.006e-10	-9.508	-9.522	-0.014	(0)
BaCO3	6.071e-12	6.073e-12	-11.217	-11.217	0.000	-10.69
BaNO3+	1.502e-12	1.453e-12	-11.823	-11.838	-0.014	(0)
BaOH+	1.779e-14	1.722e-14	-13.750	-13.764	-0.014	(0)
Br	7.144e-35					
Br-	7.144e-35	6.909e-35	-34.146	-34.161	-0.014	24.60
PbBr+	0.000e+00	0.000e+00	-40.184	-40.199	-0.014	(0)
CdBr+	0.000e+00	0.000e+00	-40.201	-40.216	-0.014	(0)
ZnBr+	0.000e+00	0.000e+00	-41.059	-41.073	-0.014	(0)
CdBr2	0.000e+00	0.000e+00	-73.645	-73.644	0.000	(0)
PbBr2	0.000e+00	0.000e+00	-74.696	-74.696	0.000	(0)
ZnBr2	0.000e+00	0.000e+00	-75.634	-75.634	0.000	(0)
C(4)	1.547e-03					
CO2	1.055e-03	1.056e-03	-2.977	-2.977	0.000	34.48
HCO3-	4.906e-04	4.749e-04	-3.309	-3.323	-0.014	24.75
CaHCO3+	7.187e-07	6.958e-07	-6.143	-6.158	-0.014	9.70
MgHCO3+	2.798e-07	2.707e-07	-6.553	-6.568	-0.014	5.50
NaHCO3	4.689e-08	4.690e-08	-7.329	-7.329	0.000	1.80
MnHCO3+	4.031e-08	3.901e-08	-7.395	-7.409	-0.014	(0)
ZnHCO3+	2.872e-08	2.779e-08	-7.542	-7.556	-0.014	(0)
CO3-2	2.586e-08	2.270e-08	-7.587	-7.644	-0.057	-5.21
(CO2)2	2.110e-08	2.110e-08	-7.676	-7.676	0.000	68.96
FeHCO3+	1.478e-08	1.430e-08	-7.830	-7.845	-0.014	(0)
PbCO3	6.040e-09	6.041e-09	-8.219	-8.219	0.000	(0)
PbHCO3+	5.971e-09	5.777e-09	-8.224	-8.238	-0.014	(0)
CaCO3	4.401e-09	4.401e-09	-8.356	-8.356	0.000	-14.60
CuHCO3+	4.121e-09	3.987e-09	-8.385	-8.399	-0.014	(0)
BaHCO3+	2.463e-09	2.383e-09	-8.608	-8.623	-0.014	(0)
ZnCO3	2.104e-09	2.105e-09	-8.677	-8.677	0.000	(0)

CuCO3	2.041e-09	2.042e-09	-8.690	-8.690	0.000	(0)
MnCO3	1.661e-09	1.662e-09	-8.780	-8.779	0.000	(0)
MgCO3	1.066e-09	1.066e-09	-8.972	-8.972	0.000	-17.09
FeCO3	1.639e-10	1.640e-10	-9.785	-9.785	0.000	(0)
CdHCO3+	9.282e-11	8.980e-11	-10.032	-10.047	-0.014	(0)
NaCO3-	8.090e-11	7.827e-11	-10.092	-10.106	-0.014	-0.95
BaCO3	6.071e-12	6.073e-12	-11.217	-11.217	0.000	-10.69
Zn(CO3)2-2	1.165e-12	1.021e-12	-11.934	-11.991	-0.057	(0)
Pb(CO3)2-2	3.930e-13	3.444e-13	-12.406	-12.463	-0.057	(0)
CdCO3	1.078e-13	1.078e-13	-12.967	-12.967	0.000	(0)
Cu(CO3)2-2	6.658e-14	5.834e-14	-13.177	-13.234	-0.057	(0)
Cd(CO3)2-2	8.830e-18	7.738e-18	-17.054	-17.111	-0.057	(0)
Ca	1.297e-04					
Ca+2	1.290e-04	1.132e-04	-3.889	-3.946	-0.057	-18.14
CaHCO3+	7.187e-07	6.958e-07	-6.143	-6.158	-0.014	9.70
CaCO3	4.401e-09	4.401e-09	-8.356	-8.356	0.000	-14.60
CaHPO4	1.826e-09	1.826e-09	-8.739	-8.738	0.000	(0)
CaH2PO4+	1.411e-09	1.366e-09	-8.850	-8.865	-0.014	(0)
CaOH+	1.942e-11	1.879e-11	-10.712	-10.726	-0.014	(0)
CaPO4-	4.544e-12	4.398e-12	-11.343	-11.357	-0.014	(0)
Cd	7.029e-09					
Cd+2	6.825e-09	5.980e-09	-8.166	-8.223	-0.057	-18.72
CdCl+	1.098e-10	1.062e-10	-9.960	-9.974	-0.014	6.07
CdHCO3+	9.282e-11	8.980e-11	-10.032	-10.047	-0.014	(0)
CdOH+	5.515e-13	5.336e-13	-12.258	-12.273	-0.014	(0)
CdNO3+	3.430e-13	3.319e-13	-12.465	-12.479	-0.014	17.49
CdF+	3.289e-13	3.182e-13	-12.483	-12.497	-0.014	(0)
CdCO3	1.078e-13	1.078e-13	-12.967	-12.967	0.000	(0)
CdCl2	8.234e-14	8.235e-14	-13.084	-13.084	0.000	23.14
CdOHCl	4.475e-14	4.476e-14	-13.349	-13.349	0.000	(0)
Cd(OH)2	2.671e-17	2.671e-17	-16.573	-16.573	0.000	(0)
CdCl3-	1.010e-17	9.770e-18	-16.996	-17.010	-0.014	68.65
Cd(CO3)2-2	8.830e-18	7.738e-18	-17.054	-17.111	-0.057	(0)
CdF2	3.377e-18	3.378e-18	-17.471	-17.471	0.000	(0)
Cd2OH+3	2.079e-20	1.544e-20	-19.682	-19.811	-0.129	(0)
Cd(OH)3-	3.097e-24	2.997e-24	-23.509	-23.523	-0.014	(0)
Cd(OH)4-2	3.048e-32	2.671e-32	-31.516	-31.573	-0.057	(0)
CdBr+	0.000e+00	0.000e+00	-40.201	-40.216	-0.014	(0)
CdBr2	0.000e+00	0.000e+00	-73.645	-73.644	0.000	(0)
Cl	1.918e-04					
Cl-	1.916e-04	1.854e-04	-3.718	-3.732	-0.014	18.10
NaCl	1.971e-07	1.972e-07	-6.705	-6.705	0.000	(0)
CuCl2-	1.564e-09	1.514e-09	-8.806	-8.820	-0.014	(0)
MnCl+	7.192e-10	6.961e-10	-9.143	-9.157	-0.014	-2.87
BaCl+	3.106e-10	3.006e-10	-9.508	-9.522	-0.014	(0)
ZnCl+	2.499e-10	2.418e-10	-9.602	-9.617	-0.014	-12.99
PbCl+	1.196e-10	1.157e-10	-9.922	-9.937	-0.014	7.98
CdCl+	1.098e-10	1.062e-10	-9.960	-9.974	-0.014	6.07
FeCl+	7.965e-11	7.706e-11	-10.099	-10.113	-0.014	(0)
CuCl+	9.049e-12	8.755e-12	-11.043	-11.058	-0.014	0.39
ZnOHCl	2.852e-12	2.853e-12	-11.545	-11.545	0.000	(0)
CuCl3-2	5.087e-13	4.463e-13	-12.294	-12.350	-0.057	(0)
CdCl2	8.234e-14	8.235e-14	-13.084	-13.084	0.000	23.14
MnCl2	5.631e-14	5.632e-14	-13.249	-13.249	0.000	84.74
ZnCl2	4.710e-14	4.711e-14	-13.327	-13.327	0.000	100.20
CdOHCl	4.475e-14	4.476e-14	-13.349	-13.349	0.000	(0)
PbCl2	3.339e-14	3.340e-14	-13.476	-13.476	0.000	35.05
CuCl2	8.803e-16	8.805e-16	-15.055	-15.055	0.000	32.10
ZnCl3-	1.018e-17	9.854e-18	-16.992	-17.006	-0.014	17.07
CdCl3-	1.010e-17	9.770e-18	-16.996	-17.010	-0.014	68.65
PbCl3-	5.113e-18	4.947e-18	-17.291	-17.306	-0.014	66.06
MnCl3-	2.971e-18	2.876e-18	-17.527	-17.541	-0.014	43.31
FeCl+2	1.266e-20	1.110e-20	-19.898	-19.955	-0.057	(0)
ZnCl4-2	1.051e-21	9.224e-22	-20.978	-21.035	-0.057	145.28
CuCl3-	6.087e-22	5.889e-22	-21.216	-21.230	-0.014	(0)
PbCl4-2	5.046e-22	4.421e-22	-21.297	-21.354	-0.057	101.48
FeCl2+	9.218e-24	8.921e-24	-23.035	-23.050	-0.014	(0)
CuCl4-2	6.375e-28	5.593e-28	-27.196	-27.252	-0.057	(0)

FeCl3	1.653e-28	1.654e-28	-27.782	-27.782	0.000	(0)
Cu(1)	1.459e-07					
Cu+	1.444e-07	1.396e-07	-6.841	-6.855	-0.015	(0)
CuCl2-	1.564e-09	1.514e-09	-8.806	-8.820	-0.014	(0)
CuCl3-2	5.087e-13	4.463e-13	-12.294	-12.350	-0.057	(0)
Cu(2)	2.577e-08					
Cu+2	1.907e-08	1.675e-08	-7.720	-7.776	-0.056	-26.63
CuHCO3+	4.121e-09	3.987e-09	-8.385	-8.399	-0.014	(0)
CuCO3	2.041e-09	2.042e-09	-8.690	-8.690	0.000	(0)
Cu(OH)2	3.499e-10	3.500e-10	-9.456	-9.456	0.000	(0)
CuOH+	1.731e-10	1.675e-10	-9.762	-9.776	-0.014	(0)
CuCl+	9.049e-12	8.755e-12	-11.043	-11.058	-0.014	0.39
CuF+	1.343e-12	1.300e-12	-11.872	-11.886	-0.014	(0)
Cu(CO3)2-2	6.658e-14	5.834e-14	-13.177	-13.234	-0.057	(0)
Cu2(OH)2+2	1.539e-14	1.349e-14	-13.813	-13.870	-0.057	(0)
CuCl2	8.803e-16	8.805e-16	-15.055	-15.055	0.000	32.10
Cu(OH)3-	2.180e-17	2.109e-17	-16.662	-16.676	-0.014	(0)
CuCl3-	6.087e-22	5.889e-22	-21.216	-21.230	-0.014	(0)
Cu(OH)4-2	4.801e-24	4.207e-24	-23.319	-23.376	-0.057	(0)
CuCl4-2	6.375e-28	5.593e-28	-27.196	-27.252	-0.057	(0)
F	4.737e-06					
F-	4.369e-06	4.226e-06	-5.360	-5.374	-0.014	-1.31
AlF2+	1.300e-07	1.259e-07	-6.886	-6.900	-0.014	(0)
AlF+2	6.737e-08	5.913e-08	-7.172	-7.228	-0.057	(0)
MgF+	1.424e-08	1.378e-08	-7.847	-7.861	-0.014	-10.58
AlF3	6.701e-09	6.703e-09	-8.174	-8.174	0.000	(0)
HF	6.446e-09	6.448e-09	-8.191	-8.191	0.000	12.54
NaF	4.293e-10	4.294e-10	-9.367	-9.367	0.000	7.30
ZnF+	2.902e-11	2.808e-11	-10.537	-10.552	-0.014	(0)
MnF+	2.785e-11	2.695e-11	-10.555	-10.569	-0.014	(0)
FeF+	1.315e-11	1.273e-11	-10.881	-10.895	-0.014	(0)
AlF4-	1.166e-11	1.128e-11	-10.933	-10.948	-0.014	(0)
CuF+	1.343e-12	1.300e-12	-11.872	-11.886	-0.014	(0)
BF(OH)3-	1.267e-12	1.226e-12	-11.897	-11.912	-0.014	(0)
PbF+	1.190e-12	1.151e-12	-11.925	-11.939	-0.014	(0)
CdF+	3.289e-13	3.182e-13	-12.483	-12.497	-0.014	(0)
HF2-	1.088e-13	1.053e-13	-12.963	-12.978	-0.014	22.10
BF2(OH)2-	5.730e-16	5.543e-16	-15.242	-15.256	-0.014	(0)
PbF2	9.930e-17	9.932e-17	-16.003	-16.003	0.000	(0)
FeF+2	1.491e-17	1.308e-17	-16.827	-16.883	-0.057	(0)
CdF2	3.377e-18	3.378e-18	-17.471	-17.471	0.000	(0)
FeF2+	2.299e-18	2.225e-18	-17.638	-17.653	-0.014	(0)
FeF3	1.495e-20	1.495e-20	-19.825	-19.825	0.000	(0)
PbF3-	3.143e-21	3.041e-21	-20.503	-20.517	-0.014	(0)
BF3OH-	2.610e-21	2.525e-21	-20.583	-20.598	-0.014	(0)
BF4-	4.487e-26	4.341e-26	-25.348	-25.362	-0.014	(0)
PbF4-2	7.019e-27	6.151e-27	-26.154	-26.211	-0.057	(0)
SiF6-2	1.410e-30	1.237e-30	-29.851	-29.908	-0.057	42.62
Fe(2)	3.581e-07					
Fe+2	3.429e-07	3.012e-07	-6.465	-6.521	-0.056	-22.09
FeHCO3+	1.478e-08	1.430e-08	-7.830	-7.845	-0.014	(0)
FeCO3	1.639e-10	1.640e-10	-9.785	-9.785	0.000	(0)
FeOH+	1.056e-10	1.022e-10	-9.976	-9.990	-0.014	(0)
FeCl+	7.965e-11	7.706e-11	-10.099	-10.113	-0.014	(0)
FeH2PO4+	7.221e-11	6.989e-11	-10.141	-10.156	-0.014	(0)
FeHPO4	3.464e-11	3.465e-11	-10.460	-10.460	0.000	(0)
FeF+	1.315e-11	1.273e-11	-10.881	-10.895	-0.014	(0)
Fe(OH)2	9.445e-16	9.446e-16	-15.025	-15.025	0.000	(0)
Fe(OH)3-	3.660e-20	3.542e-20	-19.436	-19.451	-0.014	(0)
Fe(3)	5.280e-12					
Fe(OH)2+	4.659e-12	4.509e-12	-11.332	-11.346	-0.014	(0)
Fe(OH)3	6.053e-13	6.054e-13	-12.218	-12.218	0.000	(0)
FeOH+2	1.498e-14	1.314e-14	-13.825	-13.881	-0.057	(0)
Fe(OH)4-	5.925e-16	5.735e-16	-15.227	-15.241	-0.014	(0)
FeF+2	1.491e-17	1.308e-17	-16.827	-16.883	-0.057	(0)
Fe+3	2.557e-18	1.925e-18	-17.592	-17.716	-0.123	(0)
FeF2+	2.299e-18	2.225e-18	-17.638	-17.653	-0.014	(0)
FeH2PO4+2	2.733e-19	2.399e-19	-18.563	-18.620	-0.057	(0)

FeHPO4+	1.595e-20	1.544e-20	-19.797	-19.811	-0.014	(0)
FeF3	1.495e-20	1.495e-20	-19.825	-19.825	0.000	(0)
FeCl+2	1.266e-20	1.110e-20	-19.898	-19.955	-0.057	(0)
FeCl2+	9.218e-24	8.921e-24	-23.035	-23.050	-0.014	(0)
Fe2(OH)2+4	7.578e-27	4.468e-27	-26.120	-26.350	-0.230	(0)
FeCl3	1.653e-28	1.654e-28	-27.782	-27.782	0.000	(0)
Fe3(OH)4+5	8.807e-36	3.857e-36	-35.055	-35.414	-0.359	(0)
H(0)	3.474e-19					
H2	1.737e-19	1.737e-19	-18.760	-18.760	0.000	28.61
K	5.627e-05					
K+	5.627e-05	5.443e-05	-4.250	-4.264	-0.014	9.04
KHPO4-	3.169e-12	3.067e-12	-11.499	-11.513	-0.014	38.04
Mg	5.553e-05					
Mg+2	5.523e-05	4.850e-05	-4.258	-4.314	-0.056	-21.87
MgHCO3+	2.798e-07	2.707e-07	-6.553	-6.568	-0.014	5.50
MgF+	1.424e-08	1.378e-08	-7.847	-7.861	-0.014	-10.58
MgCO3	1.066e-09	1.066e-09	-8.972	-8.972	0.000	-17.09
MgHPO4	1.058e-09	1.058e-09	-8.976	-8.976	0.000	(0)
MgH2PO4+	7.700e-10	7.453e-10	-9.114	-9.128	-0.014	(0)
MgOH+	1.981e-10	1.918e-10	-9.703	-9.717	-0.014	(0)
MgPO4-	2.626e-12	2.542e-12	-11.581	-11.595	-0.014	(0)
Mn(2)	1.092e-06					
Mn+2	1.049e-06	9.218e-07	-5.979	-6.035	-0.056	-21.07
MnHCO3+	4.031e-08	3.901e-08	-7.395	-7.409	-0.014	(0)
MnCO3	1.661e-09	1.662e-09	-8.780	-8.779	0.000	(0)
MnCl+	7.192e-10	6.961e-10	-9.143	-9.157	-0.014	-2.87
MnF+	2.785e-11	2.695e-11	-10.555	-10.569	-0.014	(0)
MnOH+	2.644e-11	2.559e-11	-10.578	-10.592	-0.014	(0)
MnCl2	5.631e-14	5.632e-14	-13.249	-13.249	0.000	84.74
Mn(NO3)2	1.890e-15	1.890e-15	-14.724	-14.723	0.000	40.79
MnCl3-	2.971e-18	2.876e-18	-17.527	-17.541	-0.014	43.31
Mn(OH)3-	1.509e-23	1.461e-23	-22.821	-22.835	-0.014	(0)
Mn(3)	2.761e-30					
Mn+3	2.761e-30	2.078e-30	-29.559	-29.682	-0.123	(0)
N(-3)	4.998e-07					
NH4+	4.995e-07	4.830e-07	-6.301	-6.316	-0.015	17.99
NH3	2.943e-10	2.943e-10	-9.531	-9.531	0.000	24.46
N(3)	3.570e-07					
NO2-	3.570e-07	3.453e-07	-6.447	-6.462	-0.014	25.01
N(5)	2.349e-05					
NO3-	2.349e-05	2.272e-05	-4.629	-4.644	-0.014	29.58
PbNO3+	5.320e-12	5.147e-12	-11.274	-11.288	-0.014	(0)
BaNO3+	1.502e-12	1.453e-12	-11.823	-11.838	-0.014	(0)
CdNO3+	3.430e-13	3.319e-13	-12.465	-12.479	-0.014	17.49
Mn(NO3)2	1.890e-15	1.890e-15	-14.724	-14.723	0.000	40.79
Na	1.827e-04					
Na+	1.825e-04	1.766e-04	-3.739	-3.753	-0.014	-1.43
NaCl	1.971e-07	1.972e-07	-6.705	-6.705	0.000	(0)
NaHCO3	4.689e-08	4.690e-08	-7.329	-7.329	0.000	1.80
NaF	4.293e-10	4.294e-10	-9.367	-9.367	0.000	7.30
NaCO3-	8.090e-11	7.827e-11	-10.092	-10.106	-0.014	-0.95
NaHPO4-	1.028e-11	9.950e-12	-10.988	-11.002	-0.014	33.45
NaOH	1.920e-22	1.921e-22	-21.717	-21.717	0.000	(0)
O(0)	0.000e+00					
O2	0.000e+00	0.000e+00	-54.554	-54.554	0.000	30.47
P	5.166e-07					
H2PO4-	4.784e-07	4.630e-07	-6.320	-6.334	-0.014	33.18
HPO4-2	3.294e-08	2.890e-08	-7.482	-7.539	-0.057	6.67
CaHPO4	1.826e-09	1.826e-09	-8.739	-8.738	0.000	(0)
CaH2PO4+	1.411e-09	1.366e-09	-8.850	-8.865	-0.014	(0)
MgHPO4	1.058e-09	1.058e-09	-8.976	-8.976	0.000	(0)
MgH2PO4+	7.700e-10	7.453e-10	-9.114	-9.128	-0.014	(0)
FeH2PO4+	7.221e-11	6.989e-11	-10.141	-10.156	-0.014	(0)
H3PO4	6.893e-11	6.895e-11	-10.162	-10.161	0.000	47.46
FeHPO4	3.464e-11	3.465e-11	-10.460	-10.460	0.000	(0)
NaHPO4-	1.028e-11	9.950e-12	-10.988	-11.002	-0.014	33.45
CaPO4-	4.544e-12	4.398e-12	-11.343	-11.357	-0.014	(0)
KHPO4-	3.169e-12	3.067e-12	-11.499	-11.513	-0.014	38.04

MgPO4-	2.626e-12	2.542e-12	-11.581	-11.595	-0.014	(0)
PO4-3	1.788e-14	1.328e-14	-13.748	-13.877	-0.129	-23.35
FeH2PO4+2	2.733e-19	2.399e-19	-18.563	-18.620	-0.057	(0)
FeHPO4+	1.595e-20	1.544e-20	-19.797	-19.811	-0.014	(0)
Pb	2.993e-08					
Pb+2	1.748e-08	1.532e-08	-7.757	-7.815	-0.057	-15.56
PbCO3	6.040e-09	6.041e-09	-8.219	-8.219	0.000	(0)
PbHCO3+	5.971e-09	5.777e-09	-8.224	-8.238	-0.014	(0)
PbOH+	3.087e-10	2.986e-10	-9.511	-9.525	-0.014	(0)
PbCl+	1.196e-10	1.157e-10	-9.922	-9.937	-0.014	7.98
PbNO3+	5.320e-12	5.147e-12	-11.274	-11.288	-0.014	(0)
PbF+	1.190e-12	1.151e-12	-11.925	-11.939	-0.014	(0)
Pb(CO3)2-2	3.930e-13	3.444e-13	-12.406	-12.463	-0.057	(0)
Pb(OH)2	1.162e-13	1.162e-13	-12.935	-12.935	0.000	(0)
PbCl2	3.339e-14	3.340e-14	-13.476	-13.476	0.000	35.05
Pb2OH+3	1.378e-16	1.024e-16	-15.861	-15.990	-0.129	(0)
PbF2	9.930e-17	9.932e-17	-16.003	-16.003	0.000	(0)
PbCl3-	5.113e-18	4.947e-18	-17.291	-17.306	-0.014	66.06
Pb(OH)3-	1.379e-18	1.334e-18	-17.861	-17.875	-0.014	(0)
PbF3-	3.143e-21	3.041e-21	-20.503	-20.517	-0.014	(0)
PbCl4-2	5.046e-22	4.421e-22	-21.297	-21.354	-0.057	101.48
Pb3(OH)4+2	6.230e-24	5.459e-24	-23.206	-23.263	-0.057	(0)
Pb(OH)4-2	3.487e-24	3.055e-24	-23.458	-23.515	-0.057	(0)
PbF4-2	7.019e-27	6.151e-27	-26.154	-26.211	-0.057	(0)
PbBr+	0.000e+00	0.000e+00	-40.184	-40.199	-0.014	(0)
PbBr2	0.000e+00	0.000e+00	-74.696	-74.696	0.000	(0)
Si	1.565e-04					
H4SiO4	1.564e-04	1.565e-04	-3.806	-3.806	0.000	52.00
H3SiO4-	2.464e-08	2.384e-08	-7.608	-7.623	-0.014	27.99
H2SiO4-2	1.965e-15	1.725e-15	-14.707	-14.763	-0.057	(0)
SiF6-2	1.410e-30	1.237e-30	-29.851	-29.908	-0.057	42.62
Zn	5.615e-07					
Zn+2	5.298e-07	4.648e-07	-6.276	-6.333	-0.057	-25.43
ZnHCO3+	2.872e-08	2.779e-08	-7.542	-7.556	-0.014	(0)
ZnCO3	2.104e-09	2.105e-09	-8.677	-8.677	0.000	(0)
ZnOH+	5.659e-10	5.475e-10	-9.247	-9.262	-0.014	(0)
ZnCl+	2.499e-10	2.418e-10	-9.602	-9.617	-0.014	-12.99
ZnF+	2.902e-11	2.808e-11	-10.537	-10.552	-0.014	(0)
Zn(OH)2	5.849e-12	5.851e-12	-11.233	-11.233	0.000	(0)
ZnOHCl	2.852e-12	2.853e-12	-11.545	-11.545	0.000	(0)
Zn(CO3)2-2	1.165e-12	1.021e-12	-11.934	-11.991	-0.057	(0)
ZnCl2	4.710e-14	4.711e-14	-13.327	-13.327	0.000	100.20
Zn(OH)3-	1.912e-17	1.850e-17	-16.718	-16.733	-0.014	(0)
ZnCl3-	1.018e-17	9.854e-18	-16.992	-17.006	-0.014	17.07
ZnCl4-2	1.051e-21	9.224e-22	-20.978	-21.035	-0.057	145.28
Zn(OH)4-2	3.346e-24	2.932e-24	-23.475	-23.533	-0.057	(0)
ZnBr+	0.000e+00	0.000e+00	-41.059	-41.073	-0.014	(0)
ZnBr2	0.000e+00	0.000e+00	-75.634	-75.634	0.000	(0)

----------Distribution of alkalinity----------

Total alkalinity (eq/kgw) = 4.914e-04

Species	Alkalinity	Molality	Alk/Mol
HCO3-	4.906e-04	4.906e-04	1.00
H+	-1.032e-06	1.032e-06	-1.00
CaHCO3+	7.187e-07	7.187e-07	1.00
MgHCO3+	2.798e-07	2.798e-07	1.00
Al(OH)2+	2.585e-07	1.292e-07	2.00
Al(OH)4-	1.559e-07	3.899e-08	4.00
Al(OH)3	5.925e-08	1.975e-08	3.00
CO3-2	5.172e-08	2.586e-08	2.00
NaHCO3	4.689e-08	4.689e-08	1.00
MnHCO3+	4.031e-08	4.031e-08	1.00
HPO4-2	3.294e-08	3.294e-08	1.00
ZnHCO3+	2.872e-08	2.872e-08	1.00
H3SiO4-	2.464e-08	2.464e-08	1.00

AlOH+2	1.675e-08	1.675e-08	1.00
FeHCO3+	1.478e-08	1.478e-08	1.00
PbCO3	1.208e-08	6.040e-09	2.00
OH-	1.124e-08	1.124e-08	1.00
CaCO3	8.801e-09	4.401e-09	2.00
HF	-6.446e-09	6.446e-09	-1.00
PbHCO3+	5.971e-09	5.971e-09	1.00
ZnCO3	4.208e-09	2.104e-09	2.00
CuHCO3+	4.121e-09	4.121e-09	1.00
CuCO3	4.083e-09	2.041e-09	2.00
MnCO3	3.323e-09	1.661e-09	2.00
BaHCO3+	2.463e-09	2.463e-09	1.00
MgCO3	2.131e-09	1.066e-09	2.00
CaHPO4	1.826e-09	1.826e-09	1.00
MgHPO4	1.058e-09	1.058e-09	1.00
Cu(OH)2	6.998e-10	3.499e-10	2.00
ZnOH+	5.659e-10	5.659e-10	1.00
H2BO3-	4.365e-10	4.365e-10	1.00
FeCO3	3.279e-10	1.639e-10	2.00
PbOH+	3.087e-10	3.087e-10	1.00
NH3	2.943e-10	2.943e-10	1.00
MgOH+	1.981e-10	1.981e-10	1.00
CuOH+	1.731e-10	1.731e-10	1.00
NaCO3-	1.618e-10	8.090e-11	2.00
FeOH+	1.056e-10	1.056e-10	1.00
CdHCO3+	9.282e-11	9.282e-11	1.00
H3PO4	-6.893e-11	6.893e-11	-1.00
FeHPO4	3.464e-11	3.464e-11	1.00
MnOH+	2.644e-11	2.644e-11	1.00
CaOH+	1.942e-11	1.942e-11	1.00
BaCO3	1.214e-11	6.071e-12	2.00
Zn(OH)2	1.170e-11	5.849e-12	2.00
NaHPO4-	1.028e-11	1.028e-11	1.00
CaPO4-	9.088e-12	4.544e-12	2.00
MgPO4-	5.252e-12	2.626e-12	2.00
Zn(CO3)2-2	4.662e-12	1.165e-12	4.00
KHPO4-	3.169e-12	3.169e-12	1.00
ZnOHCl	2.852e-12	2.852e-12	1.00
Pb(CO3)2-2	1.572e-12	3.930e-13	4.00
Fe(OH)3	6.053e-13	6.053e-13	1.00
CdOH+	5.515e-13	5.515e-13	1.00
Cu(CO3)2-2	2.663e-13	6.658e-14	4.00
Pb(OH)2	2.323e-13	1.162e-13	2.00
CdCO3	2.156e-13	1.078e-13	2.00
HF2-	-1.088e-13	1.088e-13	-1.00
CdOHCl	4.475e-14	4.475e-14	1.00
PO4-3	3.575e-14	1.788e-14	2.00
Cu2(OH)2+2	3.079e-14	1.539e-14	2.00
BaOH+	1.779e-14	1.779e-14	1.00
FeOH+2	-1.498e-14	1.498e-14	-1.00
H2SiO4-2	3.930e-15	1.965e-15	2.00
Fe(OH)2	1.889e-15	9.445e-16	2.00
Fe(OH)4-	1.185e-15	5.925e-16	2.00
BF2(OH)2-	-5.730e-16	5.730e-16	-1.00
Pb2OH+3	1.378e-16	1.378e-16	1.00
Cu(OH)3-	6.539e-17	2.180e-17	3.00
Zn(OH)3-	5.736e-17	1.912e-17	3.00
Cd(OH)2	5.341e-17	2.671e-17	2.00
Cd(CO3)2-2	3.532e-17	8.830e-18	4.00
FeF+2	-2.982e-17	1.491e-17	-2.00
Fe+3	-5.114e-18	2.557e-18	-2.00
FeF2+	-4.599e-18	2.299e-18	-2.00
Pb(OH)3-	4.136e-18	1.379e-18	3.00
FeH2PO4+2	-5.466e-19	2.733e-19	-2.00
Fe(OH)3-	1.098e-19	3.660e-20	3.00
FeF3	-2.990e-20	1.495e-20	-2.00
FeCl+2	-2.531e-20	1.266e-20	-2.00
Cd2OH+3	2.079e-20	2.079e-20	1.00

FeHPO4+	-1.595e-20	1.595e-20	-1.00
BF3OH-	-5.219e-21	2.610e-21	-2.00
NaOH	1.920e-22	1.920e-22	1.00
Mn(OH)3-	4.528e-23	1.509e-23	3.00
Pb3(OH)4+2	2.492e-23	6.230e-24	4.00
Cu(OH)4-2	1.921e-23	4.801e-24	4.00
FeCl2+	-1.844e-23	9.218e-24	-2.00
Pb(OH)4-2	1.395e-23	3.487e-24	4.00
Zn(OH)4-2	1.338e-23	3.346e-24	4.00
Cd(OH)3-	9.292e-24	3.097e-24	3.00
BF4-	-1.346e-25	4.487e-26	-3.00
Fe2(OH)2+4	-1.516e-26	7.578e-27	-2.00
FeCl3	-3.307e-28	1.653e-28	-2.00
SiF6-2	-5.639e-30	1.410e-30	-4.00
Cd(OH)4-2	1.219e-31	3.048e-32	4.00
Fe3(OH)4+5	-1.761e-35	8.807e-36	-2.00

----------Saturation indices----------

Phase	SI**	log IAP	log K(299 K, 1 atm)	
Al(OH)3(a)	-1.59	9.14	10.74	Al(OH)3
Albite	-4.65	-22.59	-17.94	NaAlSi3O8
Anorthite	-6.72	-26.40	-19.69	CaAl2Si2O8
Aragonite	-3.25	-11.59	-8.34	CaCO3
BaCl2	-15.98	-13.76	2.22	BaCl2
BaCl2:2H2O	-13.97	-13.76	0.22	BaCl2:2H2O
BaCl2:H2O	-14.58	-13.76	0.83	BaCl2:H2O
Ca-Montmorillonite	0.98	-43.91	-44.89	Ca0.165Al2.33Si3.67O10(OH)2
Calcite	-3.10	-11.59	-8.49	CaCO3
Cd(OH)2	-9.87	3.78	13.65	Cd(OH)2
CdSiO3	-9.05	-0.03	9.02	CdSiO3
Cerussite	-2.34	-15.46	-13.12	PbCO3
Chalcedony	-0.27	-3.81	-3.54	SiO2
Chlorite(14A)	-22.73	45.30	68.03	Mg5Al2Si3O10(OH)8
Chrysotile	-16.64	15.45	32.08	Mg3Si2O5(OH)4
CO2(g)	-1.50	-2.98	-1.48	CO2
Dolomite	-6.44	-23.55	-17.11	CaMg(CO3)2
Fe(OH)3(a)	-4.61	0.28	4.89	Fe(OH)3
Fluorite	-4.11	-14.69	-10.59	CaF2
Gibbsite	1.09	9.14	8.06	Al(OH)3
Goethite	1.32	0.28	-1.03	FeOOH
H2(g)	-15.66	-18.76	-3.10	H2
H2O(g)	-1.48	-0.00	1.48	H2O
Halite	-9.06	-7.49	1.57	NaCl
Hausmannite	-27.30	33.50	60.80	Mn3O4
Hematite	4.65	0.57	-4.08	Fe2O3
Hydroxyapatite	-14.84	-18.35	-3.51	Ca5(PO4)3OH
Illite	-1.09	-41.23	-40.14	K0.6Mg0.25Al2.3Si3.5O10(OH)2
K-feldspar	-2.60	-23.10	-20.50	KAlSi3O8
K-mica	5.18	17.75	12.56	KAl3Si3O10(OH)2
Kaolinite	3.32	10.68	7.35	Al2Si2O5(OH)4
Manganite	-11.57	13.77	25.34	MnOOH
NH3(g)	-11.31	-9.53	1.78	NH3
O2(g)	-51.66	-54.55	-2.90	O2
Otavite	-3.77	-15.87	-12.10	CdCO3
Pb(OH)2	-3.93	4.19	8.12	Pb(OH)2
Pyrochroite	-9.24	5.96	15.20	Mn(OH)2
Pyrolusite	-19.66	21.57	41.23	MnO2:H2O
Quartz	0.16	-3.81	-3.97	SiO2
Rhodochrosite	-2.55	-13.68	-11.13	MnCO3
Sepiolite	-11.78	3.95	15.74	Mg2Si3O7.5OH:3H2O
Sepiolite(d)	-14.71	3.95	18.66	Mg2Si3O7.5OH:3H2O
Siderite	-3.27	-14.17	-10.90	FeCO3
SiO2(a)	-1.10	-3.81	-2.70	SiO2
Smithsonite	-3.97	-13.98	-10.01	ZnCO3
Sylvite	-8.90	-8.00	0.90	KCl
Talc	-13.46	7.84	21.29	Mg3Si4O10(OH)2

Vivianite	-11.32	-47.32	-36.00	Fe3(PO4)2:8H2O
Willemite	-7.72	7.53	15.25	Zn2SiO4
Witherite	-5.38	-13.94	-8.56	BaCO3
Zn(OH)2(e)	-5.83	5.67	11.50	Zn(OH)2

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
For ideal gases, phi = 1.

Initial solution 34.

----------Solution composition----------

Elements	Molality	Moles
Al	3.032e-07	3.032e-07
Alkalinity	1.310e-03	1.310e-03
B	9.714e-07	9.714e-07
Ba	1.238e-06	1.238e-06
Br	1.628e-33	1.628e-33
Ca	1.822e-04	1.822e-04
Cd	8.809e-09	8.809e-09
Cl	1.072e-04	1.072e-04
Cu	9.818e-07	9.818e-07
F	1.948e-05	1.948e-05
Fe	1.791e-07	1.791e-07
K	1.330e-04	1.330e-04
Mg	8.556e-05	8.556e-05
Mn	5.279e-06	5.279e-06
N(-3)	2.856e-07	2.856e-07
N(3)	2.856e-07	2.856e-07
N(5)	3.142e-06	3.142e-06
Na	8.004e-04	8.004e-04
P	1.905e-06	1.905e-06
Pb	2.780e-08	2.780e-08
Si	8.655e-05	8.655e-05
Zn	1.170e-06	1.170e-06

----------Description of solution----------

pH	= 6.700
pe	= 1.481
Specific Conductance (µS/cm, 26°C)	= 145
Density (g/cm³)	= 0.99682
Volume (L)	= 1.00335
Activity of water	= 1.000
Ionic strength (mol/kgw)	= 1.730e-03
Mass of water (kg)	= 1.000e+00
Total carbon (mol/kg)	= 1.858e-03
Total CO2 (mol/kg)	= 1.858e-03
Temperature (°C)	= 26.24
Electrical balance (eq)	= 4.469e-05
Percent error, 100*(Cat-|An|)/(Cat+|An|)	= 1.53
Iterations	= 10 (365 overall)
Total H	= 1.110141e+02
Total O	= 5.551161e+01

----------Redox couples----------

Redox couple	pe	Eh (volts)
N(-3)/N(3)	6.0789	0.3611
N(-3)/N(5)	6.5690	0.3902
N(3)/N(5)	8.0393	0.4776

----------Distribution of species----------

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma	mole V cm³/mol

H+	2.084e-07	1.995e-07	-6.681	-6.700	-0.019	0.00
OH-	5.839e-08	5.572e-08	-7.234	-7.254	-0.020	-4.05
H2O	5.551e+01	9.999e-01	1.744	-0.000	0.000	18.08
Al	3.032e-07					
Al(OH)4-	2.232e-07	2.132e-07	-6.651	-6.671	-0.020	(0)
Al(OH)2+	2.872e-08	2.744e-08	-7.542	-7.562	-0.020	(0)
Al(OH)3	2.217e-08	2.218e-08	-7.654	-7.654	0.000	(0)
AlF2+	2.101e-08	2.008e-08	-7.677	-7.697	-0.020	(0)
AlF3	4.663e-09	4.665e-09	-8.331	-8.331	0.000	(0)
AlF+2	2.592e-09	2.160e-09	-8.586	-8.666	-0.079	(0)
AlOH+2	7.530e-10	6.275e-10	-9.123	-9.202	-0.079	-27.77
AlF4-	3.585e-11	3.424e-11	-10.445	-10.466	-0.020	(0)
Al+3	1.722e-11	1.163e-11	-10.764	-10.934	-0.170	-42.31
B	9.714e-07					
H3BO3	9.684e-07	9.688e-07	-6.014	-6.014	0.000	39.32
H2BO3-	2.993e-09	2.858e-09	-8.524	-8.544	-0.020	(0)
BF(OH)3-	7.543e-12	7.201e-12	-11.122	-11.143	-0.020	(0)
BF2(OH)2-	2.968e-15	2.833e-15	-14.528	-14.548	-0.020	(0)
BF3OH-	1.170e-20	1.117e-20	-19.932	-19.952	-0.020	(0)
BF4-	1.750e-25	1.671e-25	-24.757	-24.777	-0.020	(0)
Ba	1.238e-06					
Ba+2	1.224e-06	1.017e-06	-5.912	-5.993	-0.080	-12.65
BaHCO3+	1.322e-08	1.262e-08	-7.879	-7.899	-0.020	(0)
BaCl+	3.479e-10	3.321e-10	-9.459	-9.479	-0.020	(0)
BaCO3	1.615e-10	1.616e-10	-9.792	-9.792	0.000	-10.69
BaNO3+	4.021e-13	3.839e-13	-12.396	-12.416	-0.020	(0)
BaOH+	1.809e-13	1.728e-13	-12.743	-12.763	-0.020	(0)
Br	1.628e-33					
Br-	1.628e-33	1.553e-33	-32.788	-32.809	-0.020	24.62
CdBr+	1.678e-39	1.602e-39	-38.775	-38.795	-0.020	(0)
PbBr+	3.596e-40	3.433e-40	-39.444	-39.464	-0.020	(0)
ZnBr+	3.496e-40	3.338e-40	-39.456	-39.477	-0.020	(0)
CdBr2	0.000e+00	0.000e+00	-70.872	-70.872	0.000	(0)
PbBr2	0.000e+00	0.000e+00	-72.612	-72.612	0.000	(0)
ZnBr2	0.000e+00	0.000e+00	-72.685	-72.685	0.000	(0)
C(4)	1.858e-03					
HCO3-	1.303e-03	1.245e-03	-2.885	-2.905	-0.020	24.78
CO2	5.499e-04	5.501e-04	-3.260	-3.260	0.000	34.49
CaHCO3+	2.531e-06	2.419e-06	-5.597	-5.616	-0.020	9.73
MgHCO3+	1.079e-06	1.030e-06	-5.967	-5.987	-0.020	5.52
NaHCO3	5.304e-07	5.306e-07	-6.275	-6.275	0.000	1.80
MnHCO3+	4.578e-07	4.373e-07	-6.339	-6.359	-0.020	(0)
CO3-2	3.598e-07	2.998e-07	-6.444	-6.523	-0.079	-5.15
ZnHCO3+	1.341e-07	1.280e-07	-6.873	-6.893	-0.020	(0)
MnCO3	9.386e-08	9.390e-08	-7.028	-7.027	0.000	(0)
CaCO3	7.723e-08	7.726e-08	-7.112	-7.112	0.000	-14.59
CuCO3	7.026e-08	7.029e-08	-7.153	-7.153	0.000	(0)
ZnCO3	4.885e-08	4.887e-08	-7.311	-7.311	0.000	(0)
CuHCO3+	2.852e-08	2.723e-08	-7.545	-7.565	-0.020	(0)
MgCO3	2.051e-08	2.052e-08	-7.688	-7.688	0.000	-17.09
PbCO3	1.916e-08	1.916e-08	-7.718	-7.718	0.000	(0)
FeHCO3+	1.741e-08	1.662e-08	-7.759	-7.779	-0.020	(0)
BaHCO3+	1.322e-08	1.262e-08	-7.879	-7.899	-0.020	(0)
(CO2)2	5.783e-09	5.786e-09	-8.238	-8.238	0.000	68.99
NaCO3-	4.751e-09	4.536e-09	-8.323	-8.343	-0.020	-0.91
PbHCO3+	3.809e-09	3.636e-09	-8.419	-8.439	-0.020	(0)
FeCO3	9.603e-10	9.607e-10	-9.018	-9.017	0.000	(0)
Zn(CO3)2-2	3.771e-10	3.132e-10	-9.424	-9.504	-0.081	(0)
CdHCO3+	2.891e-10	2.760e-10	-9.539	-9.559	-0.020	(0)
BaCO3	1.615e-10	1.616e-10	-9.792	-9.792	0.000	-10.69
Cu(CO3)2-2	3.194e-11	2.653e-11	-10.496	-10.576	-0.081	(0)
Pb(CO3)2-2	1.737e-11	1.443e-11	-10.760	-10.841	-0.081	(0)
CdCO3	1.669e-12	1.670e-12	-11.777	-11.777	0.000	(0)
Cd(CO3)2-2	1.906e-15	1.583e-15	-14.720	-14.800	-0.081	(0)
Ca	1.822e-04					
Ca+2	1.795e-04	1.495e-04	-3.746	-3.825	-0.079	-18.10
CaHCO3+	2.531e-06	2.419e-06	-5.597	-5.616	-0.020	9.73

CaCO3	7.723e-08	7.726e-08	-7.112	-7.112	0.000	-14.59
CaHPO4	3.397e-08	3.398e-08	-7.469	-7.469	0.000	(0)
CaH2PO4+	5.301e-09	5.064e-09	-8.276	-8.295	-0.020	(0)
CaPO4-	4.317e-10	4.124e-10	-9.365	-9.385	-0.020	(0)
CaOH+	1.303e-10	1.244e-10	-9.885	-9.905	-0.020	(0)
Cd	8.809e-09					
Cd+2	8.441e-09	7.012e-09	-8.074	-8.154	-0.081	-18.66
CdHCO3+	2.891e-10	2.760e-10	-9.539	-9.559	-0.020	(0)
CdCl+	7.174e-11	6.849e-11	-10.144	-10.164	-0.020	6.16
CdOH+	3.355e-12	3.203e-12	-11.474	-11.494	-0.020	(0)
CdF+	1.704e-12	1.627e-12	-11.768	-11.789	-0.020	(0)
CdCO3	1.669e-12	1.670e-12	-11.777	-11.777	0.000	(0)
CdOHCl	1.455e-13	1.456e-13	-12.837	-12.837	0.000	(0)
CdNO3+	5.332e-14	5.091e-14	-13.273	-13.293	-0.020	17.49
CdCl2	2.920e-14	2.922e-14	-13.535	-13.534	0.000	23.14
Cd(CO3)2-2	1.906e-15	1.583e-15	-14.720	-14.800	-0.081	(0)
Cd(OH)2	7.863e-16	7.866e-16	-15.104	-15.104	0.000	(0)
CdF2	7.529e-17	7.532e-17	-16.123	-16.123	0.000	(0)
CdCl3-	2.004e-18	1.913e-18	-17.698	-17.718	-0.020	68.46
Cd2OH+3	1.644e-19	1.083e-19	-18.784	-18.965	-0.181	(0)
Cd(OH)3-	4.633e-22	4.423e-22	-21.334	-21.354	-0.020	(0)
Cd(OH)4-2	2.378e-29	1.976e-29	-28.624	-28.704	-0.081	(0)
CdBr+	1.678e-39	1.602e-39	-38.775	-38.795	-0.020	(0)
CdBr2	0.000e+00	0.000e+00	-70.872	-70.872	0.000	(0)
Cl	1.072e-04					
Cl-	1.067e-04	1.019e-04	-3.972	-3.992	-0.020	18.12
NaCl	4.693e-07	4.694e-07	-6.329	-6.328	0.000	(0)
CuCl2-	2.624e-09	2.505e-09	-8.581	-8.601	-0.020	(0)
MnCl+	1.713e-09	1.636e-09	-8.766	-8.786	-0.020	-2.79
BaCl+	3.479e-10	3.321e-10	-9.459	-9.479	-0.020	(0)
ZnCl+	2.477e-10	2.365e-10	-9.606	-9.626	-0.020	-12.70
CdCl+	7.174e-11	6.849e-11	-10.144	-10.164	-0.020	6.16
FeCl+	1.967e-11	1.878e-11	-10.706	-10.726	-0.020	(0)
PbCl+	1.611e-11	1.538e-11	-10.793	-10.813	-0.020	8.00
ZnOHCl	1.380e-11	1.381e-11	-10.860	-10.860	0.000	(0)
CuCl+	1.332e-11	1.271e-11	-10.876	-10.896	-0.020	0.33
CuCl3-2	4.881e-13	4.063e-13	-12.312	-12.391	-0.080	(0)
CdOHCl	1.455e-13	1.456e-13	-12.837	-12.837	0.000	(0)
MnCl2	7.272e-14	7.275e-14	-13.138	-13.138	0.000	84.40
CdCl2	2.920e-14	2.922e-14	-13.535	-13.534	0.000	23.14
ZnCl2	2.534e-14	2.535e-14	-13.596	-13.596	0.000	99.65
PbCl2	2.425e-15	2.426e-15	-14.615	-14.615	0.000	35.07
CuCl2	7.046e-16	7.049e-16	-15.152	-15.152	0.000	32.42
ZnCl3-	3.058e-18	2.919e-18	-17.515	-17.535	-0.020	17.10
MnCl3-	2.137e-18	2.041e-18	-17.670	-17.690	-0.020	43.31
CdCl3-	2.004e-18	1.913e-18	-17.698	-17.718	-0.020	68.46
PbCl3-	2.072e-19	1.978e-19	-18.684	-18.704	-0.020	66.11
FeCl+2	1.588e-21	1.322e-21	-20.799	-20.879	-0.080	(0)
CuCl3-	2.728e-22	2.604e-22	-21.564	-21.584	-0.020	(0)
ZnCl4-2	1.808e-22	1.505e-22	-21.743	-21.822	-0.080	145.36
PbCl4-2	1.172e-23	9.736e-24	-22.931	-23.012	-0.081	101.57
FeCl2+	6.054e-25	5.783e-25	-24.218	-24.238	-0.020	(0)
CuCl4-2	1.643e-28	1.368e-28	-27.784	-27.864	-0.080	(0)
FeCl3	5.888e-30	5.891e-30	-29.230	-29.230	0.000	(0)
Cu(1)	8.054e-07					
Cu+	8.028e-07	7.657e-07	-6.095	-6.116	-0.021	(0)
CuCl2-	2.624e-09	2.505e-09	-8.581	-8.601	-0.020	(0)
CuCl3-2	4.881e-13	4.063e-13	-12.312	-12.391	-0.080	(0)
Cu(2)	1.764e-07					
CuCO3	7.026e-08	7.029e-08	-7.153	-7.153	0.000	(0)
Cu+2	5.231e-08	4.365e-08	-7.281	-7.360	-0.079	-26.59
CuHCO3+	2.852e-08	2.723e-08	-7.545	-7.565	-0.020	(0)
Cu(OH)2	2.290e-08	2.291e-08	-7.640	-7.640	0.000	(0)
CuOH+	2.292e-09	2.188e-09	-8.640	-8.660	-0.020	(0)
Cu(CO3)2-2	3.194e-11	2.653e-11	-10.496	-10.576	-0.081	(0)
CuF+	1.551e-11	1.481e-11	-10.809	-10.829	-0.020	(0)
CuCl+	1.332e-11	1.271e-11	-10.876	-10.896	-0.020	0.33
Cu2(OH)2+2	2.850e-12	2.368e-12	-11.545	-11.626	-0.081	(0)

Cu(OH)3-	7.246e-15	6.918e-15	-14.140	-14.160	-0.020	(0)
CuCl2	7.046e-16	7.049e-16	-15.152	-15.152	0.000	32.42
Cu(OH)4-2	8.327e-21	6.917e-21	-20.079	-20.160	-0.081	(0)
CuCl3-	2.728e-22	2.604e-22	-21.564	-21.584	-0.020	(0)
CuCl4-2	1.643e-28	1.368e-28	-27.784	-27.864	-0.080	(0)
F	1.948e-05					
F-	1.931e-05	1.843e-05	-4.714	-4.734	-0.020	-1.30
MgF+	9.175e-08	8.762e-08	-7.037	-7.057	-0.020	-10.57
AlF2+	2.101e-08	2.008e-08	-7.677	-7.697	-0.020	(0)
NaF	8.094e-09	8.097e-09	-8.092	-8.092	0.000	7.31
HF	5.638e-09	5.640e-09	-8.249	-8.249	0.000	12.56
AlF3	4.663e-09	4.665e-09	-8.331	-8.331	0.000	(0)
AlF+2	2.592e-09	2.160e-09	-8.586	-8.666	-0.079	(0)
MnF+	5.263e-10	5.027e-10	-9.279	-9.299	-0.020	(0)
ZnF+	2.263e-10	2.160e-10	-9.645	-9.666	-0.020	(0)
AlF4-	3.585e-11	3.424e-11	-10.445	-10.466	-0.020	(0)
FeF+	2.579e-11	2.462e-11	-10.589	-10.609	-0.020	(0)
CuF+	1.551e-11	1.481e-11	-10.809	-10.829	-0.020	(0)
BF(OH)3-	7.543e-12	7.201e-12	-11.122	-11.143	-0.020	(0)
CdF+	1.704e-12	1.627e-12	-11.768	-11.789	-0.020	(0)
PbF+	1.263e-12	1.205e-12	-11.899	-11.919	-0.020	(0)
HF2-	4.218e-13	4.026e-13	-12.375	-12.395	-0.020	22.12
BF2(OH)2-	2.968e-15	2.833e-15	-14.528	-14.548	-0.020	(0)
PbF2	4.535e-16	4.536e-16	-15.343	-15.343	0.000	(0)
CdF2	7.529e-17	7.532e-17	-16.123	-16.123	0.000	(0)
FeF+2	1.477e-17	1.230e-17	-16.831	-16.910	-0.080	(0)
FeF2+	9.587e-18	9.158e-18	-17.018	-17.038	-0.020	(0)
FeF3	2.685e-19	2.686e-19	-18.571	-18.571	0.000	(0)
PbF3-	6.345e-20	6.057e-20	-19.198	-19.218	-0.020	(0)
BF3OH-	1.170e-20	1.117e-20	-19.932	-19.952	-0.020	(0)
PbF4-2	6.432e-25	5.343e-25	-24.192	-24.272	-0.081	(0)
BF4-	1.750e-25	1.671e-25	-24.757	-24.777	-0.020	(0)
SiF6-2	8.724e-30	7.263e-30	-29.059	-29.139	-0.080	42.68
Fe(2)	1.790e-07					
Fe+2	1.601e-07	1.336e-07	-6.796	-6.874	-0.079	-22.03
FeHCO3+	1.741e-08	1.662e-08	-7.759	-7.779	-0.020	(0)
FeCO3	9.603e-10	9.607e-10	-9.018	-9.017	0.000	(0)
FeOH+	2.430e-10	2.322e-10	-9.614	-9.634	-0.020	(0)
FeHPO4	2.153e-10	2.154e-10	-9.667	-9.667	0.000	(0)
FeH2PO4+	9.056e-11	8.653e-11	-10.043	-10.063	-0.020	(0)
FeF+	2.579e-11	2.462e-11	-10.589	-10.609	-0.020	(0)
FeCl+	1.967e-11	1.878e-11	-10.706	-10.726	-0.020	(0)
Fe(OH)2	1.102e-14	1.103e-14	-13.958	-13.958	0.000	(0)
Fe(OH)3-	2.175e-18	2.078e-18	-17.662	-17.682	-0.020	(0)
Fe(3)	4.330e-11					
Fe(OH)2+	2.617e-11	2.500e-11	-10.582	-10.602	-0.020	(0)
Fe(OH)3	1.703e-11	1.703e-11	-10.769	-10.769	0.000	(0)
Fe(OH)4-	8.564e-14	8.182e-14	-13.067	-13.087	-0.020	(0)
FeOH+2	1.727e-14	1.438e-14	-13.763	-13.842	-0.080	(0)
FeF+2	1.477e-17	1.230e-17	-16.831	-16.910	-0.080	(0)
FeF2+	9.587e-18	9.158e-18	-17.018	-17.038	-0.020	(0)
Fe+3	6.116e-19	4.132e-19	-18.214	-18.384	-0.170	(0)
FeF3	2.685e-19	2.686e-19	-18.571	-18.571	0.000	(0)
FeH2PO4+2	1.725e-19	1.437e-19	-18.763	-18.842	-0.079	(0)
FeHPO4+	4.908e-20	4.688e-20	-19.309	-19.329	-0.020	(0)
FeCl+2	1.588e-21	1.322e-21	-20.799	-20.879	-0.080	(0)
FeCl2+	6.054e-25	5.783e-25	-24.218	-24.238	-0.020	(0)
Fe2(OH)2+4	1.110e-26	5.286e-27	-25.955	-26.277	-0.322	(0)
FeCl3	5.888e-30	5.891e-30	-29.230	-29.230	0.000	(0)
Fe3(OH)4+5	7.856e-35	2.464e-35	-34.105	-34.608	-0.504	(0)
H(0)	6.075e-20					
H2	3.037e-20	3.039e-20	-19.518	-19.517	0.000	28.60
K	1.330e-04					
K+	1.330e-04	1.269e-04	-3.876	-3.896	-0.020	9.06
KHPO4-	1.049e-10	1.002e-10	-9.979	-9.999	-0.020	38.03
Mg	8.556e-05					
Mg+2	8.435e-05	7.036e-05	-4.074	-4.153	-0.079	-21.84
MgHCO3+	1.079e-06	1.030e-06	-5.967	-5.987	-0.020	5.52

MgF+	9.175e-08	8.762e-08	-7.037	-7.057	-0.020	-10.57
MgHPO4	2.161e-08	2.162e-08	-7.665	-7.665	0.000	(0)
MgCO3	2.051e-08	2.052e-08	-7.688	-7.688	0.000	-17.09
MgH2PO4+	3.176e-09	3.034e-09	-8.498	-8.518	-0.020	(0)
MgOH+	1.497e-09	1.431e-09	-8.825	-8.844	-0.020	(0)
MgPO4-	2.740e-10	2.618e-10	-9.562	-9.582	-0.020	(0)
Mn(2)	5.279e-06					
Mn+2	4.725e-06	3.943e-06	-5.326	-5.404	-0.079	-20.76
MnHCO3+	4.578e-07	4.373e-07	-6.339	-6.359	-0.020	(0)
MnCO3	9.386e-08	9.390e-08	-7.028	-7.027	0.000	(0)
MnCl+	1.713e-09	1.636e-09	-8.766	-8.786	-0.020	-2.79
MnOH+	5.880e-10	5.617e-10	-9.231	-9.251	-0.020	(0)
MnF+	5.263e-10	5.027e-10	-9.279	-9.299	-0.020	(0)
MnCl2	7.272e-14	7.275e-14	-13.138	-13.138	0.000	84.40
Mn(NO3)2	1.406e-16	1.406e-16	-15.852	-15.852	0.000	40.71
MnCl3-	2.137e-18	2.041e-18	-17.670	-17.690	-0.020	43.31
Mn(OH)3-	8.234e-21	7.865e-21	-20.084	-20.104	-0.020	(0)
Mn(3)	6.538e-30					
Mn+3	6.538e-30	4.417e-30	-29.185	-29.355	-0.170	(0)
N(-3)	2.856e-07					
NH4+	2.848e-07	2.716e-07	-6.546	-6.566	-0.021	18.01
NH3	8.461e-10	8.464e-10	-9.073	-9.072	0.000	24.47
N(3)	2.856e-07					
NO2-	2.856e-07	2.725e-07	-6.544	-6.565	-0.020	25.04
N(5)	3.142e-06					
NO3-	3.142e-06	2.997e-06	-5.503	-5.523	-0.020	29.61
BaNO3+	4.021e-13	3.839e-13	-12.396	-12.416	-0.020	(0)
PbNO3+	1.708e-13	1.631e-13	-12.768	-12.788	-0.020	(0)
CdNO3+	5.332e-14	5.091e-14	-13.273	-13.293	-0.020	17.49
Mn(NO3)2	1.406e-16	1.406e-16	-15.852	-15.852	0.000	40.71
Na	8.004e-04					
Na+	7.994e-04	7.635e-04	-3.097	-3.117	-0.020	-1.40
NaHCO3	5.304e-07	5.306e-07	-6.275	-6.275	0.000	1.80
NaCl	4.693e-07	4.694e-07	-6.329	-6.328	0.000	(0)
NaF	8.094e-09	8.097e-09	-8.092	-8.092	0.000	7.31
NaCO3-	4.751e-09	4.536e-09	-8.323	-8.343	-0.020	-0.91
NaHPO4-	6.310e-10	6.029e-10	-9.200	-9.220	-0.020	33.52
NaOH	4.253e-21	4.254e-21	-20.371	-20.371	0.000	(0)
O(0)	0.000e+00					
O2	0.000e+00	0.000e+00	-52.947	-52.947	0.000	30.50
P	1.905e-06					
H2PO4-	1.353e-06	1.292e-06	-5.869	-5.889	-0.020	33.19
HPO4-2	4.864e-07	4.050e-07	-6.313	-6.393	-0.080	6.71
CaHPO4	3.397e-08	3.398e-08	-7.469	-7.469	0.000	(0)
MgHPO4	2.161e-08	2.162e-08	-7.665	-7.665	0.000	(0)
CaH2PO4+	5.301e-09	5.064e-09	-8.276	-8.295	-0.020	(0)
MgH2PO4+	3.176e-09	3.034e-09	-8.498	-8.518	-0.020	(0)
NaHPO4-	6.310e-10	6.029e-10	-9.200	-9.220	-0.020	33.52
CaPO4-	4.317e-10	4.124e-10	-9.365	-9.385	-0.020	(0)
MgPO4-	2.740e-10	2.618e-10	-9.562	-9.582	-0.020	(0)
FeHPO4	2.153e-10	2.154e-10	-9.667	-9.667	0.000	(0)
KHPO4-	1.049e-10	1.002e-10	-9.979	-9.999	-0.020	38.03
FeH2PO4+	9.056e-11	8.653e-11	-10.043	-10.063	-0.020	(0)
H3PO4	3.852e-11	3.853e-11	-10.414	-10.414	0.000	47.47
PO4-3	1.424e-12	9.379e-13	-11.846	-12.028	-0.181	-23.27
FeH2PO4+2	1.725e-19	1.437e-19	-18.763	-18.842	-0.079	(0)
FeHPO4+	4.908e-20	4.688e-20	-19.309	-19.329	-0.020	(0)
Pb	2.780e-08					
PbCO3	1.916e-08	1.916e-08	-7.718	-7.718	0.000	(0)
Pb+2	4.428e-09	3.678e-09	-8.354	-8.434	-0.081	-15.52
PbHCO3+	3.809e-09	3.636e-09	-8.419	-8.439	-0.020	(0)
PbOH+	3.765e-10	3.594e-10	-9.424	-9.444	-0.020	(0)
Pb(CO3)2-2	1.737e-11	1.443e-11	-10.760	-10.841	-0.081	(0)
PbCl+	1.611e-11	1.538e-11	-10.793	-10.813	-0.020	8.00
PbF+	1.263e-12	1.205e-12	-11.899	-11.919	-0.020	(0)
Pb(OH)2	7.005e-13	7.007e-13	-12.155	-12.154	0.000	(0)
PbNO3+	1.708e-13	1.631e-13	-12.768	-12.788	-0.020	(0)
PbCl2	2.425e-15	2.426e-15	-14.615	-14.615	0.000	35.07

PbF2	4.535e-16	4.536e-16	-15.343	-15.343	0.000	(0)
Pb2OH+3	4.492e-17	2.959e-17	-16.348	-16.529	-0.181	(0)
Pb(OH)3-	4.224e-17	4.032e-17	-16.374	-16.394	-0.020	(0)
PbCl3-	2.072e-19	1.978e-19	-18.684	-18.704	-0.020	66.11
PbF3-	6.345e-20	6.057e-20	-19.198	-19.218	-0.020	(0)
Pb(OH)4-2	5.573e-22	4.629e-22	-21.254	-21.334	-0.081	(0)
Pb3(OH)4+2	5.994e-23	4.979e-23	-22.222	-22.303	-0.081	(0)
PbCl4-2	1.172e-23	9.736e-24	-22.931	-23.012	-0.081	101.57
PbF4-2	6.432e-25	5.343e-25	-24.192	-24.272	-0.081	(0)
PbBr+	3.596e-40	3.433e-40	-39.444	-39.464	-0.020	(0)
PbBr2	0.000e+00	0.000e+00	-72.612	-72.612	0.000	(0)
Si	8.655e-05					
H4SiO4	8.648e-05	8.652e-05	-4.063	-4.063	0.000	51.98
H3SiO4-	6.990e-08	6.673e-08	-7.156	-7.176	-0.020	28.01
H2SiO4-2	2.958e-14	2.465e-14	-13.529	-13.608	-0.079	(0)
SiF6-2	8.724e-30	7.263e-30	-29.059	-29.139	-0.080	42.68
Zn	1.170e-06					
Zn+2	9.812e-07	8.169e-07	-6.008	-6.088	-0.080	-25.41
ZnHCO3+	1.341e-07	1.280e-07	-6.873	-6.893	-0.020	(0)
ZnCO3	4.885e-08	4.887e-08	-7.311	-7.311	0.000	(0)
ZnOH+	5.164e-09	4.930e-09	-8.287	-8.307	-0.020	(0)
Zn(CO3)2-2	3.771e-10	3.132e-10	-9.424	-9.504	-0.081	(0)
Zn(OH)2	2.582e-10	2.583e-10	-9.588	-9.588	0.000	(0)
ZnCl+	2.477e-10	2.365e-10	-9.606	-9.626	-0.020	-12.70
ZnF+	2.263e-10	2.160e-10	-9.645	-9.666	-0.020	(0)
ZnOHCl	1.380e-11	1.381e-11	-10.860	-10.860	0.000	(0)
ZnCl2	2.534e-14	2.535e-14	-13.596	-13.596	0.000	99.65
Zn(OH)3-	4.288e-15	4.093e-15	-14.368	-14.388	-0.020	(0)
ZnCl3-	3.058e-18	2.919e-18	-17.515	-17.535	-0.020	17.10
Zn(OH)4-2	3.914e-21	3.251e-21	-20.407	-20.488	-0.081	(0)
ZnCl4-2	1.808e-22	1.505e-22	-21.743	-21.822	-0.080	145.36
ZnBr+	3.496e-40	3.338e-40	-39.456	-39.477	-0.020	(0)
ZnBr2	0.000e+00	0.000e+00	-72.685	-72.685	0.000	(0)

----------Distribution of alkalinity----------

Total alkalinity (eq/kgw) = 1.310e-03

Species	Alkalinity	Molality	Alk/Mol
HCO3-	1.303e-03	1.303e-03	1.00
CaHCO3+	2.531e-06	2.531e-06	1.00
MgHCO3+	1.079e-06	1.079e-06	1.00
Al(OH)4-	8.929e-07	2.232e-07	4.00
CO3-2	7.196e-07	3.598e-07	2.00
NaHCO3	5.304e-07	5.304e-07	1.00
HPO4-2	4.864e-07	4.864e-07	1.00
MnHCO3+	4.578e-07	4.578e-07	1.00
H+	-2.084e-07	2.084e-07	-1.00
MnCO3	1.877e-07	9.386e-08	2.00
CaCO3	1.545e-07	7.723e-08	2.00
CuCO3	1.405e-07	7.026e-08	2.00
ZnHCO3+	1.341e-07	1.341e-07	1.00
ZnCO3	9.769e-08	4.885e-08	2.00
H3SiO4-	6.990e-08	6.990e-08	1.00
Al(OH)3	6.652e-08	2.217e-08	3.00
OH-	5.839e-08	5.839e-08	1.00
Al(OH)2+	5.744e-08	2.872e-08	2.00
Cu(OH)2	4.580e-08	2.290e-08	2.00
MgCO3	4.102e-08	2.051e-08	2.00
PbCO3	3.831e-08	1.916e-08	2.00
CaHPO4	3.397e-08	3.397e-08	1.00
CuHCO3+	2.852e-08	2.852e-08	1.00
MgHPO4	2.161e-08	2.161e-08	1.00
FeHCO3+	1.741e-08	1.741e-08	1.00
BaHCO3+	1.322e-08	1.322e-08	1.00
NaCO3-	9.503e-09	4.751e-09	2.00
HF	-5.638e-09	5.638e-09	-1.00

ZnOH+	5.164e-09	5.164e-09	1.00
PbHCO3+	3.809e-09	3.809e-09	1.00
H2BO3-	2.993e-09	2.993e-09	1.00
CuOH+	2.292e-09	2.292e-09	1.00
FeCO3	1.921e-09	9.603e-10	2.00
Zn(CO3)2-2	1.508e-09	3.771e-10	4.00
MgOH+	1.497e-09	1.497e-09	1.00
CaPO4-	8.633e-10	4.317e-10	2.00
NH3	8.461e-10	8.461e-10	1.00
AlOH+2	7.530e-10	7.530e-10	1.00
NaHPO4-	6.310e-10	6.310e-10	1.00
MnOH+	5.880e-10	5.880e-10	1.00
MgPO4-	5.479e-10	2.740e-10	2.00
Zn(OH)2	5.164e-10	2.582e-10	2.00
PbOH+	3.765e-10	3.765e-10	1.00
BaCO3	3.230e-10	1.615e-10	2.00
CdHCO3+	2.891e-10	2.891e-10	1.00
FeOH+	2.430e-10	2.430e-10	1.00
FeHPO4	2.153e-10	2.153e-10	1.00
CaOH+	1.303e-10	1.303e-10	1.00
Cu(CO3)2-2	1.278e-10	3.194e-11	4.00
KHPO4-	1.049e-10	1.049e-10	1.00
Pb(CO3)2-2	6.949e-11	1.737e-11	4.00
H3PO4	-3.852e-11	3.852e-11	-1.00
Fe(OH)3	1.703e-11	1.703e-11	1.00
ZnOHCl	1.380e-11	1.380e-11	1.00
Cu2(OH)2+2	5.701e-12	2.850e-12	2.00
CdOH+	3.355e-12	3.355e-12	1.00
CdCO3	3.338e-12	1.669e-12	2.00
PO4-3	2.848e-12	1.424e-12	2.00
Pb(OH)2	1.401e-12	7.005e-13	2.00
HF2-	-4.218e-13	4.218e-13	-1.00
BaOH+	1.809e-13	1.809e-13	1.00
Fe(OH)4-	1.713e-13	8.564e-14	2.00
CdOHCl	1.455e-13	1.455e-13	1.00
H2SiO4-2	5.916e-14	2.958e-14	2.00
Fe(OH)2	2.204e-14	1.102e-14	2.00
Cu(OH)3-	2.174e-14	7.246e-15	3.00
FeOH+2	-1.727e-14	1.727e-14	-1.00
Zn(OH)3-	1.286e-14	4.288e-15	3.00
Cd(CO3)2-2	7.624e-15	1.906e-15	4.00
BF2(OH)2-	-2.968e-15	2.968e-15	-1.00
Cd(OH)2	1.573e-15	7.863e-16	2.00
Pb(OH)3-	1.267e-16	4.224e-17	3.00
Pb2OH+3	4.492e-17	4.492e-17	1.00
FeF+2	-2.954e-17	1.477e-17	-2.00
FeF2+	-1.917e-17	9.587e-18	-2.00
Fe(OH)3-	6.526e-18	2.175e-18	3.00
Fe+3	-1.223e-18	6.116e-19	-2.00
FeF3	-5.370e-19	2.685e-19	-2.00
FeH2PO4+2	-3.449e-19	1.725e-19	-2.00
Cd2OH+3	1.644e-19	1.644e-19	1.00
FeHPO4+	-4.908e-20	4.908e-20	-1.00
Cu(OH)4-2	3.331e-20	8.327e-21	4.00
Mn(OH)3-	2.470e-20	8.234e-21	3.00
BF3OH-	-2.340e-20	1.170e-20	-2.00
Zn(OH)4-2	1.566e-20	3.914e-21	4.00
NaOH	4.253e-21	4.253e-21	1.00
FeCl+2	-3.175e-21	1.588e-21	-2.00
Pb(OH)4-2	2.229e-21	5.573e-22	4.00
Cd(OH)3-	1.390e-21	4.633e-22	3.00
Pb3(OH)4+2	2.398e-22	5.994e-23	4.00
FeCl2+	-1.211e-24	6.054e-25	-2.00
BF4-	-5.250e-25	1.750e-25	-3.00
Fe2(OH)2+4	-2.221e-26	1.110e-26	-2.00
Cd(OH)4-2	9.514e-29	2.378e-29	4.00
SiF6-2	-3.490e-29	8.724e-30	-4.00
FeCl3	-1.178e-29	5.888e-30	-2.00

Fe3(OH)4+5	-1.571e-34	7.856e-35	-2.00

----------Saturation indices----------

Phase	SI**	log IAP	log K(299 K, 1 atm)	
Al(OH)3(a)	-1.55	9.17	10.72	Al(OH)3
Albite	-4.05	-21.98	-17.92	NaAlSi3O8
Anorthite	-5.61	-25.29	-19.68	CaAl2Si2O8
Aragonite	-2.00	-10.35	-8.34	CaCO3
BaCl2	-16.19	-13.98	2.22	BaCl2
BaCl2:2H2O	-14.20	-13.98	0.22	BaCl2:2H2O
BaCl2:H2O	-14.80	-13.98	0.83	BaCl2:H2O
Ca-Montmorillonite	0.36	-44.49	-44.85	Ca0.165Al2.33Si3.67O10(OH)2
Calcite	-1.86	-10.35	-8.49	CaCO3
Cd(OH)2	-8.40	5.25	13.65	Cd(OH)2
CdSiO3	-7.83	1.18	9.01	CdSiO3
Cerussite	-1.84	-14.96	-13.12	PbCO3
Chalcedony	-0.53	-4.06	-3.54	SiO2
Chlorite(14A)	-15.54	52.38	67.92	Mg5Al2Si3O10(OH)8
Chrysotile	-12.43	19.62	32.05	Mg3Si2O5(OH)4
CO2(g)	-1.78	-3.26	-1.48	CO2
Dolomite	-3.91	-21.02	-17.12	CaMg(CO3)2
Fe(OH)3(a)	-3.17	1.72	4.89	Fe(OH)3
Fluorite	-2.71	-13.29	-10.59	CaF2
Gibbsite	1.12	9.17	8.04	Al(OH)3
Goethite	2.76	1.72	-1.04	FeOOH
H2(g)	-16.41	-19.52	-3.10	H2
H2O(g)	-1.47	-0.00	1.47	H2O
Halite	-8.68	-7.11	1.57	NaCl
Hausmannite	-20.38	40.35	60.72	Mn3O4
Hematite	7.53	3.43	-4.10	Fe2O3
Hydroxyapatite	-7.97	-11.50	-3.53	Ca5(PO4)3OH
Illite	-0.88	-40.98	-40.10	K0.6Mg0.25Al2.3Si3.5O10(OH)2
K-feldspar	-2.28	-22.76	-20.48	KAlSi3O8
K-mica	5.59	18.11	12.52	KAl3Si3O10(OH)2
Kaolinite	2.88	10.21	7.33	Al2Si2O5(OH)4
Manganite	-9.16	16.18	25.34	MnOOH
NH3(g)	-10.84	-9.07	1.77	NH3
O2(g)	-50.05	-52.95	-2.90	O2
Otavite	-2.58	-14.68	-12.10	CdCO3
Pb(OH)2	-3.14	4.97	8.11	Pb(OH)2
Pyrochroite	-7.20	8.00	15.20	Mn(OH)2
Pyrolusite	-16.82	24.36	41.18	MnO2:H2O
Quartz	-0.10	-4.06	-3.96	SiO2
Rhodochrosite	-0.79	-11.93	-11.13	MnCO3
Sepiolite	-9.42	6.31	15.73	Mg2Si3O7.5OH:3H2O
Sepiolite(d)	-12.35	6.31	18.66	Mg2Si3O7.5OH:3H2O
Siderite	-2.50	-13.40	-10.90	FeCO3
SiO2(a)	-1.36	-4.06	-2.70	SiO2
Smithsonite	-2.60	-12.61	-10.01	ZnCO3
Sylvite	-8.79	-7.89	0.91	KCl
Talc	-9.77	11.49	21.26	Mg3Si4O10(OH)2
Vivianite	-8.68	-44.68	-36.00	Fe3(PO4)2:8H2O
Willemite	-4.67	10.56	15.23	Zn2SiO4
Witherite	-3.96	-12.52	-8.56	BaCO3
Zn(OH)2(e)	-4.19	7.31	11.50	Zn(OH)2

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
For ideal gases, phi = 1.

Initial solution 35.

----------Solution composition----------

Elements	Molality	Moles
Al	5.791e-07	5.791e-07

Alkalinity	5.374e-03	5.374e-03
B	2.461e-06	2.461e-06
Ba	3.132e-06	3.132e-06
Br	1.875e-33	1.875e-33
Ca	1.223e-04	1.223e-04
Cd	8.365e-09	8.365e-09
Cu	1.385e-08	1.385e-08
Fe	1.612e-06	1.612e-06
K	4.093e-05	4.093e-05
Mg	3.250e-05	3.250e-05
Mn	5.462e-06	5.462e-06
N(-3)	7.856e-07	7.856e-07
N(3)	2.857e-07	2.857e-07
N(5)	1.500e-06	1.500e-06
Na	1.392e-04	1.392e-04
P	4.101e-06	4.101e-06
Pb	8.014e-09	8.014e-09
Si	3.246e-04	3.246e-04
Zn	3.045e-07	3.045e-07

----------Description of solution----------

pH	= 8.800
pe	= -2.010
Specific Conductance (µS/cm, 25°C)	= 259
Density (g/cm³)	= 0.99720
Volume (L)	= 1.00316
Activity of water	= 1.000
Ionic strength (mol/kgw)	= 3.192e-03
Mass of water (kg)	= 1.000e+00
Total carbon (mol/kg)	= 5.143e-03
Total CO2 (mol/kg)	= 5.143e-03
Temperature (°C)	= 25.24
Electrical balance (eq)	= -4.866e-03
Percent error, 100*(Cat-|An|)/(Cat+|An|)	= -84.43
Iterations	= 9 (374 overall)
Total H	= 1.110186e+02
Total O	= 5.552297e+01

----------Redox couples----------

Redox couple	pe	Eh (volts)
N(-3)/N(3)	3.2853	0.1945
N(-3)/N(5)	3.9220	0.2322
N(3)/N(5)	5.8322	0.3453

----------Distribution of species----------

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma	mole V cm³/mol
OH-	6.922e-06	6.503e-06	-5.160	-5.187	-0.027	-4.07
H+	1.678e-09	1.585e-09	-8.775	-8.800	-0.025	0.00
H2O	5.551e+01	9.999e-01	1.744	-0.000	0.000	18.07
Al	5.791e-07					
Al(OH)4-	5.786e-07	5.442e-07	-6.238	-6.264	-0.027	(0)
Al(OH)3	4.559e-10	4.562e-10	-9.341	-9.341	0.000	(0)
Al(OH)2+	5.122e-12	4.822e-12	-11.291	-11.317	-0.026	(0)
AlOH+2	1.216e-15	9.550e-16	-14.915	-15.020	-0.105	-27.69
Al+3	2.503e-19	1.500e-19	-18.602	-18.824	-0.222	-42.14
B	2.461e-06					
H3BO3	1.773e-06	1.774e-06	-5.751	-5.751	0.000	39.25
H2BO3-	6.883e-07	6.471e-07	-6.162	-6.189	-0.027	(0)
Ba	3.132e-06					
Ba+2	2.865e-06	2.240e-06	-5.543	-5.650	-0.107	-12.65
BaCO3	1.600e-07	1.601e-07	-6.796	-6.796	0.000	-10.70
BaHCO3+	1.065e-07	1.002e-07	-6.973	-6.999	-0.027	(0)

BaOH+	5.089e-11	4.789e-11	-10.293	-10.320	-0.026	(0)
BaNO3+	4.225e-13	3.972e-13	-12.374	-12.401	-0.027	(0)
Br	1.875e-33					
Br-	1.875e-33	1.761e-33	-32.727	-32.754	-0.027	24.59
CdBr+	1.391e-39	1.308e-39	-38.857	-38.884	-0.027	(0)
ZnBr+	0.000e+00	0.000e+00	-41.965	-41.992	-0.027	(0)
PbBr+	0.000e+00	0.000e+00	-42.592	-42.619	-0.027	(0)
CdBr2	0.000e+00	0.000e+00	-70.908	-70.907	0.000	(0)
ZnBr2	0.000e+00	0.000e+00	-75.147	-75.147	0.000	(0)
PbBr2	0.000e+00	0.000e+00	-75.705	-75.705	0.000	(0)
C(4)	5.143e-03					
HCO3-	4.917e-03	4.629e-03	-2.308	-2.335	-0.026	24.73
CO3-2	1.752e-04	1.376e-04	-3.756	-3.861	-0.105	-5.16
CaCO3	1.805e-05	1.807e-05	-4.743	-4.743	0.000	-14.60
CO2	1.644e-05	1.645e-05	-4.784	-4.784	0.000	34.44
CaHCO3+	4.893e-06	4.609e-06	-5.310	-5.336	-0.026	9.70
MnCO3	4.717e-06	4.721e-06	-5.326	-5.326	0.000	(0)
MgCO3	2.917e-06	2.919e-06	-5.535	-5.535	0.000	-17.09
MgHCO3+	1.277e-06	1.201e-06	-5.894	-5.921	-0.027	5.50
FeCO3	9.849e-07	9.856e-07	-6.007	-6.006	0.000	(0)
NaCO3-	3.596e-07	3.381e-07	-6.444	-6.471	-0.027	-0.97
NaHCO3	3.385e-07	3.388e-07	-6.470	-6.470	0.000	1.80
Zn(CO3)2-2	2.273e-07	1.776e-07	-6.643	-6.750	-0.107	(0)
MnHCO3+	1.893e-07	1.781e-07	-6.723	-6.749	-0.026	(0)
BaCO3	1.600e-07	1.601e-07	-6.796	-6.796	0.000	-10.70
FeHCO3+	1.470e-07	1.382e-07	-6.833	-6.860	-0.027	(0)
BaHCO3+	1.065e-07	1.002e-07	-6.973	-6.999	-0.027	(0)
ZnCO3	6.032e-08	6.036e-08	-7.220	-7.219	0.000	(0)
PbCO3	5.521e-09	5.525e-09	-8.258	-8.258	0.000	(0)
Pb(CO3)2-2	2.445e-09	1.910e-09	-8.612	-8.719	-0.107	(0)
ZnHCO3+	1.363e-09	1.281e-09	-8.866	-8.892	-0.027	(0)
CdHCO3+	7.826e-10	7.357e-10	-9.106	-9.133	-0.027	(0)
CdCO3	5.491e-10	5.495e-10	-9.260	-9.260	0.000	(0)
Cd(CO3)2-2	3.061e-10	2.392e-10	-9.514	-9.621	-0.107	(0)
CuCO3	1.537e-10	1.538e-10	-9.813	-9.813	0.000	(0)
Cu(CO3)2-2	3.411e-11	2.665e-11	-10.467	-10.574	-0.107	(0)
PbHCO3+	9.033e-12	8.493e-12	-11.044	-11.071	-0.027	(0)
(CO2)2	5.002e-12	5.005e-12	-11.301	-11.301	0.000	68.89
CuHCO3+	5.135e-13	4.827e-13	-12.289	-12.316	-0.027	(0)
Ca	1.223e-04					
Ca+2	9.903e-05	7.776e-05	-4.004	-4.109	-0.105	-18.06
CaCO3	1.805e-05	1.807e-05	-4.743	-4.743	0.000	-14.60
CaHCO3+	4.893e-06	4.609e-06	-5.310	-5.336	-0.026	9.70
CaPO4-	1.919e-07	1.807e-07	-6.717	-6.743	-0.026	(0)
CaHPO4	1.204e-07	1.205e-07	-6.919	-6.919	0.000	(0)
CaOH+	8.660e-09	8.142e-09	-8.062	-8.089	-0.027	(0)
CaH2PO4+	1.523e-10	1.433e-10	-9.817	-9.844	-0.026	(0)
Cd	8.365e-09					
Cd+2	6.433e-09	5.026e-09	-8.192	-8.299	-0.107	-18.66
CdHCO3+	7.826e-10	7.357e-10	-9.106	-9.133	-0.027	(0)
CdCO3	5.491e-10	5.495e-10	-9.260	-9.260	0.000	(0)
Cd(CO3)2-2	3.061e-10	2.392e-10	-9.514	-9.621	-0.107	(0)
CdOH+	2.856e-10	2.685e-10	-9.544	-9.571	-0.027	(0)
Cd(OH)2	8.930e-12	8.936e-12	-11.049	-11.049	0.000	(0)
CdNO3+	1.878e-14	1.766e-14	-13.726	-13.753	-0.027	17.54
Cd(OH)3-	6.728e-16	6.326e-16	-15.172	-15.199	-0.027	(0)
Cd2OH+3	1.148e-17	6.590e-18	-16.940	-17.181	-0.241	(0)
Cd(OH)4-2	4.553e-21	3.557e-21	-20.342	-20.449	-0.107	(0)
CdBr+	1.391e-39	1.308e-39	-38.857	-38.884	-0.027	(0)
CdBr2	0.000e+00	0.000e+00	-70.908	-70.907	0.000	(0)
Cu(1)	1.193e-08					
Cu+	1.193e-08	1.120e-08	-7.923	-7.951	-0.028	(0)
Cu(2)	1.919e-09					
Cu(OH)2	1.729e-09	1.730e-09	-8.762	-8.762	0.000	(0)
CuCO3	1.537e-10	1.538e-10	-9.813	-9.813	0.000	(0)
Cu(CO3)2-2	3.411e-11	2.665e-11	-10.467	-10.574	-0.107	(0)
CuOH+	1.396e-12	1.313e-12	-11.855	-11.882	-0.027	(0)
CuHCO3+	5.135e-13	4.827e-13	-12.289	-12.316	-0.027	(0)

Cu+2	2.642e-13	2.081e-13	-12.578	-12.682	-0.104	-26.53
Cu(OH)3-	6.997e-14	6.578e-14	-13.155	-13.182	-0.027	(0)
Cu(OH)4-2	1.060e-17	8.281e-18	-16.975	-17.082	-0.107	(0)
Cu2(OH)2+2	9.885e-19	7.723e-19	-18.005	-18.112	-0.107	(0)
Fe(2)	1.579e-06					
FeCO3	9.849e-07	9.856e-07	-6.007	-6.006	0.000	(0)
Fe+2	3.791e-07	2.985e-07	-6.421	-6.525	-0.104	-22.04
FeHCO3+	1.470e-07	1.382e-07	-6.833	-6.860	-0.027	(0)
FeOH+	6.443e-08	6.064e-08	-7.191	-7.217	-0.026	(0)
FeHPO4	3.341e-09	3.344e-09	-8.476	-8.476	0.000	(0)
Fe(OH)2	3.322e-10	3.325e-10	-9.479	-9.478	0.000	(0)
FeH2PO4+	1.140e-11	1.073e-11	-10.943	-10.969	-0.026	(0)
Fe(OH)3-	8.301e-12	7.811e-12	-11.081	-11.107	-0.026	(0)
Fe(3)	3.290e-08					
Fe(OH)3	2.018e-08	2.019e-08	-7.695	-7.695	0.000	(0)
Fe(OH)4-	1.246e-08	1.173e-08	-7.904	-7.931	-0.026	(0)
Fe(OH)2+	2.612e-10	2.459e-10	-9.583	-9.609	-0.026	(0)
FeOH+2	1.487e-15	1.166e-15	-14.828	-14.933	-0.106	(0)
Fe+3	4.710e-22	2.823e-22	-21.327	-21.549	-0.222	(0)
FeHPO4+	2.289e-22	2.154e-22	-21.640	-21.667	-0.026	(0)
FeH2PO4+2	6.936e-24	5.449e-24	-23.159	-23.264	-0.105	(0)
Fe2(OH)2+4	9.728e-29	3.625e-29	-28.012	-28.441	-0.429	(0)
Fe3(OH)4+5	8.517e-36	1.821e-36	-35.070	-35.740	-0.670	(0)
H(0)	3.713e-17					
H2	1.856e-17	1.858e-17	-16.731	-16.731	0.000	28.61
K	4.093e-05					
K+	4.093e-05	3.846e-05	-4.388	-4.415	-0.027	9.04
KHPO4-	2.241e-10	2.110e-10	-9.650	-9.676	-0.026	38.12
Mg	3.250e-05					
Mg+2	2.813e-05	2.214e-05	-4.551	-4.655	-0.104	-21.75
MgCO3	2.917e-06	2.919e-06	-5.535	-5.535	0.000	-17.09
MgHCO3+	1.277e-06	1.201e-06	-5.894	-5.921	-0.027	5.50
MgPO4-	7.372e-08	6.940e-08	-7.132	-7.159	-0.026	(0)
MgOH+	5.500e-08	5.183e-08	-7.260	-7.285	-0.026	(0)
MgHPO4	4.636e-08	4.639e-08	-7.334	-7.334	0.000	(0)
MgH2PO4+	5.522e-11	5.199e-11	-10.258	-10.284	-0.026	(0)
Mn(2)	5.462e-06					
MnCO3	4.717e-06	4.721e-06	-5.326	-5.326	0.000	(0)
Mn+2	5.483e-07	4.318e-07	-6.261	-6.365	-0.104	-20.48
MnHCO3+	1.893e-07	1.781e-07	-6.723	-6.749	-0.026	(0)
MnOH+	7.588e-09	7.140e-09	-8.120	-8.146	-0.026	(0)
Mn(OH)3-	1.826e-15	1.718e-15	-14.738	-14.765	-0.026	(0)
Mn(NO3)2	3.405e-18	3.408e-18	-17.468	-17.468	0.000	40.97
Mn(3)	2.253e-34					
Mn+3	2.253e-34	1.350e-34	-33.647	-33.870	-0.222	(0)
N(-3)	7.856e-07					
NH4+	5.849e-07	5.490e-07	-6.233	-6.260	-0.028	17.99
NH3	2.006e-07	2.008e-07	-6.698	-6.697	0.000	24.43
N(3)	2.857e-07					
NO2-	2.857e-07	2.683e-07	-6.544	-6.571	-0.027	25.00
N(5)	1.500e-06					
NO3-	1.500e-06	1.408e-06	-5.824	-5.851	-0.027	29.54
BaNO3+	4.225e-13	3.972e-13	-12.374	-12.401	-0.027	(0)
CdNO3+	1.878e-14	1.766e-14	-13.726	-13.753	-0.027	17.54
PbNO3+	5.118e-17	4.812e-17	-16.291	-16.318	-0.027	(0)
Mn(NO3)2	3.405e-18	3.408e-18	-17.468	-17.468	0.000	40.97
Na	1.392e-04					
Na+	1.385e-04	1.303e-04	-3.858	-3.885	-0.027	-1.43
NaCO3-	3.596e-07	3.381e-07	-6.444	-6.471	-0.027	-0.97
NaHCO3	3.385e-07	3.388e-07	-6.470	-6.470	0.000	1.80
NaHPO4-	7.593e-10	7.149e-10	-9.120	-9.146	-0.026	33.66
NaOH	8.469e-20	8.476e-20	-19.072	-19.072	0.000	(0)
O(0)	0.000e+00					
O2	0.000e+00	0.000e+00	-58.841	-58.841	0.000	30.42
P	4.101e-06					
HPO4-2	3.587e-06	2.813e-06	-5.445	-5.551	-0.106	6.80
CaPO4-	1.919e-07	1.807e-07	-6.717	-6.743	-0.026	(0)
CaHPO4	1.204e-07	1.205e-07	-6.919	-6.919	0.000	(0)

H2PO4-	7.618e-08	7.172e-08	-7.118	-7.144	-0.026	33.23
MgPO4-	7.372e-08	6.940e-08	-7.132	-7.159	-0.026	(0)
MgHPO4	4.636e-08	4.639e-08	-7.334	-7.334	0.000	(0)
FeHPO4	3.341e-09	3.344e-09	-8.476	-8.476	0.000	(0)
PO4-3	1.402e-09	8.041e-10	-8.853	-9.095	-0.242	-23.05
NaHPO4-	7.593e-10	7.149e-10	-9.120	-9.146	-0.026	33.66
KHPO4-	2.241e-10	2.110e-10	-9.650	-9.676	-0.026	38.12
CaH2PO4+	1.523e-10	1.433e-10	-9.817	-9.844	-0.026	(0)
MgH2PO4+	5.522e-11	5.199e-11	-10.258	-10.284	-0.026	(0)
FeH2PO4+	1.140e-11	1.073e-11	-10.943	-10.969	-0.026	(0)
H3PO4	1.677e-14	1.678e-14	-13.775	-13.775	0.000	47.42
FeHPO4+	2.289e-22	2.154e-22	-21.640	-21.667	-0.026	(0)
FeH2PO4+2	6.936e-24	5.449e-24	-23.159	-23.264	-0.105	(0)
Pb	8.014e-09					
PbCO3	5.521e-09	5.525e-09	-8.258	-8.258	0.000	(0)
Pb(CO3)2-2	2.445e-09	1.910e-09	-8.612	-8.719	-0.107	(0)
PbOH+	3.022e-11	2.841e-11	-10.520	-10.546	-0.027	(0)
PbHCO3+	9.033e-12	8.493e-12	-11.044	-11.071	-0.027	(0)
Pb(OH)2	6.969e-12	6.974e-12	-11.157	-11.157	0.000	(0)
Pb+2	2.956e-12	2.310e-12	-11.529	-11.636	-0.107	-15.46
Pb(OH)3-	5.373e-14	5.052e-14	-13.270	-13.297	-0.027	(0)
Pb(OH)4-2	9.345e-17	7.301e-17	-16.029	-16.137	-0.107	(0)
PbNO3+	5.118e-17	4.812e-17	-16.291	-16.318	-0.027	(0)
Pb2OH+3	2.560e-21	1.469e-21	-20.592	-20.833	-0.241	(0)
Pb3(OH)4+2	3.415e-24	2.668e-24	-23.467	-23.574	-0.107	(0)
PbBr+	0.000e+00	0.000e+00	-42.592	-42.619	-0.027	(0)
PbBr2	0.000e+00	0.000e+00	-75.705	-75.705	0.000	(0)
Si	3.246e-04					
H4SiO4	2.952e-04	2.954e-04	-3.530	-3.530	0.000	52.06
H3SiO4-	2.948e-05	2.771e-05	-4.531	-4.557	-0.027	28.00
H2SiO4-2	1.538e-09	1.208e-09	-8.813	-8.918	-0.105	(0)
Zn	3.045e-07					
Zn(CO3)2-2	2.273e-07	1.776e-07	-6.643	-6.750	-0.107	(0)
ZnCO3	6.032e-08	6.036e-08	-7.220	-7.219	0.000	(0)
Zn(OH)2	1.101e-08	1.101e-08	-7.958	-7.958	0.000	(0)
Zn+2	2.803e-09	2.198e-09	-8.552	-8.658	-0.106	-25.29
ZnOH+	1.647e-09	1.549e-09	-8.783	-8.810	-0.027	(0)
ZnHCO3+	1.363e-09	1.281e-09	-8.866	-8.892	-0.027	(0)
Zn(OH)3-	2.337e-11	2.198e-11	-10.631	-10.658	-0.027	(0)
Zn(OH)4-2	2.812e-15	2.197e-15	-14.551	-14.658	-0.107	(0)
ZnBr+	0.000e+00	0.000e+00	-41.965	-41.992	-0.027	(0)
ZnBr2	0.000e+00	0.000e+00	-75.147	-75.147	0.000	(0)

----------Distribution of alkalinity----------

Total alkalinity (eq/kgw) = 5.374e-03

Species	Alkalinity	Molality	Alk/Mol
HCO3-	4.917e-03	4.917e-03	1.00
CO3-2	3.504e-04	1.752e-04	2.00
CaCO3	3.611e-05	1.805e-05	2.00
H3SiO4-	2.948e-05	2.948e-05	1.00
MnCO3	9.434e-06	4.717e-06	2.00
OH-	6.922e-06	6.922e-06	1.00
MgCO3	5.834e-06	2.917e-06	2.00
CaHCO3+	4.893e-06	4.893e-06	1.00
HPO4-2	3.587e-06	3.587e-06	1.00
Al(OH)4-	2.315e-06	5.786e-07	4.00
FeCO3	1.970e-06	9.849e-07	2.00
MgHCO3+	1.277e-06	1.277e-06	1.00
Zn(CO3)2-2	9.094e-07	2.273e-07	4.00
NaCO3-	7.192e-07	3.596e-07	2.00
H2BO3-	6.883e-07	6.883e-07	1.00
CaPO4-	3.838e-07	1.919e-07	2.00
NaHCO3	3.385e-07	3.385e-07	1.00
BaCO3	3.199e-07	1.600e-07	2.00
NH3	2.006e-07	2.006e-07	1.00

MnHCO3+	1.893e-07	1.893e-07	1.00
MgPO4-	1.474e-07	7.372e-08	2.00
FeHCO3+	1.470e-07	1.470e-07	1.00
ZnCO3	1.206e-07	6.032e-08	2.00
CaHPO4	1.204e-07	1.204e-07	1.00
BaHCO3+	1.065e-07	1.065e-07	1.00
FeOH+	6.443e-08	6.443e-08	1.00
MgOH+	5.500e-08	5.500e-08	1.00
MgHPO4	4.636e-08	4.636e-08	1.00
Fe(OH)4-	2.492e-08	1.246e-08	2.00
Zn(OH)2	2.201e-08	1.101e-08	2.00
Fe(OH)3	2.018e-08	2.018e-08	1.00
PbCO3	1.104e-08	5.521e-09	2.00
Pb(CO3)2-2	9.778e-09	2.445e-09	4.00
CaOH+	8.660e-09	8.660e-09	1.00
MnOH+	7.588e-09	7.588e-09	1.00
Cu(OH)2	3.458e-09	1.729e-09	2.00
FeHPO4	3.341e-09	3.341e-09	1.00
H2SiO4-2	3.075e-09	1.538e-09	2.00
PO4-3	2.804e-09	1.402e-09	2.00
H+	-1.678e-09	1.678e-09	-1.00
ZnOH+	1.647e-09	1.647e-09	1.00
Al(OH)3	1.368e-09	4.559e-10	3.00
ZnHCO3+	1.363e-09	1.363e-09	1.00
Cd(CO3)2-2	1.224e-09	3.061e-10	4.00
CdCO3	1.098e-09	5.491e-10	2.00
CdHCO3+	7.826e-10	7.826e-10	1.00
NaHPO4-	7.593e-10	7.593e-10	1.00
Fe(OH)2	6.644e-10	3.322e-10	2.00
CuCO3	3.074e-10	1.537e-10	2.00
CdOH+	2.856e-10	2.856e-10	1.00
KHPO4-	2.241e-10	2.241e-10	1.00
Cu(CO3)2-2	1.364e-10	3.411e-11	4.00
Zn(OH)3-	7.012e-11	2.337e-11	3.00
BaOH+	5.089e-11	5.089e-11	1.00
PbOH+	3.022e-11	3.022e-11	1.00
Fe(OH)3-	2.490e-11	8.301e-12	3.00
Cd(OH)2	1.786e-11	8.930e-12	2.00
Pb(OH)2	1.394e-11	6.969e-12	2.00
Al(OH)2+	1.024e-11	5.122e-12	2.00
PbHCO3+	9.033e-12	9.033e-12	1.00
CuOH+	1.396e-12	1.396e-12	1.00
CuHCO3+	5.135e-13	5.135e-13	1.00
Cu(OH)3-	2.099e-13	6.997e-14	3.00
Pb(OH)3-	1.612e-13	5.373e-14	3.00
H3PO4	-1.677e-14	1.677e-14	-1.00
Zn(OH)4-2	1.125e-14	2.812e-15	4.00
Mn(OH)3-	5.478e-15	1.826e-15	3.00
Cd(OH)3-	2.019e-15	6.728e-16	3.00
FeOH+2	-1.487e-15	1.487e-15	-1.00
AlOH+2	1.216e-15	1.216e-15	1.00
Pb(OH)4-2	3.738e-16	9.345e-17	4.00
Cu(OH)4-2	4.239e-17	1.060e-17	4.00
Cd2OH+3	1.148e-17	1.148e-17	1.00
Cu2(OH)2+2	1.977e-18	9.885e-19	2.00
NaOH	8.469e-20	8.469e-20	1.00
Cd(OH)4-2	1.821e-20	4.553e-21	4.00
Pb2OH+3	2.560e-21	2.560e-21	1.00
Fe+3	-9.420e-22	4.710e-22	-2.00
FeHPO4+	-2.289e-22	2.289e-22	-1.00
FeH2PO4+2	-1.387e-23	6.936e-24	-2.00
Pb3(OH)4+2	1.366e-23	3.415e-24	4.00
Fe2(OH)2+4	-1.946e-28	9.728e-29	-2.00
Fe3(OH)4+5	-1.703e-35	8.517e-36	-2.00

-------------------------------Saturation indices--------------------------------

Phase	SI**	log IAP	log K(298 K, 1 atm)

Al(OH)3(a)	-3.21	7.58	10.78	Al(OH)3
Albite	-2.75	-20.74	-17.99	NaAlSi3O8
Anorthite	-3.99	-23.70	-19.71	CaAl2Si2O8
Aragonite	0.37	-7.97	-8.34	CaCO3
Ca-Montmorillonite	-0.83	-45.83	-44.99	Ca0.165Al2.33Si3.67O10(OH)2
Calcite	0.51	-7.97	-8.48	CaCO3
Cd(OH)2	-4.35	9.30	13.65	Cd(OH)2
CdSiO3	-3.28	5.77	9.05	CdSiO3
Cerussite	-2.37	-15.50	-13.13	PbCO3
Chalcedony	0.02	-3.53	-3.55	SiO2
Chlorite(14A)	1.00	69.29	68.29	Mg5Al2Si3O10(OH)8
Chrysotile	-0.39	31.78	32.17	Mg3Si2O5(OH)4
CO2(g)	-3.31	-4.78	-1.47	CO2
Dolomite	0.61	-16.49	-17.10	CaMg(CO3)2
Fe(OH)3(a)	-0.04	4.85	4.89	Fe(OH)3
Gibbsite	-0.52	7.58	8.10	Al(OH)3
Goethite	5.86	4.85	-1.01	FeOOH
H2(g)	-13.63	-16.73	-3.10	H2
H2O(g)	-1.50	-0.00	1.50	H2O
Hausmannite	-13.69	47.29	60.97	Mn3O4
Hematite	13.73	9.70	-4.03	Fe2O3
Hydroxyapatite	1.44	-2.00	-3.44	Ca5(PO4)3OH
Illite	-0.90	-41.13	-40.23	K0.6Mg0.25Al2.3Si3.5O10(OH)2
K-feldspar	-0.71	-21.27	-20.55	KAlSi3O8
K-mica	3.86	16.52	12.67	KAl3Si3O10(OH)2
Kaolinite	0.68	8.09	7.41	Al2Si2O5(OH)4
Manganite	-7.31	18.03	25.34	MnOOH
NH3(g)	-8.49	-6.70	1.79	NH3
O2(g)	-55.95	-58.84	-2.89	O2
Otavite	-0.06	-12.16	-12.10	CdCO3
Pb(OH)2	-2.18	5.96	8.14	Pb(OH)2
Pyrochroite	-3.96	11.24	15.20	Mn(OH)2
Pyrolusite	-16.53	24.82	41.34	MnO2:H2O
Quartz	0.45	-3.53	-3.98	SiO2
Rhodochrosite	0.90	-10.23	-11.13	MnCO3
Sepiolite	-0.45	15.30	15.75	Mg2Si3O7.5OH:3H2O
Sepiolite(d)	-3.36	15.30	18.66	Mg2Si3O7.5OH:3H2O
Siderite	0.51	-10.39	-10.89	FeCO3
SiO2(a)	-0.82	-3.53	-2.71	SiO2
Smithsonite	-2.52	-12.52	-10.00	ZnCO3
Talc	3.35	24.72	21.37	Mg3Si4O10(OH)2
Vivianite	-1.76	-37.76	-36.00	Fe3(PO4)2:8H2O
Willemite	-0.96	14.35	15.31	Zn2SiO4
Witherite	-0.95	-9.51	-8.56	BaCO3
Zn(OH)2(e)	-2.56	8.94	11.50	Zn(OH)2

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
For ideal gases, phi = 1.

Initial solution 36.

-----------------------------Solution composition--------------------------------

Elements	Molality	Moles
Al	1.692e-06	1.692e-06
Alkalinity	3.932e-03	3.932e-03
B	1.305e-06	1.305e-06
Ba	1.384e-06	1.384e-06
Br	5.992e-33	5.992e-33
Ca	1.023e-04	1.023e-04
Cd	7.832e-09	7.832e-09
Cl	2.201e-04	2.201e-04
Cu	3.322e-08	3.322e-08
F	9.583e-05	9.583e-05
Fe	3.582e-07	3.582e-07
K	2.814e-05	2.814e-05

Mg	3.621e-05	3.621e-05
Mn	1.074e-05	1.074e-05
N(-3)	4.999e-07	4.999e-07
N(3)	4.285e-07	4.285e-07
N(5)	4.356e-06	4.356e-06
Na	3.925e-03	3.925e-03
P	3.068e-06	3.068e-06
Pb	8.063e-09	8.063e-09
S(6)	5.415e-05	5.415e-05
Si	3.147e-04	3.147e-04
Zn	1.836e-07	1.836e-07

----------Description of solution----------

pH	= 8.600
pe	= -0.422
Specific Conductance (µS/cm, 25°C)	= 400
Density (g/cm³)	= 0.99721
Volume (L)	= 1.00317
Activity of water	= 1.000
Ionic strength (mol/kgw)	= 4.517e-03
Mass of water (kg)	= 1.000e+00
Total carbon (mol/kg)	= 3.810e-03
Total CO2 (mol/kg)	= 3.810e-03
Temperature (°C)	= 25.40
Electrical balance (eq)	= -1.033e-04
Percent error, 100*(Cat-|An|)/(Cat+|An|)	= -1.22
Iterations	= 8 (382 overall)
Total H	= 1.110174e+02
Total O	= 5.551914e+01

----------Redox couples----------

Redox couple	pe	Eh (volts)
N(-3)/N(3)	3.5975	0.2131
N(-3)/N(5)	4.2399	0.2512
N(3)/N(5)	6.1671	0.3653

----------Distribution of species----------

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma	mole V cm³/mol
OH-	4.469e-06	4.153e-06	-5.350	-5.382	-0.032	-4.06
H+	2.683e-09	2.512e-09	-8.571	-8.600	-0.029	0.00
H2O	5.551e+01	9.999e-01	1.744	-0.000	0.000	18.07
Al	1.692e-06					
Al(OH)4-	1.690e-06	1.573e-06	-5.772	-5.803	-0.031	(0)
Al(OH)3	2.083e-09	2.085e-09	-8.681	-8.681	0.000	(0)
Al(OH)2+	3.705e-11	3.452e-11	-10.431	-10.462	-0.031	(0)
AlF3	1.165e-13	1.167e-13	-12.934	-12.933	0.000	(0)
AlF2+	1.120e-13	1.044e-13	-12.951	-12.981	-0.031	(0)
AlOH+2	1.417e-14	1.069e-14	-13.849	-13.971	-0.123	-27.66
AlF4-	4.428e-15	4.122e-15	-14.354	-14.385	-0.031	(0)
AlF+2	3.106e-15	2.342e-15	-14.508	-14.630	-0.123	(0)
Al+3	4.765e-18	2.634e-18	-17.322	-17.579	-0.258	-42.08
AlSO4+	3.559e-19	3.313e-19	-18.449	-18.480	-0.031	(0)
Al(SO4)2-	4.462e-22	4.153e-22	-21.350	-21.382	-0.031	(0)
AlHSO4+2	9.892e-29	7.404e-29	-28.005	-28.131	-0.126	(0)
B	1.305e-06					
H3BO3	1.045e-06	1.046e-06	-5.981	-5.980	0.000	39.26
H2BO3-	2.596e-07	2.414e-07	-6.586	-6.617	-0.031	(0)
BF(OH)3-	3.990e-11	3.711e-11	-10.399	-10.430	-0.031	(0)
BF2(OH)2-	9.526e-16	8.861e-16	-15.021	-15.053	-0.031	(0)
BF3OH-	2.311e-22	2.150e-22	-21.636	-21.668	-0.031	(0)
BF4-	2.098e-28	1.951e-28	-27.678	-27.710	-0.031	(0)
Ba	1.384e-06					

Ba+2	1.297e-06	9.716e-07	-5.887	-6.013	-0.125	-12.61
BaHCO3+	3.468e-08	3.226e-08	-7.460	-7.491	-0.031	(0)
BaCO3	3.254e-08	3.258e-08	-7.488	-7.487	0.000	-10.69
BaSO4	1.925e-08	1.927e-08	-7.716	-7.715	0.000	(0)
BaCl+	6.629e-10	6.166e-10	-9.179	-9.210	-0.031	(0)
BaOH+	1.407e-11	1.310e-11	-10.852	-10.883	-0.031	(0)
BaNO3+	5.320e-13	4.948e-13	-12.274	-12.306	-0.031	(0)
Br	5.992e-33					
Br-	5.992e-33	5.564e-33	-32.222	-32.255	-0.032	24.61
CdBr+	4.348e-39	4.044e-39	-38.362	-38.393	-0.031	(0)
ZnBr+	0.000e+00	0.000e+00	-41.149	-41.181	-0.031	(0)
PbBr+	0.000e+00	0.000e+00	-41.682	-41.713	-0.031	(0)
CdBr2	0.000e+00	0.000e+00	-69.917	-69.917	0.000	(0)
ZnBr2	0.000e+00	0.000e+00	-73.836	-73.835	0.000	(0)
PbBr2	0.000e+00	0.000e+00	-74.301	-74.300	0.000	(0)
C(4)	3.810e-03					
HCO3-	3.671e-03	3.421e-03	-2.435	-2.466	-0.031	24.75
CO3-2	8.538e-05	6.438e-05	-4.069	-4.191	-0.123	-5.11
CO2	1.921e-05	1.923e-05	-4.717	-4.716	0.000	34.45
MnCO3	8.097e-06	8.106e-06	-5.092	-5.091	0.000	(0)
CaCO3	7.469e-06	7.477e-06	-5.127	-5.126	0.000	-14.60
NaHCO3	6.975e-06	6.982e-06	-5.156	-5.156	0.000	1.80
NaCO3-	4.784e-06	4.450e-06	-5.320	-5.352	-0.031	-0.94
CaHCO3+	3.229e-06	3.011e-06	-5.491	-5.521	-0.030	9.72
MgCO3	1.544e-06	1.546e-06	-5.811	-5.811	0.000	-17.09
MgHCO3+	1.078e-06	1.003e-06	-5.967	-5.999	-0.032	5.52
MnHCO3+	5.189e-07	4.832e-07	-6.285	-6.316	-0.031	(0)
FeCO3	1.271e-07	1.272e-07	-6.896	-6.895	0.000	(0)
Zn(CO3)2-2	1.065e-07	7.970e-08	-6.973	-7.099	-0.126	(0)
ZnCO3	5.784e-08	5.790e-08	-7.238	-7.237	0.000	(0)
BaHCO3+	3.468e-08	3.226e-08	-7.460	-7.491	-0.031	(0)
BaCO3	3.254e-08	3.258e-08	-7.488	-7.487	0.000	-10.69
FeHCO3+	3.029e-08	2.818e-08	-7.519	-7.550	-0.031	(0)
PbCO3	6.562e-09	6.569e-09	-8.183	-8.182	0.000	(0)
CuCO3	2.199e-09	2.202e-09	-8.658	-8.657	0.000	(0)
ZnHCO3+	2.087e-09	1.941e-09	-8.680	-8.712	-0.031	(0)
Pb(CO3)2-2	1.419e-09	1.062e-09	-8.848	-8.974	-0.126	(0)
CdHCO3+	5.725e-10	5.325e-10	-9.242	-9.274	-0.031	(0)
CdCO3	2.515e-10	2.517e-10	-9.600	-9.599	0.000	(0)
Cu(CO3)2-2	2.384e-10	1.784e-10	-9.623	-9.749	-0.126	(0)
Cd(CO3)2-2	6.847e-11	5.125e-11	-10.165	-10.290	-0.126	(0)
PbHCO3+	1.715e-11	1.595e-11	-10.766	-10.797	-0.031	(0)
CuHCO3+	1.174e-11	1.092e-11	-10.930	-10.962	-0.031	(0)
(CO2)2	6.869e-12	6.876e-12	-11.163	-11.163	0.000	68.90
Ca	1.023e-04					
Ca+2	9.099e-05	6.857e-05	-4.041	-4.164	-0.123	-18.02
CaCO3	7.469e-06	7.477e-06	-5.127	-5.126	0.000	-14.60
CaHCO3+	3.229e-06	3.011e-06	-5.491	-5.521	-0.030	9.72
CaSO4	4.835e-07	4.840e-07	-6.316	-6.315	0.000	7.52
CaPO4-	7.917e-08	7.378e-08	-7.101	-7.132	-0.031	(0)
CaHPO4	7.766e-08	7.774e-08	-7.110	-7.109	0.000	(0)
CaOH+	4.870e-09	4.530e-09	-8.312	-8.344	-0.031	(0)
CaH2PO4+	1.572e-10	1.465e-10	-9.804	-9.834	-0.031	(0)
CaHSO4+	8.641e-15	8.037e-15	-14.063	-14.095	-0.031	(0)
Cd	7.832e-09					
Cd+2	6.576e-09	4.922e-09	-8.182	-8.308	-0.126	-18.62
CdHCO3+	5.725e-10	5.325e-10	-9.242	-9.274	-0.031	(0)
CdCO3	2.515e-10	2.517e-10	-9.600	-9.599	0.000	(0)
CdOH+	1.805e-10	1.679e-10	-9.744	-9.775	-0.031	(0)
CdCl+	1.015e-10	9.439e-11	-9.994	-10.025	-0.031	5.99
Cd(CO3)2-2	6.847e-11	5.125e-11	-10.165	-10.290	-0.126	(0)
CdSO4	5.625e-11	5.631e-11	-10.250	-10.249	0.000	77.85
CdOHCl	1.564e-11	1.565e-11	-10.806	-10.805	0.000	(0)
CdF+	5.912e-12	5.499e-12	-11.228	-11.260	-0.031	(0)
Cd(OH)2	3.480e-12	3.484e-12	-11.458	-11.458	0.000	(0)
CdCl2	7.894e-14	7.902e-14	-13.103	-13.102	0.000	23.14
CdNO3+	5.315e-14	4.943e-14	-13.275	-13.306	-0.031	17.54
Cd(SO4)2-2	3.256e-14	2.437e-14	-13.487	-13.613	-0.126	-105.29

CdF2	1.224e-15	1.226e-15	-14.912	-14.912	0.000	(0)
Cd(OH)3-	1.673e-16	1.556e-16	-15.777	-15.808	-0.031	(0)
CdCl3-	1.081e-17	1.006e-17	-16.966	-16.997	-0.031	69.07
Cd2OH+3	7.727e-18	4.027e-18	-17.112	-17.395	-0.283	(0)
Cd(OH)4-2	7.374e-22	5.520e-22	-21.132	-21.258	-0.126	(0)
CdBr+	4.348e-39	4.044e-39	-38.362	-38.393	-0.031	(0)
CdBr2	0.000e+00	0.000e+00	-69.917	-69.917	0.000	(0)
Cl	2.201e-04					
Cl-	2.157e-04	2.005e-04	-3.666	-3.698	-0.032	18.12
NaCl	4.373e-06	4.378e-06	-5.359	-5.359	0.000	(0)
MnCl+	1.390e-09	1.295e-09	-8.857	-8.888	-0.031	-2.97
BaCl+	6.629e-10	6.166e-10	-9.179	-9.210	-0.031	(0)
CuCl2-	1.211e-10	1.126e-10	-9.917	-9.948	-0.032	(0)
CdCl+	1.015e-10	9.439e-11	-9.994	-10.025	-0.031	5.99
FeCl+	2.451e-11	2.280e-11	-10.611	-10.642	-0.031	(0)
CdOHCl	1.564e-11	1.565e-11	-10.806	-10.805	0.000	(0)
ZnOHCl	1.190e-11	1.191e-11	-10.924	-10.924	0.000	(0)
ZnCl+	2.662e-12	2.476e-12	-11.575	-11.606	-0.032	-13.50
MnCl2	1.132e-13	1.133e-13	-12.946	-12.946	0.000	85.40
CdCl2	7.894e-14	7.902e-14	-13.103	-13.102	0.000	23.14
PbCl+	5.090e-14	4.734e-14	-13.293	-13.325	-0.031	7.99
CuCl3-2	4.764e-14	3.584e-14	-13.322	-13.446	-0.124	(0)
CuCl+	3.768e-15	3.505e-15	-14.424	-14.455	-0.032	0.56
ZnCl2	5.202e-16	5.208e-16	-15.284	-15.283	0.000	101.25
PbCl2	1.492e-17	1.493e-17	-16.826	-16.826	0.000	35.00
CdCl3-	1.081e-17	1.006e-17	-16.966	-16.997	-0.031	69.07
MnCl3-	6.722e-18	6.260e-18	-17.173	-17.203	-0.031	43.37
CuCl2	3.787e-19	3.791e-19	-18.422	-18.421	0.000	31.48
ZnCl3-	1.263e-19	1.175e-19	-18.899	-18.930	-0.032	17.02
PbCl3-	2.564e-21	2.385e-21	-20.591	-20.623	-0.031	66.03
FeCl+2	2.480e-23	1.866e-23	-22.605	-22.729	-0.124	(0)
ZnCl4-2	1.574e-23	1.184e-23	-22.803	-22.927	-0.124	145.36
PbCl4-2	3.067e-25	2.296e-25	-24.513	-24.639	-0.126	101.54
CuCl3-	2.921e-25	2.716e-25	-24.535	-24.566	-0.032	(0)
FeCl2+	1.772e-26	1.651e-26	-25.751	-25.782	-0.031	(0)
CuCl4-2	3.662e-31	2.755e-31	-30.436	-30.560	-0.124	(0)
FeCl3	3.307e-31	3.310e-31	-30.481	-30.480	0.000	(0)
Cu(1)	9.673e-09					
Cu+	9.552e-09	8.863e-09	-8.020	-8.052	-0.033	(0)
CuCl2-	1.211e-10	1.126e-10	-9.917	-9.948	-0.032	(0)
CuCl3-2	4.764e-14	3.584e-14	-13.322	-13.446	-0.124	(0)
Cu(2)	2.354e-08					
Cu(OH)2	2.106e-08	2.108e-08	-7.677	-7.676	0.000	(0)
CuCO3	2.199e-09	2.202e-09	-8.658	-8.657	0.000	(0)
Cu(CO3)2-2	2.384e-10	1.784e-10	-9.623	-9.749	-0.126	(0)
CuOH+	2.725e-11	2.535e-11	-10.565	-10.596	-0.032	(0)
CuHCO3+	1.174e-11	1.092e-11	-10.930	-10.962	-0.031	(0)
Cu+2	8.416e-12	6.367e-12	-11.075	-11.196	-0.121	-26.50
Cu(OH)3-	5.435e-13	5.056e-13	-12.265	-12.296	-0.031	(0)
CuSO4	5.153e-14	5.159e-14	-13.288	-13.287	0.000	13.14
CuF+	1.109e-14	1.032e-14	-13.955	-13.986	-0.031	(0)
CuCl+	3.768e-15	3.505e-15	-14.424	-14.455	-0.032	0.56
Cu2(OH)2+2	3.907e-16	2.925e-16	-15.408	-15.534	-0.126	(0)
Cu(OH)4-2	5.364e-17	4.015e-17	-16.270	-16.396	-0.126	(0)
CuCl2	3.787e-19	3.791e-19	-18.422	-18.421	0.000	31.48
CuCl3-	2.921e-25	2.716e-25	-24.535	-24.566	-0.032	(0)
CuCl4-2	3.662e-31	2.755e-31	-30.436	-30.560	-0.124	(0)
F	9.583e-05					
F-	9.548e-05	8.873e-05	-4.020	-4.052	-0.032	-1.28
NaF	1.855e-07	1.857e-07	-6.732	-6.731	0.000	7.28
MgF+	1.587e-07	1.477e-07	-6.800	-6.831	-0.031	-10.55
MnF+	1.045e-09	9.730e-10	-8.981	-9.012	-0.031	(0)
HF	3.363e-10	3.367e-10	-9.473	-9.473	0.000	12.52
FeF+	7.858e-11	7.309e-11	-10.105	-10.136	-0.031	(0)
BF(OH)3-	3.990e-11	3.711e-11	-10.399	-10.430	-0.031	(0)
ZnF+	6.104e-12	5.678e-12	-11.214	-11.246	-0.031	(0)
CdF+	5.912e-12	5.499e-12	-11.228	-11.260	-0.031	(0)
HF2-	1.236e-13	1.150e-13	-12.908	-12.939	-0.031	22.11

AlF3	1.165e-13	1.167e-13	-12.934	-12.933	0.000	(0)
AlF2+	1.120e-13	1.044e-13	-12.951	-12.981	-0.031	(0)
CuF+	1.109e-14	1.032e-14	-13.955	-13.986	-0.031	(0)
PbF+	9.961e-15	9.265e-15	-14.002	-14.033	-0.031	(0)
AlF4-	4.428e-15	4.122e-15	-14.354	-14.385	-0.031	(0)
AlF+2	3.106e-15	2.342e-15	-14.508	-14.630	-0.123	(0)
CdF2	1.224e-15	1.226e-15	-14.912	-14.912	0.000	(0)
BF2(OH)2-	9.526e-16	8.861e-16	-15.021	-15.053	-0.031	(0)
PbF2	1.677e-17	1.679e-17	-16.776	-16.775	0.000	(0)
FeF2+	1.641e-18	1.528e-18	-17.785	-17.816	-0.031	(0)
FeF+2	5.722e-19	4.305e-19	-18.242	-18.366	-0.124	(0)
FeF3	2.150e-19	2.152e-19	-18.668	-18.667	0.000	(0)
PbF3-	1.160e-20	1.079e-20	-19.936	-19.967	-0.031	(0)
BF3OH-	2.311e-22	2.150e-22	-21.636	-21.668	-0.031	(0)
PbF4-2	6.122e-25	4.582e-25	-24.213	-24.339	-0.126	(0)
BF4-	2.098e-28	1.951e-28	-27.678	-27.710	-0.031	(0)
SiF6-2	1.116e-32	8.397e-33	-31.952	-32.076	-0.124	42.73
Fe(2)	2.791e-07					
FeCO3	1.271e-07	1.272e-07	-6.896	-6.895	0.000	(0)
Fe+2	1.089e-07	8.237e-08	-6.963	-7.084	-0.121	-22.00
FeHCO3+	3.029e-08	2.818e-08	-7.519	-7.550	-0.031	(0)
FeOH+	1.147e-08	1.068e-08	-7.940	-7.971	-0.031	(0)
FeHPO4	6.723e-10	6.730e-10	-9.172	-9.172	0.000	(0)
FeSO4	5.833e-10	5.839e-10	-9.234	-9.234	0.000	18.55
FeF+	7.858e-11	7.309e-11	-10.105	-10.136	-0.031	(0)
Fe(OH)2	3.743e-11	3.747e-11	-10.427	-10.426	0.000	(0)
FeCl+	2.451e-11	2.280e-11	-10.611	-10.642	-0.031	(0)
FeH2PO4+	3.670e-12	3.420e-12	-11.435	-11.466	-0.031	(0)
Fe(OH)3-	5.973e-13	5.563e-13	-12.224	-12.255	-0.031	(0)
FeHSO4+	1.038e-17	9.654e-18	-16.984	-17.015	-0.031	(0)
Fe(3)	7.913e-08					
Fe(OH)3	5.584e-08	5.590e-08	-7.253	-7.253	0.000	(0)
Fe(OH)4-	2.213e-08	2.062e-08	-7.655	-7.686	-0.031	(0)
Fe(OH)2+	1.150e-09	1.071e-09	-8.939	-8.970	-0.031	(0)
FeOH+2	1.064e-14	8.006e-15	-13.973	-14.097	-0.124	(0)
FeF2+	1.641e-18	1.528e-18	-17.785	-17.816	-0.031	(0)
FeF+2	5.722e-19	4.305e-19	-18.242	-18.366	-0.124	(0)
FeF3	2.150e-19	2.152e-19	-18.668	-18.667	0.000	(0)
Fe+3	5.505e-21	3.043e-21	-20.259	-20.517	-0.258	(0)
FeHPO4+	1.828e-21	1.703e-21	-20.738	-20.769	-0.031	(0)
FeSO4+	1.430e-21	1.332e-21	-20.845	-20.876	-0.031	(0)
FeH2PO4+2	8.998e-23	6.785e-23	-22.046	-22.168	-0.123	(0)
FeCl+2	2.480e-23	1.866e-23	-22.605	-22.729	-0.124	(0)
Fe(SO4)2-	1.242e-24	1.155e-24	-23.906	-23.937	-0.031	(0)
FeCl2+	1.772e-26	1.651e-26	-25.751	-25.782	-0.031	(0)
Fe2(OH)2+4	5.406e-27	1.697e-27	-26.267	-26.770	-0.503	(0)
FeHSO4+2	1.197e-29	8.958e-30	-28.922	-29.048	-0.126	(0)
FeCl3	3.307e-31	3.310e-31	-30.481	-30.480	0.000	(0)
Fe3(OH)4+5	2.238e-33	3.661e-34	-32.650	-33.436	-0.786	(0)
H(0)	6.207e-20					
H2	3.103e-20	3.107e-20	-19.508	-19.508	0.000	28.61
K	2.814e-05					
K+	2.813e-05	2.615e-05	-4.551	-4.583	-0.032	9.05
KSO4-	7.856e-09	7.321e-09	-8.105	-8.135	-0.031	34.15
KHPO4-	1.123e-10	1.046e-10	-9.950	-9.980	-0.031	38.12
Mg	3.621e-05					
Mg+2	3.308e-05	2.501e-05	-4.480	-4.602	-0.121	-21.72
MgCO3	1.544e-06	1.546e-06	-5.811	-5.811	0.000	-17.09
MgHCO3+	1.078e-06	1.003e-06	-5.967	-5.999	-0.032	5.52
MgSO4	2.341e-07	2.344e-07	-6.631	-6.630	0.000	5.85
MgF+	1.587e-07	1.477e-07	-6.800	-6.831	-0.031	-10.55
MgOH+	4.015e-08	3.747e-08	-7.396	-7.426	-0.030	(0)
MgPO4-	3.895e-08	3.629e-08	-7.410	-7.440	-0.031	(0)
MgHPO4	3.829e-08	3.833e-08	-7.417	-7.416	0.000	(0)
MgH2PO4+	7.300e-11	6.803e-11	-10.137	-10.167	-0.031	(0)
Mn(2)	1.074e-05					
MnCO3	8.097e-06	8.106e-06	-5.092	-5.091	0.000	(0)
Mn+2	2.095e-06	1.585e-06	-5.679	-5.800	-0.121	-20.30

MnHCO3+	5.189e-07	4.832e-07	-6.285	-6.316	-0.031	(0)
MnOH+	1.799e-08	1.675e-08	-7.745	-7.776	-0.031	(0)
MnSO4	1.123e-08	1.124e-08	-7.950	-7.949	0.000	22.37
MnCl+	1.390e-09	1.295e-09	-8.857	-8.888	-0.031	-2.97
MnF+	1.045e-09	9.730e-10	-8.981	-9.012	-0.031	(0)
MnCl2	1.132e-13	1.133e-13	-12.946	-12.946	0.000	85.40
Mn(OH)3-	1.701e-15	1.584e-15	-14.769	-14.800	-0.031	(0)
Mn(NO3)2	1.031e-16	1.032e-16	-15.987	-15.986	0.000	40.93
MnCl3-	6.722e-18	6.260e-18	-17.173	-17.203	-0.031	43.37
Mn(3)	3.555e-32					
Mn+3	3.555e-32	1.965e-32	-31.449	-31.707	-0.258	(0)
N(-3)	4.999e-07					
NH4+	4.108e-07	3.812e-07	-6.386	-6.419	-0.033	18.01
NH3	8.887e-08	8.896e-08	-7.051	-7.051	0.000	24.43
NH4SO4-	2.089e-10	1.943e-10	-9.680	-9.711	-0.031	37.77
N(3)	4.285e-07					
NO2-	4.285e-07	3.979e-07	-6.368	-6.400	-0.032	25.02
N(5)	4.356e-06					
NO3-	4.356e-06	4.045e-06	-5.361	-5.393	-0.032	29.56
BaNO3+	5.320e-13	4.948e-13	-12.274	-12.306	-0.031	(0)
CdNO3+	5.315e-14	4.943e-14	-13.275	-13.306	-0.031	17.54
PbNO3+	3.777e-16	3.513e-16	-15.423	-15.454	-0.031	(0)
Mn(NO3)2	1.031e-16	1.032e-16	-15.987	-15.986	0.000	40.93
Na	3.925e-03					
Na+	3.908e-03	3.638e-03	-2.408	-2.439	-0.031	-1.41
NaHCO3	6.975e-06	6.982e-06	-5.156	-5.156	0.000	1.80
NaCO3-	4.784e-06	4.450e-06	-5.320	-5.352	-0.031	-0.94
NaCl	4.373e-06	4.378e-06	-5.359	-5.359	0.000	(0)
NaSO4-	7.761e-07	7.233e-07	-6.110	-6.141	-0.031	14.03
NaF	1.855e-07	1.857e-07	-6.732	-6.731	0.000	7.28
NaHPO4-	1.562e-08	1.456e-08	-7.806	-7.837	-0.031	33.76
NaOH	1.509e-18	1.511e-18	-17.821	-17.821	0.000	(0)
O(0)	0.000e+00					
O2	0.000e+00	0.000e+00	-53.236	-53.236	0.000	30.43
P	3.068e-06					
HPO4-2	2.728e-06	2.052e-06	-5.564	-5.688	-0.124	6.83
H2PO4-	8.890e-08	8.285e-08	-7.051	-7.082	-0.031	33.24
CaPO4-	7.917e-08	7.378e-08	-7.101	-7.132	-0.031	(0)
CaHPO4	7.766e-08	7.774e-08	-7.110	-7.109	0.000	(0)
MgPO4-	3.895e-08	3.629e-08	-7.410	-7.440	-0.031	(0)
MgHPO4	3.829e-08	3.833e-08	-7.417	-7.416	0.000	(0)
NaHPO4-	1.562e-08	1.456e-08	-7.806	-7.837	-0.031	33.76
PO4-3	7.135e-10	3.713e-10	-9.147	-9.430	-0.284	-22.98
FeHPO4	6.723e-10	6.730e-10	-9.172	-9.172	0.000	(0)
CaH2PO4+	1.572e-10	1.465e-10	-9.804	-9.834	-0.031	(0)
KHPO4-	1.123e-10	1.046e-10	-9.950	-9.980	-0.031	38.12
MgH2PO4+	7.300e-11	6.803e-11	-10.137	-10.167	-0.031	(0)
FeH2PO4+	3.670e-12	3.420e-12	-11.435	-11.466	-0.031	(0)
H3PO4	3.075e-14	3.079e-14	-13.512	-13.512	0.000	47.43
FeHPO4+	1.828e-21	1.703e-21	-20.738	-20.769	-0.031	(0)
FeH2PO4+2	8.998e-23	6.785e-23	-22.046	-22.168	-0.123	(0)
Pb	8.063e-09					
PbCO3	6.562e-09	6.569e-09	-8.183	-8.182	0.000	(0)
Pb(CO3)2-2	1.419e-09	1.062e-09	-8.848	-8.974	-0.126	(0)
PbOH+	4.899e-11	4.557e-11	-10.310	-10.341	-0.031	(0)
PbHCO3+	1.715e-11	1.595e-11	-10.766	-10.797	-0.031	(0)
Pb+2	7.844e-12	5.871e-12	-11.105	-11.231	-0.126	-15.43
Pb(OH)2	7.050e-12	7.057e-12	-11.152	-11.151	0.000	(0)
PbSO4	1.305e-13	1.307e-13	-12.884	-12.884	0.000	(0)
PbCl+	5.090e-14	4.734e-14	-13.293	-13.325	-0.031	7.99
Pb(OH)3-	3.467e-14	3.225e-14	-13.460	-13.491	-0.031	(0)
PbF+	9.961e-15	9.265e-15	-14.002	-14.033	-0.031	(0)
PbNO3+	3.777e-16	3.513e-16	-15.423	-15.454	-0.031	(0)
Pb(OH)4-2	3.929e-17	2.941e-17	-16.406	-16.532	-0.126	(0)
Pb(SO4)2-2	3.625e-17	2.713e-17	-16.441	-16.567	-0.126	(0)
PbF2	1.677e-17	1.679e-17	-16.776	-16.775	0.000	(0)
PbCl2	1.492e-17	1.493e-17	-16.826	-16.826	0.000	35.00
PbF3-	1.160e-20	1.079e-20	-19.936	-19.967	-0.031	(0)

Pb2OH+3	1.149e-20	5.990e-21	-19.940	-20.223	-0.283	(0)
PbCl3-	2.564e-21	2.385e-21	-20.591	-20.623	-0.031	66.03
Pb3(OH)4+2	9.502e-24	7.112e-24	-23.022	-23.148	-0.126	(0)
PbF4-2	6.122e-25	4.582e-25	-24.213	-24.339	-0.126	(0)
PbCl4-2	3.067e-25	2.296e-25	-24.513	-24.639	-0.126	101.54
PbBr+	0.000e+00	0.000e+00	-41.682	-41.713	-0.031	(0)
PbBr2	0.000e+00	0.000e+00	-74.301	-74.300	0.000	(0)
S(6)	5.415e-05					
SO4-2	5.262e-05	3.957e-05	-4.279	-4.403	-0.124	14.70
NaSO4-	7.761e-07	7.233e-07	-6.110	-6.141	-0.031	14.03
CaSO4	4.835e-07	4.840e-07	-6.316	-6.315	0.000	7.52
MgSO4	2.341e-07	2.344e-07	-6.631	-6.630	0.000	5.85
BaSO4	1.925e-08	1.927e-08	-7.716	-7.715	0.000	(0)
MnSO4	1.123e-08	1.124e-08	-7.950	-7.949	0.000	22.37
KSO4-	7.856e-09	7.321e-09	-8.105	-8.135	-0.031	34.15
FeSO4	5.833e-10	5.839e-10	-9.234	-9.234	0.000	18.55
NH4SO4-	2.089e-10	1.943e-10	-9.680	-9.711	-0.031	37.77
CdSO4	5.625e-11	5.631e-11	-10.250	-10.249	0.000	77.85
ZnSO4	4.190e-11	4.194e-11	-10.378	-10.377	0.000	21.65
HSO4-	1.048e-11	9.749e-12	-10.980	-11.011	-0.031	40.34
PbSO4	1.305e-13	1.307e-13	-12.884	-12.884	0.000	(0)
CuSO4	5.153e-14	5.159e-14	-13.288	-13.287	0.000	13.14
Cd(SO4)2-2	3.256e-14	2.437e-14	-13.487	-13.613	-0.126	-105.29
Zn(SO4)2-2	1.797e-14	1.345e-14	-13.746	-13.871	-0.126	-12.64
CaHSO4+	8.641e-15	8.037e-15	-14.063	-14.095	-0.031	(0)
Pb(SO4)2-2	3.625e-17	2.713e-17	-16.441	-16.567	-0.126	(0)
FeHSO4+	1.038e-17	9.654e-18	-16.984	-17.015	-0.031	(0)
AlSO4+	3.559e-19	3.313e-19	-18.449	-18.480	-0.031	(0)
FeSO4+	1.430e-21	1.332e-21	-20.845	-20.876	-0.031	(0)
Al(SO4)2-	4.462e-22	4.153e-22	-21.350	-21.382	-0.031	(0)
Fe(SO4)2-	1.242e-24	1.155e-24	-23.906	-23.937	-0.031	(0)
AlHSO4+2	9.892e-29	7.404e-29	-28.005	-28.131	-0.126	(0)
FeHSO4+2	1.197e-29	8.958e-30	-28.922	-29.048	-0.126	(0)
Si	3.147e-04					
H4SiO4	2.957e-04	2.960e-04	-3.529	-3.529	0.000	52.04
H3SiO4-	1.895e-05	1.762e-05	-4.722	-4.754	-0.032	28.02
H2SiO4-2	6.494e-10	4.897e-10	-9.187	-9.310	-0.123	(0)
SiF6-2	1.116e-32	8.397e-33	-31.952	-32.076	-0.124	42.73
Zn	1.836e-07					
Zn(CO3)2-2	1.065e-07	7.970e-08	-6.973	-7.099	-0.126	(0)
ZnCO3	5.784e-08	5.790e-08	-7.238	-7.237	0.000	(0)
Zn(OH)2	8.982e-09	8.991e-09	-8.047	-8.046	0.000	(0)
Zn+2	5.991e-09	4.507e-09	-8.223	-8.346	-0.124	-25.27
ZnOH+	2.180e-09	2.028e-09	-8.662	-8.693	-0.031	(0)
ZnHCO3+	2.087e-09	1.941e-09	-8.680	-8.712	-0.031	(0)
ZnSO4	4.190e-11	4.194e-11	-10.378	-10.377	0.000	21.65
Zn(OH)3-	1.217e-11	1.132e-11	-10.915	-10.946	-0.031	(0)
ZnOHCl	1.190e-11	1.191e-11	-10.924	-10.924	0.000	(0)
ZnF+	6.104e-12	5.678e-12	-11.214	-11.246	-0.031	(0)
ZnCl+	2.662e-12	2.476e-12	-11.575	-11.606	-0.032	-13.50
Zn(SO4)2-2	1.797e-14	1.345e-14	-13.746	-13.871	-0.126	-12.64
Zn(OH)4-2	9.538e-16	7.140e-16	-15.021	-15.146	-0.126	(0)
ZnCl2	5.202e-16	5.208e-16	-15.284	-15.283	0.000	101.25
ZnCl3-	1.263e-19	1.175e-19	-18.899	-18.930	-0.032	17.02
ZnCl4-2	1.574e-23	1.184e-23	-22.803	-22.927	-0.124	145.36
ZnBr+	0.000e+00	0.000e+00	-41.149	-41.181	-0.031	(0)
ZnBr2	0.000e+00	0.000e+00	-73.836	-73.835	0.000	(0)

----------Distribution of alkalinity----------

Total alkalinity (eq/kgw) = 3.932e-03

Species	Alkalinity	Molality	Alk/Mol
HCO3-	3.671e-03	3.671e-03	1.00
CO3-2	1.708e-04	8.538e-05	2.00
H3SiO4-	1.895e-05	1.895e-05	1.00
MnCO3	1.619e-05	8.097e-06	2.00

CaCO3	1.494e-05	7.469e-06	2.00
NaCO3-	9.568e-06	4.784e-06	2.00
NaHCO3	6.975e-06	6.975e-06	1.00
Al(OH)4-	6.760e-06	1.690e-06	4.00
OH-	4.469e-06	4.469e-06	1.00
CaHCO3+	3.229e-06	3.229e-06	1.00
MgCO3	3.088e-06	1.544e-06	2.00
HPO4-2	2.728e-06	2.728e-06	1.00
MgHCO3+	1.078e-06	1.078e-06	1.00
MnHCO3+	5.189e-07	5.189e-07	1.00
Zn(CO3)2-2	4.259e-07	1.065e-07	4.00
H2BO3-	2.596e-07	2.596e-07	1.00
FeCO3	2.542e-07	1.271e-07	2.00
CaPO4-	1.583e-07	7.917e-08	2.00
ZnCO3	1.157e-07	5.784e-08	2.00
NH3	8.887e-08	8.887e-08	1.00
MgPO4-	7.789e-08	3.895e-08	2.00
CaHPO4	7.766e-08	7.766e-08	1.00
BaCO3	6.508e-08	3.254e-08	2.00
Fe(OH)3	5.584e-08	5.584e-08	1.00
Fe(OH)4-	4.426e-08	2.213e-08	2.00
Cu(OH)2	4.211e-08	2.106e-08	2.00
MgOH+	4.015e-08	4.015e-08	1.00
MgHPO4	3.829e-08	3.829e-08	1.00
BaHCO3+	3.468e-08	3.468e-08	1.00
FeHCO3+	3.029e-08	3.029e-08	1.00
MnOH+	1.799e-08	1.799e-08	1.00
Zn(OH)2	1.796e-08	8.982e-09	2.00
NaHPO4-	1.562e-08	1.562e-08	1.00
PbCO3	1.312e-08	6.562e-09	2.00
FeOH+	1.147e-08	1.147e-08	1.00
Al(OH)3	6.248e-09	2.083e-09	3.00
Pb(CO3)2-2	5.677e-09	1.419e-09	4.00
CaOH+	4.870e-09	4.870e-09	1.00
CuCO3	4.398e-09	2.199e-09	2.00
H+	-2.683e-09	2.683e-09	-1.00
ZnOH+	2.180e-09	2.180e-09	1.00
ZnHCO3+	2.087e-09	2.087e-09	1.00
PO4-3	1.427e-09	7.135e-10	2.00
H2SiO4-2	1.299e-09	6.494e-10	2.00
Cu(CO3)2-2	9.535e-10	2.384e-10	4.00
FeHPO4	6.723e-10	6.723e-10	1.00
CdHCO3+	5.725e-10	5.725e-10	1.00
CdCO3	5.029e-10	2.515e-10	2.00
HF	-3.363e-10	3.363e-10	-1.00
Cd(CO3)2-2	2.739e-10	6.847e-11	4.00
CdOH+	1.805e-10	1.805e-10	1.00
KHPO4-	1.123e-10	1.123e-10	1.00
Fe(OH)2	7.486e-11	3.743e-11	2.00
Al(OH)2+	7.409e-11	3.705e-11	2.00
PbOH+	4.899e-11	4.899e-11	1.00
Zn(OH)3-	3.650e-11	1.217e-11	3.00
CuOH+	2.725e-11	2.725e-11	1.00
PbHCO3+	1.715e-11	1.715e-11	1.00
CdOHCl	1.564e-11	1.564e-11	1.00
Pb(OH)2	1.410e-11	7.050e-12	2.00
BaOH+	1.407e-11	1.407e-11	1.00
ZnOHCl	1.190e-11	1.190e-11	1.00
CuHCO3+	1.174e-11	1.174e-11	1.00
HSO4-	-1.048e-11	1.048e-11	-1.00
Cd(OH)2	6.960e-12	3.480e-12	2.00
Fe(OH)3-	1.792e-12	5.973e-13	3.00
Cu(OH)3-	1.631e-12	5.435e-13	3.00
HF2-	-1.236e-13	1.236e-13	-1.00
Pb(OH)3-	1.040e-13	3.467e-14	3.00
H3PO4	-3.075e-14	3.075e-14	-1.00
AlOH+2	1.417e-14	1.417e-14	1.00
FeOH+2	-1.064e-14	1.064e-14	-1.00

CaHSO4+	-8.641e-15	8.641e-15	-1.00
Mn(OH)3-	5.103e-15	1.701e-15	3.00
Zn(OH)4-2	3.815e-15	9.538e-16	4.00
BF2(OH)2-	-9.526e-16	9.526e-16	-1.00
Cu2(OH)2+2	7.815e-16	3.907e-16	2.00
Cd(OH)3-	5.018e-16	1.673e-16	3.00
Cu(OH)4-2	2.146e-16	5.364e-17	4.00
Pb(OH)4-2	1.572e-16	3.929e-17	4.00
FeHSO4+	-1.038e-17	1.038e-17	-1.00
Cd2OH+3	7.727e-18	7.727e-18	1.00
FeF2+	-3.282e-18	1.641e-18	-2.00
NaOH	1.509e-18	1.509e-18	1.00
FeF+2	-1.144e-18	5.722e-19	-2.00
FeF3	-4.299e-19	2.150e-19	-2.00
Pb2OH+3	1.149e-20	1.149e-20	1.00
Fe+3	-1.101e-20	5.505e-21	-2.00
Cd(OH)4-2	2.950e-21	7.374e-22	4.00
FeSO4+	-2.860e-21	1.430e-21	-2.00
FeHPO4+	-1.828e-21	1.828e-21	-1.00
BF3OH-	-4.623e-22	2.311e-22	-2.00
FeH2PO4+2	-1.800e-22	8.998e-23	-2.00
FeCl+2	-4.961e-23	2.480e-23	-2.00
Pb3(OH)4+2	3.801e-23	9.502e-24	4.00
Fe(SO4)2-	-2.483e-24	1.242e-24	-2.00
FeCl2+	-3.545e-26	1.772e-26	-2.00
Fe2(OH)2+4	-1.081e-26	5.406e-27	-2.00
BF4-	-6.294e-28	2.098e-28	-3.00
AlHSO4+2	-9.892e-29	9.892e-29	-1.00
FeHSO4+2	-3.590e-29	1.197e-29	-3.00
FeCl3	-6.613e-31	3.307e-31	-2.00
SiF6-2	-4.464e-32	1.116e-32	-4.00
Fe3(OH)4+5	-4.475e-33	2.238e-33	-2.00

------------------------------Saturation indices--------------------------------

Phase	SI**	log IAP	log K(298 K, 1 atm)	
Al(OH)3(a)	-2.55	8.22	10.77	Al(OH)3
Albite	-0.85	-18.83	-17.98	NaAlSi3O8
Alunite	-13.08	-14.53	-1.45	KAl3(SO4)2(OH)6
Anglesite	-7.85	-15.63	-7.79	PbSO4
Anhydrite	-4.28	-8.57	-4.28	CaSO4
Anorthite	-3.12	-22.83	-19.70	CaAl2Si2O8
Aragonite	-0.02	-8.36	-8.34	CaCO3
BaCl2	-15.63	-13.41	2.23	BaCl2
BaCl2:2H2O	-13.62	-13.41	0.21	BaCl2:2H2O
BaCl2:H2O	-14.23	-13.41	0.83	BaCl2:H2O
Barite	-0.58	-10.42	-9.84	BaSO4
Ca-Montmorillonite	0.61	-44.36	-44.97	Ca0.165Al2.33Si3.67O10(OH)2
Calcite	0.13	-8.36	-8.48	CaCO3
Cd(OH)2	-4.76	8.89	13.65	Cd(OH)2
CdSiO3	-3.68	5.36	9.04	CdSiO3
CdSO4	-12.60	-12.71	-0.11	CdSO4
Cerussite	-2.30	-15.42	-13.13	PbCO3
Chalcedony	0.02	-3.53	-3.55	SiO2
Chlorite(14A)	0.61	68.85	68.23	Mg5Al2Si3O10(OH)8
Chrysotile	-1.41	30.74	32.15	Mg3Si2O5(OH)4
CO2(g)	-3.24	-4.72	-1.47	CO2
Dolomite	-0.05	-17.15	-17.10	CaMg(CO3)2
Fe(OH)3(a)	0.39	5.28	4.89	Fe(OH)3
Fluorite	-1.67	-12.27	-10.60	CaF2
Gibbsite	0.13	8.22	8.09	Al(OH)3
Goethite	6.30	5.28	-1.01	FeOOH
Gypsum	-3.98	-8.57	-4.58	CaSO4:2H2O
H2(g)	-16.41	-19.51	-3.10	H2
H2O(g)	-1.49	-0.00	1.49	H2O
Halite	-7.71	-6.14	1.57	NaCl
Hausmannite	-10.38	50.56	60.93	Mn3O4

Hematite	14.60	10.57	-4.04	Fe2O3
Hydroxyapatite	-0.03	-3.48	-3.46	Ca5(PO4)3OH
Illite	0.30	-39.92	-40.21	K0.6Mg0.25Al2.3Si3.5O10(OH)2
Jarosite-K	-14.10	-23.34	-9.24	KFe3(SO4)2(OH)6
K-feldspar	-0.43	-20.97	-20.54	KAlSi3O8
K-mica	5.45	18.09	12.64	KAl3Si3O10(OH)2
Kaolinite	1.98	9.38	7.40	Al2Si2O5(OH)4
Manganite	-5.76	19.58	25.34	MnOOH
Melanterite	-9.28	-11.49	-2.20	FeSO4:7H2O
NH3(g)	-8.84	-7.05	1.79	NH3
O2(g)	-50.34	-53.24	-2.90	O2
Otavite	-0.40	-12.50	-12.10	CdCO3
Pb(OH)2	-2.17	5.97	8.14	Pb(OH)2
Pyrochroite	-3.80	11.40	15.20	Mn(OH)2
Pyrolusite	-13.56	27.76	41.32	MnO2:H2O
Quartz	0.45	-3.53	-3.97	SiO2
Rhodochrosite	1.14	-9.99	-11.13	MnCO3
Sepiolite	-1.14	14.61	15.75	Mg2Si3O7.5OH:3H2O
Sepiolite(d)	-4.05	14.61	18.66	Mg2Si3O7.5OH:3H2O
Siderite	-0.38	-11.28	-10.89	FeCO3
SiO2(a)	-0.82	-3.53	-2.71	SiO2
Smithsonite	-2.53	-12.54	-10.00	ZnCO3
Sylvite	-9.18	-8.28	0.90	KCl
Talc	2.33	23.68	21.35	Mg3Si4O10(OH)2
Vivianite	-4.11	-40.11	-36.00	Fe3(PO4)2:8H2O
Willemite	-1.12	14.18	15.30	Zn2SiO4
Witherite	-1.64	-10.20	-8.56	BaCO3
Zn(OH)2(e)	-2.65	8.85	11.50	Zn(OH)2

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
For ideal gases, phi = 1.

Initial solution 37.

-----------------------------Solution composition-------------------------------

Elements	Molality	Moles
Al	4.263e-08	4.263e-08
Alkalinity	8.191e-04	8.191e-04
B	1.129e-06	1.129e-06
Ba	1.894e-06	1.894e-06
Br	2.572e-35	2.572e-35
Ca	4.018e-04	4.018e-04
Cd	6.141e-09	6.141e-09
Cl	3.442e-03	3.442e-03
Cu	5.289e-08	5.289e-08
F	3.233e-04	3.233e-04
Fe	2.723e-05	2.723e-05
K	2.047e-04	2.047e-04
Mg	2.736e-04	2.736e-04
Mn	2.458e-05	2.458e-05
N(-3)	3.499e-06	3.499e-06
N(3)	4.999e-07	4.999e-07
N(5)	1.285e-06	1.285e-06
Na	1.462e-03	1.462e-03
P	1.292e-07	1.292e-07
Pb	1.530e-08	1.530e-08
S(6)	2.343e-04	2.343e-04
Si	6.243e-04	6.243e-04
Zn	1.500e-07	1.500e-07

----------------------------Description of solution----------------------------

pH = 7.700
pe = -2.682
Specific Conductance (µS/cm, 26°C) = 486
Density (g/cm³) = 0.99712

```
                              Volume (L)  =   1.00322
                       Activity of water  =   1.000
                  Ionic strength (mol/kgw)  =   4.925e-03
                        Mass of water (kg)  =   1.000e+00
                     Total carbon (mol/kg)  =   8.389e-04
                        Total CO2 (mol/kg)  =   8.389e-04
                          Temperature (°C)  =  25.56
                   Electrical balance (eq)  =  -1.926e-03
 Percent error, 100*(Cat-|An|)/(Cat+|An|)  = -24.02
                                Iterations  =  13 (395 overall)
                                   Total H  = 1.110157e+02
                                   Total O  = 5.551215e+01
```

----------Redox couples----------

Redox couple	pe	Eh (volts)
N(-3)/N(3)	4.6464	0.2754
N(-3)/N(5)	5.1748	0.3067
N(3)/N(5)	6.7600	0.4006

----------Distribution of species----------

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma	mole V cm³/mol
OH-	5.713e-07	5.293e-07	-6.243	-6.276	-0.033	-4.05
H+	2.136e-08	1.995e-08	-7.670	-7.700	-0.030	0.00
H2O	5.551e+01	9.999e-01	1.744	-0.000	0.000	18.07
Al	4.263e-08					
Al(OH)4-	4.160e-08	3.860e-08	-7.381	-7.413	-0.032	(0)
Al(OH)3	4.051e-10	4.056e-10	-9.392	-9.392	0.000	(0)
AlF3	4.051e-10	4.055e-10	-9.392	-9.392	0.000	(0)
AlF2+	1.173e-10	1.090e-10	-9.931	-9.963	-0.032	(0)
Al(OH)2+	5.673e-11	5.272e-11	-10.246	-10.278	-0.032	(0)
AlF4-	5.140e-11	4.770e-11	-10.289	-10.322	-0.032	(0)
AlF+2	9.844e-13	7.341e-13	-12.007	-12.134	-0.127	(0)
AlOH+2	1.715e-13	1.279e-13	-12.766	-12.893	-0.127	-27.66
Al+3	4.580e-16	2.477e-16	-15.339	-15.606	-0.267	-42.08
AlSO4+	1.366e-16	1.267e-16	-15.865	-15.897	-0.032	(0)
Al(SO4)2-	6.958e-19	6.456e-19	-18.158	-18.190	-0.032	(0)
AlHSO4+2	3.046e-25	2.254e-25	-24.516	-24.647	-0.131	(0)
B	1.129e-06					
H3BO3	1.094e-06	1.096e-06	-5.961	-5.960	0.000	39.27
H2BO3-	3.442e-08	3.192e-08	-7.463	-7.496	-0.033	(0)
BF(OH)3-	1.397e-10	1.296e-10	-9.855	-9.887	-0.033	(0)
BF2(OH)2-	8.820e-14	8.180e-14	-13.055	-13.087	-0.033	(0)
BF3OH-	5.643e-19	5.233e-19	-18.249	-18.281	-0.033	(0)
BF4-	1.354e-23	1.256e-23	-22.868	-22.901	-0.033	(0)
Ba	1.894e-06					
Ba+2	1.763e-06	1.306e-06	-5.754	-5.884	-0.130	-12.59
BaSO4	1.050e-07	1.051e-07	-6.979	-6.978	0.000	(0)
BaCl+	1.414e-08	1.312e-08	-7.849	-7.882	-0.033	(0)
BaHCO3+	1.011e-08	9.373e-09	-7.995	-8.028	-0.033	(0)
BaCO3	1.192e-09	1.193e-09	-8.924	-8.923	0.000	-10.69
BaOH+	2.387e-12	2.217e-12	-11.622	-11.654	-0.032	(0)
BaNO3+	2.109e-13	1.956e-13	-12.676	-12.709	-0.033	(0)
Br	2.572e-35					
Br-	2.572e-35	2.381e-35	-34.590	-34.623	-0.034	24.62
CdBr+	0.000e+00	0.000e+00	-40.881	-40.914	-0.033	(0)
PbBr+	0.000e+00	0.000e+00	-42.161	-42.194	-0.033	(0)
ZnBr+	0.000e+00	0.000e+00	-42.287	-42.320	-0.033	(0)
CdBr2	0.000e+00	0.000e+00	-74.807	-74.806	0.000	(0)
PbBr2	0.000e+00	0.000e+00	-77.151	-77.151	0.000	(0)
ZnBr2	0.000e+00	0.000e+00	-77.343	-77.343	0.000	(0)
C(4)	8.389e-04					
HCO3-	7.918e-04	7.358e-04	-3.101	-3.133	-0.032	24.77
CO2	3.275e-05	3.279e-05	-4.485	-4.484	0.000	34.46

CaHCO3+	2.956e-06	2.749e-06	-5.529	-5.561	-0.031	9.72
CO3-2	2.345e-06	1.749e-06	-5.630	-5.757	-0.127	-5.08
MnCO3	2.143e-06	2.145e-06	-5.669	-5.669	0.000	(0)
MgHCO3+	1.809e-06	1.677e-06	-5.743	-5.775	-0.033	5.52
FeHCO3+	1.428e-06	1.325e-06	-5.845	-5.878	-0.033	(0)
MnHCO3+	1.090e-06	1.013e-06	-5.962	-5.995	-0.032	(0)
CaCO3	8.620e-07	8.630e-07	-6.064	-6.064	0.000	-14.60
FeCO3	7.544e-07	7.553e-07	-6.122	-6.122	0.000	(0)
NaHCO3	5.487e-07	5.493e-07	-6.261	-6.260	0.000	1.80
MgCO3	3.268e-07	3.272e-07	-6.486	-6.485	0.000	-17.09
NaCO3-	4.810e-08	4.461e-08	-7.318	-7.351	-0.033	-0.93
ZnCO3	2.666e-08	2.669e-08	-7.574	-7.574	0.000	(0)
PbCO3	1.373e-08	1.375e-08	-7.862	-7.862	0.000	(0)
BaHCO3+	1.011e-08	9.373e-09	-7.995	-8.028	-0.033	(0)
ZnHCO3+	7.639e-09	7.084e-09	-8.117	-8.150	-0.033	(0)
Zn(CO3)2-2	1.349e-09	9.979e-10	-8.870	-9.001	-0.131	(0)
BaCO3	1.192e-09	1.193e-09	-8.924	-8.923	0.000	-10.69
PbHCO3+	2.851e-10	2.644e-10	-9.545	-9.578	-0.033	(0)
CdHCO3+	8.702e-11	8.070e-11	-10.060	-10.093	-0.033	(0)
Pb(CO3)2-2	8.166e-11	6.041e-11	-10.088	-10.219	-0.131	(0)
(CO2)2	2.008e-11	2.010e-11	-10.697	-10.697	0.000	68.92
CdCO3	4.813e-12	4.818e-12	-11.318	-11.317	0.000	(0)
CuCO3	4.330e-13	4.334e-13	-12.364	-12.363	0.000	(0)
Cd(CO3)2-2	3.602e-14	2.665e-14	-13.443	-13.574	-0.131	(0)
CuHCO3+	1.835e-14	1.702e-14	-13.736	-13.769	-0.033	(0)
Cu(CO3)2-2	1.290e-15	9.544e-16	-14.889	-15.020	-0.131	(0)
Ca	**4.018e-04**					
Ca+2	3.897e-04	2.904e-04	-3.409	-3.537	-0.128	-18.01
CaSO4	8.323e-06	8.332e-06	-5.080	-5.079	0.000	7.52
CaHCO3+	2.956e-06	2.749e-06	-5.529	-5.561	-0.031	9.72
CaCO3	8.620e-07	8.630e-07	-6.064	-6.064	0.000	-14.60
CaHPO4	9.805e-09	9.816e-09	-8.009	-8.008	0.000	(0)
CaOH+	2.604e-09	2.415e-09	-8.584	-8.617	-0.033	(0)
CaPO4-	1.266e-09	1.176e-09	-8.898	-8.929	-0.032	(0)
CaH2PO4+	1.580e-10	1.468e-10	-9.801	-9.833	-0.032	(0)
CaHSO4+	1.188e-12	1.102e-12	-11.925	-11.958	-0.033	(0)
Cd	**6.141e-09**					
Cd+2	4.688e-09	3.468e-09	-8.329	-8.460	-0.131	-18.60
CdCl+	1.133e-09	1.051e-09	-8.946	-8.978	-0.033	6.03
CdSO4	1.611e-10	1.613e-10	-9.793	-9.792	0.000	77.77
CdHCO3+	8.702e-11	8.070e-11	-10.060	-10.093	-0.033	(0)
CdOHCl	2.199e-11	2.201e-11	-10.658	-10.657	0.000	(0)
CdOH+	1.625e-11	1.507e-11	-10.789	-10.822	-0.033	(0)
CdF+	1.391e-11	1.290e-11	-10.857	-10.889	-0.033	(0)
CdCl2	1.388e-11	1.390e-11	-10.857	-10.857	0.000	23.14
CdCO3	4.813e-12	4.818e-12	-11.318	-11.317	0.000	(0)
Cd(SO4)2-2	3.827e-13	2.831e-13	-12.417	-12.548	-0.131	-105.18
Cd(OH)2	3.886e-14	3.890e-14	-13.410	-13.410	0.000	(0)
Cd(CO3)2-2	3.602e-14	2.665e-14	-13.443	-13.574	-0.131	(0)
CdCl3-	3.020e-14	2.801e-14	-13.520	-13.553	-0.033	68.96
CdNO3+	1.100e-14	1.020e-14	-13.959	-13.991	-0.033	17.54
CdF2	9.559e-15	9.570e-15	-14.020	-14.019	0.000	(0)
Cd2OH+3	5.008e-19	2.542e-19	-18.300	-18.595	-0.295	(0)
Cd(OH)3-	2.359e-19	2.187e-19	-18.627	-18.660	-0.033	(0)
Cd(OH)4-2	1.321e-25	9.770e-26	-24.879	-25.010	-0.131	(0)
CdBr+	0.000e+00	0.000e+00	-40.881	-40.914	-0.033	(0)
CdBr2	0.000e+00	0.000e+00	-74.807	-74.806	0.000	(0)
Cl	**3.442e-03**					
Cl-	3.416e-03	3.167e-03	-2.466	-2.499	-0.033	18.13
NaCl	2.531e-05	2.534e-05	-4.597	-4.596	0.000	(0)
MnCl+	2.145e-07	1.992e-07	-6.669	-6.701	-0.032	-2.93
FeCl+	8.485e-08	7.869e-08	-7.071	-7.104	-0.033	(0)
CuCl2-	3.998e-08	3.707e-08	-7.398	-7.431	-0.033	(0)
BaCl+	1.414e-08	1.312e-08	-7.849	-7.882	-0.033	(0)
CdCl+	1.133e-09	1.051e-09	-8.946	-8.978	-0.033	6.03
ZnCl+	7.205e-10	6.681e-10	-9.142	-9.175	-0.033	-13.34
ZnOHCl	4.014e-10	4.019e-10	-9.396	-9.396	0.000	(0)
MnCl2	2.750e-10	2.753e-10	-9.561	-9.560	0.000	85.21

CuCl3-2	2.507e-10	1.865e-10	-9.601	-9.729	-0.128	(0)
PbCl+	6.236e-11	5.783e-11	-10.205	-10.238	-0.033	8.00
CdOHCl	2.199e-11	2.201e-11	-10.658	-10.657	0.000	(0)
CdCl2	1.388e-11	1.390e-11	-10.857	-10.857	0.000	23.14
ZnCl2	2.218e-12	2.220e-12	-11.654	-11.654	0.000	100.94
PbCl2	2.869e-13	2.872e-13	-12.542	-12.542	0.000	35.02
MnCl3-	2.586e-13	2.401e-13	-12.587	-12.620	-0.032	43.37
CdCl3-	3.020e-14	2.801e-14	-13.520	-13.553	-0.033	68.96
ZnCl3-	8.537e-15	7.916e-15	-14.069	-14.102	-0.033	17.04
PbCl3-	7.817e-16	7.250e-16	-15.107	-15.140	-0.033	66.05
CuCl+	4.360e-16	4.042e-16	-15.361	-15.393	-0.033	0.52
ZnCl4-2	1.696e-17	1.262e-17	-16.770	-16.899	-0.128	145.39
PbCl4-2	1.492e-18	1.104e-18	-17.826	-17.957	-0.131	101.58
CuCl2	6.908e-19	6.916e-19	-18.161	-18.160	0.000	31.66
FeCl+2	4.824e-22	3.589e-22	-21.317	-21.445	-0.128	(0)
CuCl3-	8.464e-24	7.848e-24	-23.072	-23.105	-0.033	(0)
FeCl2+	5.370e-24	4.987e-24	-23.270	-23.302	-0.032	(0)
FeCl3	1.577e-27	1.579e-27	-26.802	-26.802	0.000	(0)
CuCl4-2	1.696e-28	1.262e-28	-27.771	-27.899	-0.128	(0)
Cu(1)	5.289e-08					
CuCl2-	3.998e-08	3.707e-08	-7.398	-7.431	-0.033	(0)
Cu+	1.266e-08	1.171e-08	-7.898	-7.932	-0.034	(0)
CuCl3-2	2.507e-10	1.865e-10	-9.601	-9.729	-0.128	(0)
Cu(2)	2.960e-12					
Cu(OH)2	2.419e-12	2.421e-12	-11.616	-11.616	0.000	(0)
CuCO3	4.330e-13	4.334e-13	-12.364	-12.363	0.000	(0)
Cu+2	6.167e-14	4.615e-14	-13.210	-13.336	-0.126	-26.49
CuOH+	2.494e-14	2.313e-14	-13.603	-13.636	-0.033	(0)
CuHCO3+	1.835e-14	1.702e-14	-13.736	-13.769	-0.033	(0)
CuSO4	1.518e-15	1.520e-15	-14.819	-14.818	0.000	13.16
Cu(CO3)2-2	1.290e-15	9.544e-16	-14.889	-15.020	-0.131	(0)
CuCl+	4.360e-16	4.042e-16	-15.361	-15.393	-0.033	0.52
CuF+	2.688e-16	2.493e-16	-15.570	-15.603	-0.033	(0)
Cu(OH)3-	7.883e-18	7.311e-18	-17.103	-17.136	-0.033	(0)
CuCl2	6.908e-19	6.916e-19	-18.161	-18.160	0.000	31.66
Cu2(OH)2+2	3.344e-22	2.474e-22	-21.476	-21.607	-0.131	(0)
Cu(OH)4-2	9.881e-23	7.310e-23	-22.005	-22.136	-0.131	(0)
CuCl3-	8.464e-24	7.848e-24	-23.072	-23.105	-0.033	(0)
CuCl4-2	1.696e-28	1.262e-28	-27.771	-27.899	-0.128	(0)
F	3.233e-04					
F-	3.188e-04	2.954e-04	-3.496	-3.530	-0.033	-1.27
MgF+	4.129e-06	3.832e-06	-5.384	-5.417	-0.032	-10.54
NaF	2.261e-07	2.264e-07	-6.646	-6.645	0.000	7.28
FeF+	5.734e-08	5.318e-08	-7.242	-7.274	-0.033	(0)
MnF+	3.398e-08	3.155e-08	-7.469	-7.501	-0.032	(0)
HF	8.919e-09	8.929e-09	-8.050	-8.049	0.000	12.53
AlF3	4.051e-10	4.055e-10	-9.392	-9.392	0.000	(0)
ZnF+	3.465e-10	3.214e-10	-9.460	-9.493	-0.033	(0)
BF(OH)3-	1.397e-10	1.296e-10	-9.855	-9.887	-0.033	(0)
AlF2+	1.173e-10	1.090e-10	-9.931	-9.963	-0.032	(0)
AlF4-	5.140e-11	4.770e-11	-10.289	-10.322	-0.032	(0)
CdF+	1.391e-11	1.290e-11	-10.857	-10.889	-0.033	(0)
HF2-	1.096e-11	1.016e-11	-10.960	-10.993	-0.033	22.12
PbF+	2.562e-12	2.376e-12	-11.591	-11.624	-0.033	(0)
AlF+2	9.844e-13	7.341e-13	-12.007	-12.134	-0.127	(0)
BF2(OH)2-	8.820e-14	8.180e-14	-13.055	-13.087	-0.033	(0)
PbF2	1.432e-14	1.433e-14	-13.844	-13.844	0.000	(0)
CdF2	9.559e-15	9.570e-15	-14.020	-14.019	0.000	(0)
CuF+	2.688e-16	2.493e-16	-15.570	-15.603	-0.033	(0)
PbF3-	3.307e-17	3.067e-17	-16.481	-16.513	-0.033	(0)
FeF2+	2.219e-17	2.061e-17	-16.654	-16.686	-0.032	(0)
FeF3	9.655e-18	9.666e-18	-17.015	-17.015	0.000	(0)
FeF+2	2.340e-18	1.741e-18	-17.631	-17.759	-0.128	(0)
BF3OH-	5.643e-19	5.233e-19	-18.249	-18.281	-0.033	(0)
PbF4-2	5.862e-21	4.336e-21	-20.232	-20.363	-0.131	(0)
BF4-	1.354e-23	1.256e-23	-22.868	-22.901	-0.033	(0)
SiF6-2	1.262e-25	9.390e-26	-24.899	-25.027	-0.128	42.75
Fe(2)	2.723e-05					

Fe+2	2.406e-05	1.800e-05	-4.619	-4.745	-0.126	-21.98
FeHCO3+	1.428e-06	1.325e-06	-5.845	-5.878	-0.033	(0)
FeCO3	7.544e-07	7.553e-07	-6.122	-6.122	0.000	(0)
FeSO4	5.190e-07	5.196e-07	-6.285	-6.284	0.000	18.39
FeOH+	3.203e-07	2.975e-07	-6.494	-6.527	-0.032	(0)
FeCl+	8.485e-08	7.869e-08	-7.071	-7.104	-0.033	(0)
FeF+	5.734e-08	5.318e-08	-7.242	-7.274	-0.033	(0)
FeHPO4	4.368e-09	4.373e-09	-8.360	-8.359	0.000	(0)
FeH2PO4+	1.898e-10	1.764e-10	-9.722	-9.754	-0.032	(0)
Fe(OH)2	1.330e-10	1.332e-10	-9.876	-9.876	0.000	(0)
Fe(OH)3-	2.685e-13	2.493e-13	-12.571	-12.603	-0.032	(0)
FeHSO4+	7.363e-14	6.829e-14	-13.133	-13.166	-0.033	(0)
Fe(3)	1.675e-10					
Fe(OH)3	1.381e-10	1.382e-10	-9.860	-9.859	0.000	(0)
Fe(OH)2+	2.248e-11	2.089e-11	-10.648	-10.680	-0.032	(0)
Fe(OH)4-	6.952e-12	6.460e-12	-11.158	-11.190	-0.032	(0)
FeOH+2	1.657e-15	1.233e-15	-14.781	-14.909	-0.128	(0)
FeF2+	2.219e-17	2.061e-17	-16.654	-16.686	-0.032	(0)
FeF3	9.655e-18	9.666e-18	-17.015	-17.015	0.000	(0)
FeF+2	2.340e-18	1.741e-18	-17.631	-17.759	-0.128	(0)
FeSO4+	7.080e-21	6.576e-21	-20.150	-20.182	-0.032	(0)
Fe+3	6.818e-21	3.687e-21	-20.166	-20.433	-0.267	(0)
FeCl+2	4.824e-22	3.589e-22	-21.317	-21.445	-0.128	(0)
FeHPO4+	6.639e-23	6.165e-23	-22.178	-22.210	-0.032	(0)
FeH2PO4+2	2.601e-23	1.939e-23	-22.585	-22.712	-0.127	(0)
Fe(SO4)2-	2.498e-23	2.316e-23	-22.602	-22.635	-0.033	(0)
FeCl2+	5.370e-24	4.987e-24	-23.270	-23.302	-0.032	(0)
FeCl3	1.577e-27	1.579e-27	-26.802	-26.802	0.000	(0)
FeHSO4+2	4.748e-28	3.513e-28	-27.323	-27.454	-0.131	(0)
Fe2(OH)2+4	1.334e-28	3.997e-29	-27.875	-28.398	-0.524	(0)
Fe3(OH)4+5	1.090e-36	1.657e-37	-35.963	-36.781	-0.818	(0)
H(0)	1.295e-13					
H2	6.473e-14	6.480e-14	-13.189	-13.188	0.000	28.61
K	2.047e-04					
K+	2.044e-04	1.894e-04	-3.689	-3.723	-0.033	9.06
KSO4-	2.324e-07	2.159e-07	-6.634	-6.666	-0.032	34.15
KHPO4-	2.425e-11	2.253e-11	-10.615	-10.647	-0.032	38.11
Mg	2.736e-04					
Mg+2	2.599e-04	1.943e-04	-3.585	-3.711	-0.126	-21.72
MgSO4	7.418e-06	7.426e-06	-5.130	-5.129	0.000	5.86
MgF+	4.129e-06	3.832e-06	-5.384	-5.417	-0.032	-10.54
MgHCO3+	1.809e-06	1.677e-06	-5.743	-5.775	-0.033	5.52
MgCO3	3.268e-07	3.272e-07	-6.486	-6.485	0.000	-17.09
MgOH+	3.996e-08	3.719e-08	-7.398	-7.430	-0.031	(0)
MgHPO4	8.872e-09	8.882e-09	-8.052	-8.051	0.000	(0)
MgPO4-	1.143e-09	1.062e-09	-8.942	-8.974	-0.032	(0)
MgH2PO4+	1.346e-10	1.251e-10	-9.871	-9.903	-0.032	(0)
Mn(2)	2.458e-05					
Mn+2	2.063e-05	1.544e-05	-4.685	-4.811	-0.126	-20.25
MnCO3	2.143e-06	2.145e-06	-5.669	-5.669	0.000	(0)
MnHCO3+	1.090e-06	1.013e-06	-5.962	-5.995	-0.032	(0)
MnSO4	4.453e-07	4.459e-07	-6.351	-6.351	0.000	22.30
MnCl+	2.145e-07	1.992e-07	-6.669	-6.701	-0.032	-2.93
MnF+	3.398e-08	3.155e-08	-7.469	-7.501	-0.032	(0)
MnOH+	2.241e-08	2.081e-08	-7.650	-7.682	-0.032	(0)
MnCl2	2.750e-10	2.753e-10	-9.561	-9.560	0.000	85.21
MnCl3-	2.586e-13	2.401e-13	-12.587	-12.620	-0.032	43.37
Mn(NO3)2	8.684e-17	8.694e-17	-16.061	-16.061	0.000	40.89
Mn(OH)3-	3.316e-17	3.079e-17	-16.479	-16.512	-0.032	(0)
Mn(3)	1.991e-33					
Mn+3	1.991e-33	1.077e-33	-32.701	-32.968	-0.267	(0)
N(-3)	3.499e-06					
NH4+	3.399e-06	3.144e-06	-5.469	-5.503	-0.034	18.01
NH3	9.331e-08	9.341e-08	-7.030	-7.030	0.000	24.44
NH4SO4-	7.017e-09	6.507e-09	-8.154	-8.187	-0.033	37.83
N(3)	4.999e-07					
NO2-	4.999e-07	4.628e-07	-6.301	-6.335	-0.034	25.03
N(5)	1.285e-06					

NO3-	1.285e-06	1.190e-06	-5.891	-5.924	-0.034	29.58
BaNO3+	2.109e-13	1.956e-13	-12.676	-12.709	-0.033	(0)
CdNO3+	1.100e-14	1.020e-14	-13.959	-13.991	-0.033	17.54
PbNO3+	8.586e-15	7.963e-15	-14.066	-14.099	-0.033	(0)
Mn(NO3)2	8.684e-17	8.694e-17	-16.061	-16.061	0.000	40.89
Na	1.462e-03					
Na+	1.435e-03	1.332e-03	-2.843	-2.876	-0.032	-1.39
NaCl	2.531e-05	2.534e-05	-4.597	-4.596	0.000	(0)
NaSO4-	1.158e-06	1.076e-06	-5.936	-5.968	-0.032	14.05
NaHCO3	5.487e-07	5.493e-07	-6.261	-6.260	0.000	1.80
NaF	2.261e-07	2.264e-07	-6.646	-6.645	0.000	7.28
NaCO3-	4.810e-08	4.461e-08	-7.318	-7.351	-0.033	-0.93
NaHPO4-	1.705e-10	1.584e-10	-9.768	-9.800	-0.032	33.79
NaOH	7.040e-20	7.048e-20	-19.152	-19.152	0.000	(0)
O(0)	0.000e+00					
O2	0.000e+00	0.000e+00	-65.823	-65.823	0.000	30.44
P	1.292e-07					
HPO4-2	8.201e-08	6.101e-08	-7.086	-7.215	-0.128	6.84
H2PO4-	2.103e-08	1.955e-08	-7.677	-7.709	-0.032	33.24
CaHPO4	9.805e-09	9.816e-09	-8.009	-8.008	0.000	(0)
MgHPO4	8.872e-09	8.882e-09	-8.052	-8.051	0.000	(0)
FeHPO4	4.368e-09	4.373e-09	-8.360	-8.359	0.000	(0)
CaPO4-	1.266e-09	1.176e-09	-8.898	-8.929	-0.032	(0)
MgPO4-	1.143e-09	1.062e-09	-8.942	-8.974	-0.032	(0)
FeH2PO4+	1.898e-10	1.764e-10	-9.722	-9.754	-0.032	(0)
NaHPO4-	1.705e-10	1.584e-10	-9.768	-9.800	-0.032	33.79
CaH2PO4+	1.580e-10	1.468e-10	-9.801	-9.833	-0.032	(0)
MgH2PO4+	1.346e-10	1.251e-10	-9.871	-9.903	-0.032	(0)
KHPO4-	2.425e-11	2.253e-11	-10.615	-10.647	-0.032	38.11
PO4-3	2.751e-12	1.394e-12	-11.561	-11.856	-0.295	-22.97
H3PO4	5.773e-14	5.780e-14	-13.239	-13.238	0.000	47.44
FeHPO4+	6.639e-23	6.165e-23	-22.178	-22.210	-0.032	(0)
FeH2PO4+2	2.601e-23	1.939e-23	-22.585	-22.712	-0.127	(0)
Pb	1.530e-08					
PbCO3	1.373e-08	1.375e-08	-7.862	-7.862	0.000	(0)
Pb+2	6.115e-10	4.524e-10	-9.214	-9.344	-0.131	-15.42
PbOH+	4.767e-10	4.421e-10	-9.322	-9.355	-0.033	(0)
PbHCO3+	2.851e-10	2.644e-10	-9.545	-9.578	-0.033	(0)
Pb(CO3)2-2	8.166e-11	6.041e-11	-10.088	-10.219	-0.131	(0)
PbCl+	6.236e-11	5.783e-11	-10.205	-10.238	-0.033	8.00
PbSO4	4.083e-11	4.088e-11	-10.389	-10.389	0.000	(0)
Pb(OH)2	8.609e-12	8.618e-12	-11.065	-11.065	0.000	(0)
PbF+	2.562e-12	2.376e-12	-11.591	-11.624	-0.033	(0)
PbCl2	2.869e-13	2.872e-13	-12.542	-12.542	0.000	35.02
Pb(SO4)2-2	4.659e-14	3.447e-14	-13.332	-13.463	-0.131	(0)
PbF2	1.432e-14	1.433e-14	-13.844	-13.844	0.000	(0)
PbNO3+	8.586e-15	7.963e-15	-14.066	-14.099	-0.033	(0)
Pb(OH)3-	5.347e-15	4.959e-15	-14.272	-14.305	-0.033	(0)
PbCl3-	7.817e-16	7.250e-16	-15.107	-15.140	-0.033	66.05
PbF3-	3.307e-17	3.067e-17	-16.481	-16.513	-0.033	(0)
Pb2OH+3	8.821e-18	4.477e-18	-17.054	-17.349	-0.295	(0)
PbCl4-2	1.492e-18	1.104e-18	-17.826	-17.957	-0.131	101.58
Pb(OH)4-2	7.695e-19	5.693e-19	-18.114	-18.245	-0.131	(0)
PbF4-2	5.862e-21	4.336e-21	-20.232	-20.363	-0.131	(0)
Pb3(OH)4+2	1.132e-21	8.371e-22	-20.946	-21.077	-0.131	(0)
PbBr+	0.000e+00	0.000e+00	-42.161	-42.194	-0.033	(0)
PbBr2	0.000e+00	0.000e+00	-77.151	-77.151	0.000	(0)
S(6)	2.343e-04					
SO4-2	2.161e-04	1.607e-04	-3.665	-3.794	-0.129	14.73
CaSO4	8.323e-06	8.332e-06	-5.080	-5.079	0.000	7.52
MgSO4	7.418e-06	7.426e-06	-5.130	-5.129	0.000	5.86
NaSO4-	1.158e-06	1.076e-06	-5.936	-5.968	-0.032	14.05
FeSO4	5.190e-07	5.196e-07	-6.285	-6.284	0.000	18.39
MnSO4	4.453e-07	4.459e-07	-6.351	-6.351	0.000	22.30
KSO4-	2.324e-07	2.159e-07	-6.634	-6.666	-0.032	34.15
BaSO4	1.050e-07	1.051e-07	-6.979	-6.978	0.000	(0)
NH4SO4-	7.017e-09	6.507e-09	-8.154	-8.187	-0.033	37.83
ZnSO4	2.890e-09	2.893e-09	-8.539	-8.539	0.000	21.63

HSO4-	3.402e-10	3.155e-10	-9.468	-9.501	-0.033	40.35
CdSO4	1.611e-10	1.613e-10	-9.793	-9.792	0.000	77.77
PbSO4	4.083e-11	4.088e-11	-10.389	-10.389	0.000	(0)
Zn(SO4)2-2	5.085e-12	3.762e-12	-11.294	-11.425	-0.131	-12.49
CaHSO4+	1.188e-12	1.102e-12	-11.925	-11.958	-0.033	(0)
Cd(SO4)2-2	3.827e-13	2.831e-13	-12.417	-12.548	-0.131	-105.18
FeHSO4+	7.363e-14	6.829e-14	-13.133	-13.166	-0.033	(0)
Pb(SO4)2-2	4.659e-14	3.447e-14	-13.332	-13.463	-0.131	(0)
CuSO4	1.518e-15	1.520e-15	-14.819	-14.818	0.000	13.16
AlSO4+	1.366e-16	1.267e-16	-15.865	-15.897	-0.032	(0)
Al(SO4)2-	6.958e-19	6.456e-19	-18.158	-18.190	-0.032	(0)
FeSO4+	7.080e-21	6.576e-21	-20.150	-20.182	-0.032	(0)
Fe(SO4)2-	2.498e-23	2.316e-23	-22.602	-22.635	-0.033	(0)
AlHSO4+2	3.046e-25	2.254e-25	-24.516	-24.647	-0.131	(0)
FeHSO4+2	4.748e-28	3.513e-28	-27.323	-27.454	-0.131	(0)
Si	6.243e-04					
H4SiO4	6.193e-04	6.200e-04	-3.208	-3.208	0.000	52.03
H3SiO4-	5.038e-06	4.671e-06	-5.298	-5.331	-0.033	28.02
H2SiO4-2	2.215e-11	1.652e-11	-10.655	-10.782	-0.127	(0)
SiF6-2	1.262e-25	9.390e-26	-24.899	-25.027	-0.128	42.75
Zn	1.500e-07					
Zn+2	1.028e-07	7.648e-08	-6.988	-7.116	-0.128	-25.27
ZnCO3	2.666e-08	2.669e-08	-7.574	-7.574	0.000	(0)
ZnHCO3+	7.639e-09	7.084e-09	-8.117	-8.150	-0.033	(0)
ZnOH+	4.727e-09	4.384e-09	-8.325	-8.358	-0.033	(0)
ZnSO4	2.890e-09	2.893e-09	-8.539	-8.539	0.000	21.63
Zn(OH)2	2.415e-09	2.418e-09	-8.617	-8.617	0.000	(0)
Zn(CO3)2-2	1.349e-09	9.979e-10	-8.870	-9.001	-0.131	(0)
ZnCl+	7.205e-10	6.681e-10	-9.142	-9.175	-0.033	-13.34
ZnOHCl	4.014e-10	4.019e-10	-9.396	-9.396	0.000	(0)
ZnF+	3.465e-10	3.214e-10	-9.460	-9.493	-0.033	(0)
Zn(SO4)2-2	5.085e-12	3.762e-12	-11.294	-11.425	-0.131	-12.49
ZnCl2	2.218e-12	2.220e-12	-11.654	-11.654	0.000	100.94
Zn(OH)3-	4.131e-13	3.831e-13	-12.384	-12.417	-0.033	(0)
ZnCl3-	8.537e-15	7.916e-15	-14.069	-14.102	-0.033	17.04
ZnCl4-2	1.696e-17	1.262e-17	-16.770	-16.899	-0.128	145.39
Zn(OH)4-2	4.113e-18	3.043e-18	-17.386	-17.517	-0.131	(0)
ZnBr+	0.000e+00	0.000e+00	-42.287	-42.320	-0.033	(0)
ZnBr2	0.000e+00	0.000e+00	-77.343	-77.343	0.000	(0)

----------Distribution of alkalinity----------

Total alkalinity (eq/kgw) = 8.191e-04

Species	Alkalinity	Molality	Alk/Mol
HCO3-	7.918e-04	7.918e-04	1.00
H3SiO4-	5.038e-06	5.038e-06	1.00
CO3-2	4.691e-06	2.345e-06	2.00
MnCO3	4.285e-06	2.143e-06	2.00
CaHCO3+	2.956e-06	2.956e-06	1.00
MgHCO3+	1.809e-06	1.809e-06	1.00
CaCO3	1.724e-06	8.620e-07	2.00
FeCO3	1.509e-06	7.544e-07	2.00
FeHCO3+	1.428e-06	1.428e-06	1.00
MnHCO3+	1.090e-06	1.090e-06	1.00
MgCO3	6.536e-07	3.268e-07	2.00
OH-	5.713e-07	5.713e-07	1.00
NaHCO3	5.487e-07	5.487e-07	1.00
FeOH+	3.203e-07	3.203e-07	1.00
Al(OH)4-	1.664e-07	4.160e-08	4.00
NaCO3-	9.620e-08	4.810e-08	2.00
NH3	9.331e-08	9.331e-08	1.00
HPO4-2	8.201e-08	8.201e-08	1.00
ZnCO3	5.332e-08	2.666e-08	2.00
MgOH+	3.996e-08	3.996e-08	1.00
H2BO3-	3.442e-08	3.442e-08	1.00
PbCO3	2.747e-08	1.373e-08	2.00

MnOH+	2.241e-08	2.241e-08	1.00
H+	-2.136e-08	2.136e-08	-1.00
BaHCO3+	1.011e-08	1.011e-08	1.00
CaHPO4	9.805e-09	9.805e-09	1.00
HF	-8.919e-09	8.919e-09	-1.00
MgHPO4	8.872e-09	8.872e-09	1.00
ZnHCO3+	7.639e-09	7.639e-09	1.00
Zn(CO3)2-2	5.396e-09	1.349e-09	4.00
Zn(OH)2	4.830e-09	2.415e-09	2.00
ZnOH+	4.727e-09	4.727e-09	1.00
FeHPO4	4.368e-09	4.368e-09	1.00
CaOH+	2.604e-09	2.604e-09	1.00
CaPO4-	2.532e-09	1.266e-09	2.00
BaCO3	2.384e-09	1.192e-09	2.00
MgPO4-	2.285e-09	1.143e-09	2.00
Al(OH)3	1.215e-09	4.051e-10	3.00
PbOH+	4.767e-10	4.767e-10	1.00
ZnOHCl	4.014e-10	4.014e-10	1.00
HSO4-	-3.402e-10	3.402e-10	-1.00
Pb(CO3)2-2	3.266e-10	8.166e-11	4.00
PbHCO3+	2.851e-10	2.851e-10	1.00
Fe(OH)2	2.661e-10	1.330e-10	2.00
NaHPO4-	1.705e-10	1.705e-10	1.00
Fe(OH)3	1.381e-10	1.381e-10	1.00
Al(OH)2+	1.135e-10	5.673e-11	2.00
CdHCO3+	8.702e-11	8.702e-11	1.00
H2SiO4-2	4.429e-11	2.215e-11	2.00
KHPO4-	2.425e-11	2.425e-11	1.00
CdOHCl	2.199e-11	2.199e-11	1.00
Pb(OH)2	1.722e-11	8.609e-12	2.00
CdOH+	1.625e-11	1.625e-11	1.00
Fe(OH)4-	1.390e-11	6.952e-12	2.00
HF2-	-1.096e-11	1.096e-11	-1.00
CdCO3	9.626e-12	4.813e-12	2.00
PO4-3	5.502e-12	2.751e-12	2.00
Cu(OH)2	4.837e-12	2.419e-12	2.00
BaOH+	2.387e-12	2.387e-12	1.00
Zn(OH)3-	1.239e-12	4.131e-13	3.00
CaHSO4+	-1.188e-12	1.188e-12	-1.00
CuCO3	8.659e-13	4.330e-13	2.00
Fe(OH)3-	8.055e-13	2.685e-13	3.00
AlOH+2	1.715e-13	1.715e-13	1.00
Cd(CO3)2-2	1.441e-13	3.602e-14	4.00
BF2(OH)2-	-8.820e-14	8.820e-14	-1.00
Cd(OH)2	7.772e-14	3.886e-14	2.00
FeHSO4+	-7.363e-14	7.363e-14	-1.00
H3PO4	-5.773e-14	5.773e-14	-1.00
CuOH+	2.494e-14	2.494e-14	1.00
CuHCO3+	1.835e-14	1.835e-14	1.00
Pb(OH)3-	1.604e-14	5.347e-15	3.00
Cu(CO3)2-2	5.160e-15	1.290e-15	4.00
FeOH+2	-1.657e-15	1.657e-15	-1.00
Mn(OH)3-	9.947e-17	3.316e-17	3.00
FeF2+	-4.438e-17	2.219e-17	-2.00
Cu(OH)3-	2.365e-17	7.883e-18	3.00
FeF3	-1.931e-17	9.655e-18	-2.00
Zn(OH)4-2	1.645e-17	4.113e-18	4.00
Pb2OH+3	8.821e-18	8.821e-18	1.00
FeF+2	-4.680e-18	2.340e-18	-2.00
Pb(OH)4-2	3.078e-18	7.695e-19	4.00
BF3OH-	-1.129e-18	5.643e-19	-2.00
Cd(OH)3-	7.076e-19	2.359e-19	3.00
Cd2OH+3	5.008e-19	5.008e-19	1.00
NaOH	7.040e-20	7.040e-20	1.00
FeSO4+	-1.416e-20	7.080e-21	-2.00
Fe+3	-1.364e-20	6.818e-21	-2.00
Pb3(OH)4+2	4.526e-21	1.132e-21	4.00
FeCl+2	-9.649e-22	4.824e-22	-2.00

Cu2(OH)2+2	6.688e-22	3.344e-22	2.00
Cu(OH)4-2	3.953e-22	9.881e-23	4.00
FeHPO4+	-6.639e-23	6.639e-23	-1.00
FeH2PO4+2	-5.202e-23	2.601e-23	-2.00
Fe(SO4)2-	-4.995e-23	2.498e-23	-2.00
BF4-	-4.062e-23	1.354e-23	-3.00
FeCl2+	-1.074e-23	5.370e-24	-2.00
Cd(OH)4-2	5.282e-25	1.321e-25	4.00
SiF6-2	-5.049e-25	1.262e-25	-4.00
AlHSO4+2	-3.046e-25	3.046e-25	-1.00
FeCl3	-3.155e-27	1.577e-27	-2.00
FeHSO4+2	-1.425e-27	4.748e-28	-3.00
Fe2(OH)2+4	-2.669e-28	1.334e-28	-2.00
Fe3(OH)4+5	-2.180e-36	1.090e-36	-2.00

----------Saturation indices----------

Phase	SI**	log IAP	log K(298 K, 1 atm)	
Al(OH)3(a)	-3.27	7.49	10.76	Al(OH)3
Albite	-1.94	-19.91	-17.97	NaAlSi3O8
Alunite	-10.46	-11.93	-1.47	KAl3(SO4)2(OH)6
Anglesite	-5.35	-13.14	-7.79	PbSO4
Anhydrite	-3.05	-7.33	-4.28	CaSO4
Anorthite	-5.08	-24.78	-19.70	CaAl2Si2O8
Aragonite	-0.95	-9.29	-8.34	CaCO3
BaCl2	-13.11	-10.88	2.22	BaCl2
BaCl2:2H2O	-11.10	-10.88	0.21	BaCl2:2H2O
BaCl2:H2O	-11.71	-10.88	0.83	BaCl2:H2O
Barite	0.16	-9.68	-9.84	BaSO4
Ca-Montmorillonite	-0.08	-45.03	-44.95	Ca0.165Al2.33Si3.67O10(OH)2
Calcite	-0.81	-9.29	-8.48	CaCO3
Cd(OH)2	-6.71	6.94	13.65	Cd(OH)2
CdSiO3	-5.30	3.73	9.04	CdSiO3
CdSO4	-12.13	-12.25	-0.12	CdSO4
Cerussite	-1.98	-15.10	-13.12	PbCO3
Chalcedony	0.34	-3.21	-3.54	SiO2
Chlorite(14A)	-4.36	63.81	68.17	Mg5Al2Si3O10(OH)8
Chrysotile	-3.48	28.65	32.13	Mg3Si2O5(OH)4
CO2(g)	-3.01	-4.48	-1.47	CO2
Dolomite	-1.66	-18.76	-17.10	CaMg(CO3)2
Fe(OH)3(a)	-2.22	2.67	4.89	Fe(OH)3
Fluorite	-0.00	-10.60	-10.59	CaF2
Gibbsite	-0.58	7.49	8.08	Al(OH)3
Goethite	3.69	2.67	-1.02	FeOOH
Gypsum	-2.75	-7.33	-4.58	CaSO4:2H2O
H2(g)	-10.09	-13.19	-3.10	H2
H2O(g)	-1.49	-0.00	1.49	H2O
Halite	-6.95	-5.37	1.57	NaCl
Hausmannite	-19.09	41.80	60.89	Mn3O4
Hematite	9.38	5.33	-4.05	Fe2O3
Hydroxyapatite	-5.06	-8.53	-3.47	Ca5(PO4)3OH
Illite	-0.49	-40.68	-40.19	K0.6Mg0.25Al2.3Si3.5O10(OH)2
Jarosite-K	-17.16	-26.41	-9.25	KFe3(SO4)2(OH)6
K-feldspar	-0.23	-20.76	-20.53	KAlSi3O8
K-mica	4.21	16.84	12.62	KAl3Si3O10(OH)2
Kaolinite	1.19	8.57	7.39	Al2Si2O5(OH)4
Manganite	-9.73	15.61	25.34	MnOOH
Melanterite	-6.34	-8.54	-2.20	FeSO4:7H2O
NH3(g)	-8.81	-7.03	1.78	NH3
O2(g)	-62.93	-65.82	-2.90	O2
Otavite	-2.12	-14.22	-12.10	CdCO3
Pb(OH)2	-2.08	6.06	8.13	Pb(OH)2
Pyrochroite	-4.61	10.59	15.20	Mn(OH)2
Pyrolusite	-20.67	20.62	41.29	MnO2:H2O
Quartz	0.76	-3.21	-3.97	SiO2
Rhodochrosite	0.56	-10.57	-11.13	MnCO3
Sepiolite	-1.99	13.75	15.75	Mg2Si3O7.5OH:3H2O

Sepiolite(d)	-4.91	13.75	18.66	Mg2Si3O7.5OH:3H2O
Siderite	0.39	-10.50	-10.89	FeCO3
SiO2(a)	-0.50	-3.21	-2.71	SiO2
Smithsonite	-2.87	-12.87	-10.01	ZnCO3
Sylvite	-7.12	-6.22	0.90	KCl
Talc	0.90	22.24	21.34	Mg3Si4O10(OH)2
Vivianite	-1.95	-37.95	-36.00	Fe3(PO4)2:8H2O
Willemite	-1.92	13.36	15.28	Zn2SiO4
Witherite	-3.08	-11.64	-8.56	BaCO3
Zn(OH)2(e)	-3.22	8.28	11.50	Zn(OH)2

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
For ideal gases, phi = 1.

Initial solution 38.

-----------------------------Solution composition-----------------------------

Elements	Molality	Moles
Al	7.786e-08	7.786e-08
Alkalinity	1.114e-03	1.114e-03
B	2.934e-06	2.934e-06
Ba	1.602e-06	1.602e-06
Br	1.883e-34	1.883e-34
Ca	4.742e-04	4.742e-04
Cd	6.052e-09	6.052e-09
Cl	4.458e-03	4.458e-03
Cu	4.990e-08	4.990e-08
F	1.948e-05	1.948e-05
Fe	3.583e-07	3.583e-07
K	1.535e-04	1.535e-04
Mg	3.292e-04	3.292e-04
Mn	8.740e-06	8.740e-06
N(-3)	6.428e-07	6.428e-07
N(3)	2.857e-07	2.857e-07
N(5)	1.643e-06	1.643e-06
Na	4.221e-03	4.221e-03
P	9.689e-07	9.689e-07
Pb	1.627e-08	1.627e-08
S(6)	1.562e-04	1.562e-04
Si	3.746e-04	3.746e-04
Zn	8.876e-08	8.876e-08

----------------------------Description of solution----------------------------

pH	= 6.800
pe	= -1.839
Specific Conductance (µS/cm, 26°C)	= 672
Density (g/cm³)	= 0.99719
Volume (L)	= 1.00324
Activity of water	= 1.000
Ionic strength (mol/kgw)	= 6.764e-03
Mass of water (kg)	= 1.000e+00
Total carbon (mol/kg)	= 1.470e-03
Total CO2 (mol/kg)	= 1.470e-03
Temperature (°C)	= 25.60
Electrical balance (eq)	= 9.645e-05
Percent error, 100*(Cat-|An|)/(Cat+|An|)	= 0.83
Iterations	= 12 (407 overall)
Total H	= 1.110151e+02
Total O	= 5.551241e+01

---------------------------------Redox couples---------------------------------

Redox couple	pe	Eh (volts)
N(-3)/N(3)	5.9244	0.3512

N(-3)/N(5)	6.4015	0.3794
N(3)/N(5)	7.8327	0.4643

----------Distribution of species----------

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma	mole V cm³/mol
H+	1.713e-07	1.585e-07	-6.766	-6.800	-0.034	0.00
OH-	7.300e-08	6.683e-08	-7.137	-7.175	-0.038	-4.03
H2O	5.551e+01	9.998e-01	1.744	-0.000	0.000	18.07
Al	7.786e-08					
Al(OH)4-	6.397e-08	5.869e-08	-7.194	-7.231	-0.037	(0)
Al(OH)2+	5.484e-09	5.040e-09	-8.261	-8.298	-0.037	(0)
Al(OH)3	4.888e-09	4.895e-09	-8.311	-8.310	0.001	(0)
AlF2+	2.503e-09	2.301e-09	-8.602	-8.638	-0.037	(0)
AlF3	5.070e-10	5.078e-10	-9.295	-9.294	0.001	(0)
AlF+2	3.660e-10	2.612e-10	-9.437	-9.583	-0.147	(0)
AlOH+2	1.356e-10	9.676e-11	-9.868	-10.014	-0.147	-27.62
AlF4-	3.862e-12	3.543e-12	-11.413	-11.451	-0.037	(0)
Al+3	2.990e-12	1.485e-12	-11.524	-11.828	-0.304	-42.01
AlSO4+	5.220e-13	4.789e-13	-12.282	-12.320	-0.037	(0)
Al(SO4)2-	1.675e-15	1.537e-15	-14.776	-14.813	-0.037	(0)
AlHSO4+2	9.581e-21	6.767e-21	-20.019	-20.170	-0.151	(0)
B	2.934e-06					
H3BO3	2.922e-06	2.926e-06	-5.534	-5.534	0.001	39.28
H2BO3-	1.172e-08	1.074e-08	-7.931	-7.969	-0.038	(0)
BF(OH)3-	2.241e-11	2.054e-11	-10.650	-10.687	-0.038	(0)
BF2(OH)2-	6.664e-15	6.109e-15	-14.176	-14.214	-0.038	(0)
BF3OH-	2.007e-20	1.840e-20	-19.697	-19.735	-0.038	(0)
BF4-	2.270e-25	2.081e-25	-24.644	-24.682	-0.038	(0)
Ba	1.602e-06					
Ba+2	1.521e-06	1.076e-06	-5.818	-5.968	-0.151	-12.55
BaSO4	5.447e-08	5.455e-08	-7.264	-7.263	0.001	(0)
BaCl+	1.490e-08	1.366e-08	-7.827	-7.865	-0.038	(0)
BaHCO3+	1.160e-08	1.063e-08	-7.936	-7.973	-0.038	(0)
BaCO3	1.702e-10	1.705e-10	-9.769	-9.768	0.001	-10.69
BaOH+	2.504e-13	2.299e-13	-12.601	-12.638	-0.037	(0)
BaNO3+	2.219e-13	2.034e-13	-12.654	-12.692	-0.038	(0)
Br	1.883e-34					
Br-	1.883e-34	1.722e-34	-33.725	-33.764	-0.039	24.63
CdBr+	0.000e+00	0.000e+00	-40.056	-40.093	-0.038	(0)
PbBr+	0.000e+00	0.000e+00	-40.640	-40.677	-0.038	(0)
ZnBr+	0.000e+00	0.000e+00	-41.576	-41.614	-0.038	(0)
CdBr2	0.000e+00	0.000e+00	-73.127	-73.126	0.001	(0)
PbBr2	0.000e+00	0.000e+00	-74.776	-74.776	0.001	(0)
ZnBr2	0.000e+00	0.000e+00	-75.778	-75.778	0.001	(0)
C(4)	1.470e-03					
HCO3-	1.101e-03	1.012e-03	-2.958	-2.995	-0.037	24.79
CO2	3.575e-04	3.581e-04	-3.447	-3.446	0.001	34.46
CaHCO3+	4.679e-06	4.305e-06	-5.330	-5.366	-0.036	9.73
MgHCO3+	2.973e-06	2.724e-06	-5.527	-5.565	-0.038	5.53
NaHCO3	2.144e-06	2.148e-06	-5.669	-5.668	0.001	1.80
MnHCO3+	5.527e-07	5.076e-07	-6.258	-6.295	-0.037	(0)
CO3-2	4.248e-07	3.031e-07	-6.372	-6.518	-0.147	-5.03
CaCO3	1.700e-07	1.703e-07	-6.769	-6.769	0.001	-14.60
MnCO3	1.353e-07	1.355e-07	-6.869	-6.868	0.001	(0)
MgCO3	6.687e-08	6.697e-08	-7.175	-7.174	0.001	-17.09
FeHCO3+	2.568e-08	2.354e-08	-7.590	-7.628	-0.038	(0)
NaCO3-	2.403e-08	2.203e-08	-7.619	-7.657	-0.038	-0.90
BaHCO3+	1.160e-08	1.063e-08	-7.936	-7.973	-0.038	(0)
PbCO3	1.080e-08	1.081e-08	-7.967	-7.966	0.001	(0)
ZnHCO3+	7.471e-09	6.849e-09	-8.127	-8.164	-0.038	(0)
ZnCO3	3.246e-09	3.251e-09	-8.489	-8.488	0.001	(0)
(CO2)2	2.397e-09	2.401e-09	-8.620	-8.620	0.001	68.92
PbHCO3+	1.800e-09	1.650e-09	-8.745	-8.782	-0.038	(0)
FeCO3	1.688e-09	1.691e-09	-8.773	-8.772	0.001	(0)
BaCO3	1.702e-10	1.705e-10	-9.769	-9.768	0.001	-10.69

CdHCO3+	1.108e-10	1.016e-10	-9.955	-9.993	-0.038	(0)
Zn(CO3)2-2	2.983e-11	2.106e-11	-10.525	-10.676	-0.151	(0)
Pb(CO3)2-2	1.166e-11	8.232e-12	-10.933	-11.085	-0.151	(0)
CdCO3	7.632e-13	7.644e-13	-12.117	-12.117	0.001	(0)
CuCO3	3.346e-13	3.351e-13	-12.475	-12.475	0.001	(0)
CuHCO3+	1.139e-13	1.044e-13	-12.943	-12.981	-0.038	(0)
Cd(CO3)2-2	1.037e-15	7.326e-16	-14.984	-15.135	-0.151	(0)
Cu(CO3)2-2	1.811e-16	1.279e-16	-15.742	-15.893	-0.151	(0)
Ca	4.742e-04					
Ca+2	4.634e-04	3.304e-04	-3.334	-3.481	-0.147	-17.97
CaSO4	5.963e-06	5.973e-06	-5.225	-5.224	0.001	7.52
CaHCO3+	4.679e-06	4.305e-06	-5.330	-5.366	-0.036	9.73
CaCO3	1.700e-07	1.703e-07	-6.769	-6.769	0.001	-14.60
CaHPO4	3.862e-08	3.868e-08	-7.413	-7.412	0.001	(0)
CaH2PO4+	4.999e-09	4.594e-09	-8.301	-8.338	-0.037	(0)
CaPO4-	6.355e-10	5.840e-10	-9.197	-9.234	-0.037	(0)
CaOH+	3.774e-10	3.459e-10	-9.423	-9.461	-0.038	(0)
CaHSO4+	6.846e-12	6.276e-12	-11.165	-11.202	-0.038	(0)
Cd	6.052e-09					
Cd+2	4.496e-09	3.175e-09	-8.347	-8.498	-0.151	-18.56
CdCl+	1.326e-09	1.215e-09	-8.878	-8.915	-0.038	6.07
CdHCO3+	1.108e-10	1.016e-10	-9.955	-9.993	-0.038	(0)
CdSO4	9.285e-11	9.299e-11	-10.032	-10.032	0.001	77.75
CdCl2	2.028e-11	2.031e-11	-10.693	-10.692	0.001	23.14
CdOHCl	3.202e-12	3.207e-12	-11.495	-11.494	0.001	(0)
CdOH+	1.900e-12	1.742e-12	-11.721	-11.759	-0.038	(0)
CdF+	7.640e-13	7.004e-13	-12.117	-12.155	-0.038	(0)
CdCO3	7.632e-13	7.644e-13	-12.117	-12.117	0.001	(0)
Cd(SO4)2-2	1.456e-13	1.028e-13	-12.837	-12.988	-0.151	-105.12
CdCl3-	5.643e-14	5.173e-14	-13.249	-13.286	-0.038	68.94
CdNO3+	1.284e-14	1.177e-14	-13.891	-13.929	-0.038	17.55
Cd(CO3)2-2	1.037e-15	7.326e-16	-14.984	-15.135	-0.151	(0)
Cd(OH)2	5.635e-16	5.644e-16	-15.249	-15.248	0.001	(0)
CdF2	3.078e-17	3.083e-17	-16.512	-16.511	0.001	(0)
Cd2OH+3	5.879e-20	2.688e-20	-19.231	-19.571	-0.340	(0)
Cd(OH)3-	4.358e-22	3.995e-22	-21.361	-21.399	-0.038	(0)
Cd(OH)4-2	3.180e-29	2.246e-29	-28.498	-28.649	-0.151	(0)
CdBr+	0.000e+00	0.000e+00	-40.056	-40.093	-0.038	(0)
CdBr2	0.000e+00	0.000e+00	-73.127	-73.126	0.001	(0)
Cl	4.458e-03					
Cl-	4.367e-03	4.000e-03	-2.360	-2.398	-0.038	18.14
NaCl	9.088e-05	9.102e-05	-4.042	-4.041	0.001	(0)
MnCl+	9.985e-08	9.170e-08	-7.001	-7.038	-0.037	-2.91
CuCl2-	4.135e-08	3.790e-08	-7.383	-7.421	-0.038	(0)
BaCl+	1.490e-08	1.366e-08	-7.827	-7.865	-0.038	(0)
FeCl+	1.401e-09	1.284e-09	-8.854	-8.891	-0.038	(0)
CdCl+	1.326e-09	1.215e-09	-8.878	-8.915	-0.038	6.07
ZnCl+	6.484e-10	5.942e-10	-9.188	-9.226	-0.038	-13.30
PbCl+	3.619e-10	3.318e-10	-9.441	-9.479	-0.038	8.01
CuCl3-2	3.386e-10	2.408e-10	-9.470	-9.618	-0.148	(0)
MnCl2	1.599e-10	1.601e-10	-9.796	-9.796	0.001	85.16
ZnOHCl	4.485e-11	4.492e-11	-10.348	-10.348	0.001	(0)
CdCl2	2.028e-11	2.031e-11	-10.693	-10.692	0.001	23.14
CdOHCl	3.202e-12	3.207e-12	-11.495	-11.494	0.001	(0)
ZnCl2	2.491e-12	2.495e-12	-11.604	-11.603	0.001	100.86
PbCl2	2.077e-12	2.080e-12	-11.683	-11.682	0.001	35.02
MnCl3-	1.921e-13	1.764e-13	-12.716	-12.753	-0.037	43.39
CdCl3-	5.643e-14	5.173e-14	-13.249	-13.286	-0.038	68.94
ZnCl3-	1.226e-14	1.124e-14	-13.911	-13.949	-0.038	17.04
PbCl3-	7.237e-15	6.634e-15	-14.140	-14.178	-0.038	66.07
CuCl+	2.491e-15	2.283e-15	-14.604	-14.642	-0.038	0.53
ZnCl4-2	3.183e-17	2.264e-17	-16.497	-16.645	-0.148	145.45
PbCl4-2	1.807e-17	1.276e-17	-16.743	-16.894	-0.151	101.63
CuCl2	4.928e-18	4.936e-18	-17.307	-17.307	0.001	31.70
CuCl3-	7.726e-23	7.080e-23	-22.112	-22.150	-0.038	(0)
FeCl+2	5.756e-23	4.094e-23	-22.240	-22.388	-0.148	(0)
FeCl2+	7.816e-25	7.178e-25	-24.107	-24.144	-0.037	(0)
CuCl4-2	2.024e-27	1.439e-27	-26.694	-26.842	-0.148	(0)

FeCl3	2.867e-28	2.871e-28	-27.543	-27.542	0.001	(0)
Cu(1)	4.990e-08					
CuCl2-	4.135e-08	3.790e-08	-7.383	-7.421	-0.038	(0)
Cu+	8.211e-09	7.500e-09	-8.086	-8.125	-0.039	(0)
CuCl3-2	3.386e-10	2.408e-10	-9.470	-9.618	-0.148	(0)
Cu(2)	9.278e-13					
CuCO3	3.346e-13	3.351e-13	-12.475	-12.475	0.001	(0)
Cu+2	2.872e-13	2.059e-13	-12.542	-12.686	-0.145	-26.46
Cu(OH)2	1.709e-13	1.712e-13	-12.767	-12.767	0.001	(0)
CuHCO3+	1.139e-13	1.044e-13	-12.943	-12.981	-0.038	(0)
CuOH+	1.417e-14	1.299e-14	-13.849	-13.886	-0.038	(0)
CuSO4	4.265e-15	4.271e-15	-14.370	-14.369	0.001	13.16
CuCl+	2.491e-15	2.283e-15	-14.604	-14.642	-0.038	0.53
Cu(CO3)2-2	1.811e-16	1.279e-16	-15.742	-15.893	-0.151	(0)
CuF+	7.201e-17	6.601e-17	-16.143	-16.180	-0.038	(0)
CuCl2	4.928e-18	4.936e-18	-17.307	-17.307	0.001	31.70
Cu(OH)3-	7.098e-20	6.507e-20	-19.149	-19.187	-0.038	(0)
Cu2(OH)2+2	1.109e-22	7.834e-23	-21.955	-22.106	-0.151	(0)
CuCl3-	7.726e-23	7.080e-23	-22.112	-22.150	-0.038	(0)
Cu(OH)4-2	1.160e-25	8.190e-26	-24.936	-25.087	-0.151	(0)
CuCl4-2	2.024e-27	1.439e-27	-26.694	-26.842	-0.148	(0)
F	1.948e-05					
F-	1.914e-05	1.752e-05	-4.718	-4.756	-0.038	-1.26
MgF+	2.927e-07	2.685e-07	-6.534	-6.571	-0.037	-10.53
NaF	3.812e-08	3.818e-08	-7.419	-7.418	0.001	7.28
HF	4.204e-09	4.210e-09	-8.376	-8.376	0.001	12.53
AlF2+	2.503e-09	2.301e-09	-8.602	-8.638	-0.037	(0)
MnF+	7.427e-10	6.821e-10	-9.129	-9.166	-0.037	(0)
AlF3	5.070e-10	5.078e-10	-9.295	-9.294	0.001	(0)
AlF+2	3.660e-10	2.612e-10	-9.437	-9.583	-0.147	(0)
FeF+	4.446e-11	4.075e-11	-10.352	-10.390	-0.038	(0)
BF(OH)3-	2.241e-11	2.054e-11	-10.650	-10.687	-0.038	(0)
ZnF+	1.462e-11	1.340e-11	-10.835	-10.873	-0.038	(0)
AlF4-	3.862e-12	3.543e-12	-11.413	-11.451	-0.037	(0)
CdF+	7.640e-13	7.004e-13	-12.117	-12.155	-0.038	(0)
PbF+	6.977e-13	6.396e-13	-12.156	-12.194	-0.038	(0)
HF2-	3.102e-13	2.844e-13	-12.508	-12.546	-0.038	22.14
BF2(OH)2-	6.664e-15	6.109e-15	-14.176	-14.214	-0.038	(0)
PbF2	2.285e-16	2.288e-16	-15.641	-15.640	0.001	(0)
CuF+	7.201e-17	6.601e-17	-16.143	-16.180	-0.038	(0)
CdF2	3.078e-17	3.083e-17	-16.512	-16.511	0.001	(0)
PbF3-	3.168e-20	2.905e-20	-19.499	-19.537	-0.038	(0)
BF3OH-	2.007e-20	1.840e-20	-19.697	-19.735	-0.038	(0)
FeF+2	1.310e-20	9.320e-21	-19.883	-20.031	-0.148	(0)
FeF2+	7.130e-21	6.548e-21	-20.147	-20.184	-0.037	(0)
FeF3	1.819e-22	1.822e-22	-21.740	-21.739	0.001	(0)
PbF4-2	3.449e-25	2.436e-25	-24.462	-24.613	-0.151	(0)
BF4-	2.270e-25	2.081e-25	-24.644	-24.682	-0.038	(0)
SiF6-2	1.379e-29	9.811e-30	-28.860	-29.008	-0.148	42.80
Fe(2)	3.583e-07					
Fe+2	3.244e-07	2.326e-07	-6.489	-6.633	-0.145	-21.94
FeHCO3+	2.568e-08	2.354e-08	-7.590	-7.628	-0.038	(0)
FeSO4	4.225e-09	4.231e-09	-8.374	-8.374	0.001	18.35
FeCO3	1.688e-09	1.691e-09	-8.773	-8.772	0.001	(0)
FeCl+	1.401e-09	1.284e-09	-8.854	-8.891	-0.038	(0)
FeOH+	5.284e-10	4.852e-10	-9.277	-9.314	-0.037	(0)
FeHPO4	1.952e-10	1.955e-10	-9.709	-9.709	0.001	(0)
FeH2PO4+	6.814e-11	6.262e-11	-10.167	-10.203	-0.037	(0)
FeF+	4.446e-11	4.075e-11	-10.352	-10.390	-0.038	(0)
Fe(OH)2	2.740e-14	2.745e-14	-13.562	-13.562	0.001	(0)
FeHSO4+	4.819e-15	4.418e-15	-14.317	-14.355	-0.038	(0)
Fe(OH)3-	7.046e-18	6.471e-18	-17.152	-17.189	-0.037	(0)
Fe(3)	5.777e-14					
Fe(OH)2+	3.262e-14	2.998e-14	-13.487	-13.523	-0.037	(0)
Fe(OH)3	2.497e-14	2.501e-14	-13.603	-13.602	0.001	(0)
Fe(OH)4-	1.604e-16	1.474e-16	-15.795	-15.832	-0.037	(0)
FeOH+2	1.973e-17	1.403e-17	-16.705	-16.853	-0.148	(0)
FeF+2	1.310e-20	9.320e-21	-19.883	-20.031	-0.148	(0)

FeF2+	7.130e-21	6.548e-21	-20.147	-20.184	-0.037	(0)
Fe+3	6.696e-22	3.325e-22	-21.174	-21.478	-0.304	(0)
FeSO4+	4.071e-22	3.739e-22	-21.390	-21.427	-0.037	(0)
FeF3	1.819e-22	1.822e-22	-21.740	-21.739	0.001	(0)
FeH2PO4+2	6.738e-23	4.808e-23	-22.171	-22.318	-0.147	(0)
FeCl+2	5.756e-23	4.094e-23	-22.240	-22.388	-0.148	(0)
FeHPO4+	2.099e-23	1.927e-23	-22.678	-22.715	-0.037	(0)
Fe(SO4)2-	9.050e-25	8.296e-25	-24.043	-24.081	-0.038	(0)
FeCl2+	7.816e-25	7.178e-25	-24.107	-24.144	-0.037	(0)
FeCl3	2.867e-28	2.871e-28	-27.543	-27.542	0.001	(0)
FeHSO4+2	2.246e-28	1.587e-28	-27.648	-27.800	-0.151	(0)
Fe2(OH)2+4	2.078e-32	5.169e-33	-31.682	-32.287	-0.604	(0)
Fe3(OH)4+5	0.000e+00	0.000e+00	-42.570	-43.514	-0.944	(0)
H(0)	1.682e-13					
H2	8.409e-14	8.422e-14	-13.075	-13.075	0.001	28.61
K	1.535e-04					
K+	1.534e-04	1.405e-04	-3.814	-3.852	-0.038	9.07
KSO4-	1.098e-07	1.009e-07	-6.959	-6.996	-0.037	34.17
KHPO4-	6.292e-11	5.783e-11	-10.201	-10.238	-0.037	38.12
Mg	3.292e-04					
Mg+2	3.203e-04	2.294e-04	-3.494	-3.639	-0.145	-21.69
MgSO4	5.518e-06	5.527e-06	-5.258	-5.258	0.001	5.86
MgHCO3+	2.973e-06	2.724e-06	-5.527	-5.565	-0.038	5.53
MgF+	2.927e-07	2.685e-07	-6.534	-6.571	-0.037	-10.53
MgCO3	6.687e-08	6.697e-08	-7.175	-7.174	0.001	-17.09
MgHPO4	3.626e-08	3.632e-08	-7.441	-7.440	0.001	(0)
MgOH+	6.023e-09	5.547e-09	-8.220	-8.256	-0.036	(0)
MgH2PO4+	4.420e-09	4.063e-09	-8.355	-8.391	-0.037	(0)
MgPO4-	5.952e-10	5.470e-10	-9.225	-9.262	-0.037	(0)
Mn(2)	8.740e-06					
Mn+2	7.848e-06	5.627e-06	-5.105	-5.250	-0.145	-20.07
MnHCO3+	5.527e-07	5.076e-07	-6.258	-6.295	-0.037	(0)
MnCO3	1.353e-07	1.355e-07	-6.869	-6.868	0.001	(0)
MnSO4	1.023e-07	1.024e-07	-6.990	-6.990	0.001	22.28
MnCl+	9.985e-08	9.170e-08	-7.001	-7.038	-0.037	-2.91
MnOH+	1.043e-09	9.580e-10	-8.982	-9.019	-0.037	(0)
MnF+	7.427e-10	6.821e-10	-9.129	-9.166	-0.037	(0)
MnCl2	1.599e-10	1.601e-10	-9.796	-9.796	0.001	85.16
MnCl3-	1.921e-13	1.764e-13	-12.716	-12.753	-0.037	43.39
Mn(NO3)2	5.040e-17	5.048e-17	-16.298	-16.297	0.001	40.88
Mn(OH)3-	2.438e-20	2.239e-20	-19.613	-19.650	-0.037	(0)
Mn(3)	5.536e-33					
Mn+3	5.536e-33	2.749e-33	-32.257	-32.561	-0.304	(0)
N(-3)	6.428e-07					
NH4+	6.398e-07	5.844e-07	-6.194	-6.233	-0.039	18.02
NH3	2.189e-09	2.192e-09	-8.660	-8.659	0.001	24.44
NH4SO4-	8.310e-10	7.618e-10	-9.080	-9.118	-0.038	37.85
N(3)	2.857e-07					
NO2-	2.857e-07	2.612e-07	-6.544	-6.583	-0.039	25.04
N(5)	1.643e-06					
NO3-	1.643e-06	1.502e-06	-5.784	-5.823	-0.039	29.59
BaNO3+	2.219e-13	2.034e-13	-12.654	-12.692	-0.038	(0)
PbNO3+	4.975e-14	4.561e-14	-13.303	-13.341	-0.038	(0)
CdNO3+	1.284e-14	1.177e-14	-13.891	-13.929	-0.038	17.55
Mn(NO3)2	5.040e-17	5.048e-17	-16.298	-16.297	0.001	40.88
Na	4.221e-03					
Na+	4.126e-03	3.786e-03	-2.385	-2.422	-0.037	-1.37
NaCl	9.088e-05	9.102e-05	-4.042	-4.041	0.001	(0)
NaHCO3	2.144e-06	2.148e-06	-5.669	-5.668	0.001	1.80
NaSO4-	2.097e-06	1.928e-06	-5.678	-5.715	-0.037	14.15
NaF	3.812e-08	3.818e-08	-7.419	-7.418	0.001	7.28
NaCO3-	2.403e-08	2.203e-08	-7.619	-7.657	-0.038	-0.90
NaHPO4-	1.696e-09	1.559e-09	-8.771	-8.807	-0.037	33.93
NaOH	2.527e-20	2.530e-20	-19.597	-19.597	0.001	(0)
O(0)	0.000e+00					
O2	0.000e+00	0.000e+00	-66.038	-66.038	0.001	30.45
P	9.689e-07					
H2PO4-	5.845e-07	5.372e-07	-6.233	-6.270	-0.037	33.25

HPO4-2	2.969e-07	2.112e-07	-6.527	-6.675	-0.148	6.88
CaHPO4	3.862e-08	3.868e-08	-7.413	-7.412	0.001	(0)
MgHPO4	3.626e-08	3.632e-08	-7.441	-7.440	0.001	(0)
CaH2PO4+	4.999e-09	4.594e-09	-8.301	-8.338	-0.037	(0)
MgH2PO4+	4.420e-09	4.063e-09	-8.355	-8.391	-0.037	(0)
NaHPO4-	1.696e-09	1.559e-09	-8.771	-8.807	-0.037	33.93
CaPO4-	6.355e-10	5.840e-10	-9.197	-9.234	-0.037	(0)
MgPO4-	5.952e-10	5.470e-10	-9.225	-9.262	-0.037	(0)
FeHPO4	1.952e-10	1.955e-10	-9.709	-9.709	0.001	(0)
FeH2PO4+	6.814e-11	6.262e-11	-10.167	-10.203	-0.037	(0)
KHPO4-	6.292e-11	5.783e-11	-10.201	-10.238	-0.037	38.12
H3PO4	1.261e-11	1.263e-11	-10.899	-10.899	0.001	47.44
PO4-3	1.333e-12	6.078e-13	-11.875	-12.216	-0.341	-22.87
FeH2PO4+2	6.738e-23	4.808e-23	-22.171	-22.318	-0.147	(0)
FeHPO4+	2.099e-23	1.927e-23	-22.678	-22.715	-0.037	(0)
Pb	1.627e-08					
PbCO3	1.080e-08	1.081e-08	-7.967	-7.966	0.001	(0)
Pb+2	2.907e-09	2.053e-09	-8.537	-8.688	-0.151	-15.39
PbHCO3+	1.800e-09	1.650e-09	-8.745	-8.782	-0.038	(0)
PbCl+	3.619e-10	3.318e-10	-9.441	-9.479	-0.038	8.01
PbOH+	2.754e-10	2.525e-10	-9.560	-9.598	-0.038	(0)
PbSO4	1.166e-10	1.168e-10	-9.933	-9.933	0.001	(0)
Pb(CO3)2-2	1.166e-11	8.232e-12	-10.933	-11.085	-0.151	(0)
PbCl2	2.077e-12	2.080e-12	-11.683	-11.682	0.001	35.02
PbF+	6.977e-13	6.396e-13	-12.156	-12.194	-0.038	(0)
Pb(OH)2	6.187e-13	6.197e-13	-12.209	-12.208	0.001	(0)
Pb(SO4)2-2	8.783e-14	6.203e-14	-13.056	-13.207	-0.151	(0)
PbNO3+	4.975e-14	4.561e-14	-13.303	-13.341	-0.038	(0)
PbCl3-	7.237e-15	6.634e-15	-14.140	-14.178	-0.038	66.07
PbF2	2.285e-16	2.288e-16	-15.641	-15.640	0.001	(0)
Pb(OH)3-	4.896e-17	4.488e-17	-16.310	-16.348	-0.038	(0)
Pb2OH+3	2.538e-17	1.160e-17	-16.596	-16.935	-0.340	(0)
PbCl4-2	1.807e-17	1.276e-17	-16.743	-16.894	-0.151	101.63
PbF3-	3.168e-20	2.905e-20	-19.499	-19.537	-0.038	(0)
Pb(OH)4-2	9.184e-22	6.486e-22	-21.037	-21.188	-0.151	(0)
Pb3(OH)4+2	2.797e-23	1.976e-23	-22.553	-22.704	-0.151	(0)
PbF4-2	3.449e-25	2.436e-25	-24.462	-24.613	-0.151	(0)
PbBr+	0.000e+00	0.000e+00	-40.640	-40.677	-0.038	(0)
PbBr2	0.000e+00	0.000e+00	-74.776	-74.776	0.001	(0)
S(6)	1.562e-04					
SO4-2	1.424e-04	1.012e-04	-3.847	-3.995	-0.148	14.78
CaSO4	5.963e-06	5.973e-06	-5.225	-5.224	0.001	7.52
MgSO4	5.518e-06	5.527e-06	-5.258	-5.258	0.001	5.86
NaSO4-	2.097e-06	1.928e-06	-5.678	-5.715	-0.037	14.15
KSO4-	1.098e-07	1.009e-07	-6.959	-6.996	-0.037	34.17
MnSO4	1.023e-07	1.024e-07	-6.990	-6.990	0.001	22.28
BaSO4	5.447e-08	5.455e-08	-7.264	-7.263	0.001	(0)
FeSO4	4.225e-09	4.231e-09	-8.374	-8.374	0.001	18.35
HSO4-	1.723e-09	1.580e-09	-8.764	-8.801	-0.038	40.36
ZnSO4	1.279e-09	1.281e-09	-8.893	-8.892	0.001	21.62
NH4SO4-	8.310e-10	7.618e-10	-9.080	-9.118	-0.038	37.85
PbSO4	1.166e-10	1.168e-10	-9.933	-9.933	0.001	(0)
CdSO4	9.285e-11	9.299e-11	-10.032	-10.032	0.001	77.75
CaHSO4+	6.846e-12	6.276e-12	-11.165	-11.202	-0.038	(0)
Zn(SO4)2-2	1.485e-12	1.049e-12	-11.828	-11.979	-0.151	-12.40
AlSO4+	5.220e-13	4.789e-13	-12.282	-12.320	-0.037	(0)
Cd(SO4)2-2	1.456e-13	1.028e-13	-12.837	-12.988	-0.151	-105.12
Pb(SO4)2-2	8.783e-14	6.203e-14	-13.056	-13.207	-0.151	(0)
FeHSO4+	4.819e-15	4.418e-15	-14.317	-14.355	-0.038	(0)
CuSO4	4.265e-15	4.271e-15	-14.370	-14.369	0.001	13.16
Al(SO4)2-	1.675e-15	1.537e-15	-14.776	-14.813	-0.037	(0)
AlHSO4+2	9.581e-21	6.767e-21	-20.019	-20.170	-0.151	(0)
FeSO4+	4.071e-22	3.739e-22	-21.390	-21.427	-0.037	(0)
Fe(SO4)2-	9.050e-25	8.296e-25	-24.043	-24.081	-0.038	(0)
FeHSO4+2	2.246e-28	1.587e-28	-27.648	-27.800	-0.151	(0)
Si	3.746e-04					
H4SiO4	3.742e-04	3.748e-04	-3.427	-3.426	0.001	52.03
H3SiO4-	3.885e-07	3.560e-07	-6.411	-6.449	-0.038	28.04

H2SiO4-2	2.226e-13	1.589e-13	-12.652	-12.799	-0.147	(0)
SiF6-2	1.379e-29	9.811e-30	-28.860	-29.008	-0.148	42.80
Zn	8.876e-08					
Zn+2	7.557e-08	5.375e-08	-7.122	-7.270	-0.148	-25.24
ZnHCO3+	7.471e-09	6.849e-09	-8.127	-8.164	-0.038	(0)
ZnCO3	3.246e-09	3.251e-09	-8.489	-8.488	0.001	(0)
ZnSO4	1.279e-09	1.281e-09	-8.893	-8.892	0.001	21.62
ZnCl+	6.484e-10	5.942e-10	-9.188	-9.226	-0.038	-13.30
ZnOH+	4.244e-10	3.891e-10	-9.372	-9.410	-0.038	(0)
ZnOHCl	4.485e-11	4.492e-11	-10.348	-10.348	0.001	(0)
Zn(CO3)2-2	2.983e-11	2.106e-11	-10.525	-10.676	-0.151	(0)
Zn(OH)2	2.689e-11	2.693e-11	-10.570	-10.570	0.001	(0)
ZnF+	1.462e-11	1.340e-11	-10.835	-10.873	-0.038	(0)
ZnCl2	2.491e-12	2.495e-12	-11.604	-11.603	0.001	100.86
Zn(SO4)2-2	1.485e-12	1.049e-12	-11.828	-11.979	-0.151	-12.40
ZnCl3-	1.226e-14	1.124e-14	-13.911	-13.949	-0.038	17.04
Zn(OH)3-	5.860e-16	5.372e-16	-15.232	-15.270	-0.038	(0)
ZnCl4-2	3.183e-17	2.264e-17	-16.497	-16.645	-0.148	145.45
Zn(OH)4-2	7.605e-22	5.371e-22	-21.119	-21.270	-0.151	(0)
ZnBr+	0.000e+00	0.000e+00	-41.576	-41.614	-0.038	(0)
ZnBr2	0.000e+00	0.000e+00	-75.778	-75.778	0.001	(0)

----------Distribution of alkalinity----------

Total alkalinity (eq/kgw) = 1.114e-03

Species	Alkalinity	Molality	Alk/Mol
HCO3-	1.101e-03	1.101e-03	1.00
CaHCO3+	4.679e-06	4.679e-06	1.00
MgHCO3+	2.973e-06	2.973e-06	1.00
NaHCO3	2.144e-06	2.144e-06	1.00
CO3-2	8.495e-07	4.248e-07	2.00
MnHCO3+	5.527e-07	5.527e-07	1.00
H3SiO4-	3.885e-07	3.885e-07	1.00
CaCO3	3.401e-07	1.700e-07	2.00
HPO4-2	2.969e-07	2.969e-07	1.00
MnCO3	2.705e-07	1.353e-07	2.00
Al(OH)4-	2.559e-07	6.397e-08	4.00
H+	-1.713e-07	1.713e-07	-1.00
MgCO3	1.337e-07	6.687e-08	2.00
OH-	7.300e-08	7.300e-08	1.00
NaCO3-	4.805e-08	2.403e-08	2.00
CaHPO4	3.862e-08	3.862e-08	1.00
MgHPO4	3.626e-08	3.626e-08	1.00
FeHCO3+	2.568e-08	2.568e-08	1.00
PbCO3	2.159e-08	1.080e-08	2.00
Al(OH)3	1.466e-08	4.888e-09	3.00
H2BO3-	1.172e-08	1.172e-08	1.00
BaHCO3+	1.160e-08	1.160e-08	1.00
Al(OH)2+	1.097e-08	5.484e-09	2.00
ZnHCO3+	7.471e-09	7.471e-09	1.00
ZnCO3	6.491e-09	3.246e-09	2.00
MgOH+	6.023e-09	6.023e-09	1.00
HF	-4.204e-09	4.204e-09	-1.00
FeCO3	3.377e-09	1.688e-09	2.00
NH3	2.189e-09	2.189e-09	1.00
PbHCO3+	1.800e-09	1.800e-09	1.00
HSO4-	-1.723e-09	1.723e-09	-1.00
NaHPO4-	1.696e-09	1.696e-09	1.00
CaPO4-	1.271e-09	6.355e-10	2.00
MgPO4-	1.190e-09	5.952e-10	2.00
MnOH+	1.043e-09	1.043e-09	1.00
FeOH+	5.284e-10	5.284e-10	1.00
ZnOH+	4.244e-10	4.244e-10	1.00
CaOH+	3.774e-10	3.774e-10	1.00
BaCO3	3.404e-10	1.702e-10	2.00
PbOH+	2.754e-10	2.754e-10	1.00

FeHPO4	1.952e-10	1.952e-10	1.00
AlOH+2	1.356e-10	1.356e-10	1.00
Zn(CO3)2-2	1.193e-10	2.983e-11	4.00
CdHCO3+	1.108e-10	1.108e-10	1.00
KHPO4-	6.292e-11	6.292e-11	1.00
Zn(OH)2	5.377e-11	2.689e-11	2.00
Pb(CO3)2-2	4.662e-11	1.166e-11	4.00
ZnOHCl	4.485e-11	4.485e-11	1.00
H3PO4	-1.261e-11	1.261e-11	-1.00
CaHSO4+	-6.846e-12	6.846e-12	-1.00
CdOHCl	3.202e-12	3.202e-12	1.00
PO4-3	2.666e-12	1.333e-12	2.00
CdOH+	1.900e-12	1.900e-12	1.00
CdCO3	1.526e-12	7.632e-13	2.00
Pb(OH)2	1.237e-12	6.187e-13	2.00
CuCO3	6.692e-13	3.346e-13	2.00
H2SiO4-2	4.453e-13	2.226e-13	2.00
Cu(OH)2	3.418e-13	1.709e-13	2.00
HF2-	-3.102e-13	3.102e-13	-1.00
BaOH+	2.504e-13	2.504e-13	1.00
CuHCO3+	1.139e-13	1.139e-13	1.00
Fe(OH)2	5.481e-14	2.740e-14	2.00
Fe(OH)3	2.497e-14	2.497e-14	1.00
CuOH+	1.417e-14	1.417e-14	1.00
BF2(OH)2-	-6.664e-15	6.664e-15	-1.00
FeHSO4+	-4.819e-15	4.819e-15	-1.00
Cd(CO3)2-2	4.149e-15	1.037e-15	4.00
Zn(OH)3-	1.758e-15	5.860e-16	3.00
Cd(OH)2	1.127e-15	5.635e-16	2.00
Cu(CO3)2-2	7.243e-16	1.811e-16	4.00
Fe(OH)4-	3.207e-16	1.604e-16	2.00
Pb(OH)3-	1.469e-16	4.896e-17	3.00
Pb2OH+3	2.538e-17	2.538e-17	1.00
Fe(OH)3-	2.114e-17	7.046e-18	3.00
FeOH+2	-1.973e-17	1.973e-17	-1.00
Cu(OH)3-	2.129e-19	7.098e-20	3.00
Mn(OH)3-	7.313e-20	2.438e-20	3.00
Cd2OH+3	5.879e-20	5.879e-20	1.00
BF3OH-	-4.015e-20	2.007e-20	-2.00
FeF+2	-2.621e-20	1.310e-20	-2.00
NaOH	2.527e-20	2.527e-20	1.00
FeF2+	-1.426e-20	7.130e-21	-2.00
AlHSO4+2	-9.581e-21	9.581e-21	-1.00
Pb(OH)4-2	3.674e-21	9.184e-22	4.00
Zn(OH)4-2	3.042e-21	7.605e-22	4.00
Fe+3	-1.339e-21	6.696e-22	-2.00
Cd(OH)3-	1.307e-21	4.358e-22	3.00
FeSO4+	-8.142e-22	4.071e-22	-2.00
FeF3	-3.638e-22	1.819e-22	-2.00
Cu2(OH)2+2	2.219e-22	1.109e-22	2.00
FeH2PO4+2	-1.348e-22	6.738e-23	-2.00
FeCl+2	-1.151e-22	5.756e-23	-2.00
Pb3(OH)4+2	1.119e-22	2.797e-23	4.00
FeHPO4+	-2.099e-23	2.099e-23	-1.00
Fe(SO4)2-	-1.810e-24	9.050e-25	-2.00
FeCl2+	-1.563e-24	7.816e-25	-2.00
BF4-	-6.809e-25	2.270e-25	-3.00
Cu(OH)4-2	4.639e-25	1.160e-25	4.00
FeHSO4+2	-6.739e-28	2.246e-28	-3.00
FeCl3	-5.734e-28	2.867e-28	-2.00
Cd(OH)4-2	1.272e-28	3.180e-29	4.00
SiF6-2	-5.517e-29	1.379e-29	-4.00
Fe2(OH)2+4	-4.155e-32	2.078e-32	-2.00
Fe3(OH)4+5	-0.000e+00	0.000e+00	-2.00

-------------------------------Saturation indices--------------------------------

Phase	SI**	log IAP	log K(298 K, 1 atm)

Al(OH)3(a)	-2.19	8.57	10.76	Al(OH)3
Albite	-1.97	-19.93	-17.96	NaAlSi3O8
Alunite	-5.05	-6.53	-1.47	KAl3(SO4)2(OH)6
Anglesite	-4.90	-12.68	-7.79	PbSO4
Anhydrite	-3.19	-7.48	-4.28	CaSO4
Anorthite	-5.10	-24.80	-19.70	CaAl2Si2O8
Aragonite	-1.66	-10.00	-8.34	CaCO3
BaCl2	-12.99	-10.76	2.22	BaCl2
BaCl2:2H2O	-10.98	-10.76	0.21	BaCl2:2H2O
BaCl2:H2O	-11.59	-10.76	0.83	BaCl2:H2O
Barite	-0.13	-9.96	-9.84	BaSO4
Ca-Montmorillonite	1.34	-43.60	-44.94	Ca0.165Al2.33Si3.67O10(OH)2
Calcite	-1.52	-10.00	-8.48	CaCO3
Cd(OH)2	-8.55	5.10	13.65	Cd(OH)2
CdSiO3	-7.36	1.68	9.04	CdSiO3
CdSO4	-12.37	-12.49	-0.12	CdSO4
Cerussite	-2.08	-15.21	-13.12	PbCO3
Chalcedony	0.12	-3.43	-3.54	SiO2
Chlorite(14A)	-11.49	56.67	68.16	Mg5Al2Si3O10(OH)8
Chrysotile	-9.10	23.03	32.13	Mg3Si2O5(OH)4
CO2(g)	-1.97	-3.45	-1.48	CO2
Dolomite	-3.05	-20.16	-17.10	CaMg(CO3)2
Fe(OH)3(a)	-5.97	-1.08	4.89	Fe(OH)3
Fluorite	-2.40	-12.99	-10.59	CaF2
Gibbsite	0.50	8.57	8.08	Al(OH)3
Goethite	-0.06	-1.08	-1.02	FeOOH
Gypsum	-2.89	-7.48	-4.58	CaSO4:2H2O
H2(g)	-9.97	-13.07	-3.10	H2
H2O(g)	-1.49	-0.00	1.49	H2O
Halite	-6.39	-4.82	1.57	NaCl
Hausmannite	-25.91	34.97	60.88	Mn3O4
Hematite	1.90	-2.16	-4.05	Fe2O3
Hydroxyapatite	-6.76	-10.23	-3.47	Ca5(PO4)3OH
Illite	0.18	-40.00	-40.19	K0.6Mg0.25Al2.3Si3.5O10(OH)2
Jarosite-K	-26.22	-35.48	-9.26	KFe3(SO4)2(OH)6
K-feldspar	-0.83	-21.36	-20.53	KAlSi3O8
K-mica	5.77	18.38	12.62	KAl3Si3O10(OH)2
Kaolinite	2.91	10.29	7.38	Al2Si2O5(OH)4
Manganite	-12.03	13.31	25.34	MnOOH
Melanterite	-8.43	-10.63	-2.20	FeSO4:7H2O
NH3(g)	-10.44	-8.66	1.78	NH3
O2(g)	-63.14	-66.04	-2.90	O2
Otavite	-2.92	-15.02	-12.10	CdCO3
Pb(OH)2	-3.22	4.91	8.13	Pb(OH)2
Pyrochroite	-6.85	8.35	15.20	Mn(OH)2
Pyrolusite	-23.01	18.27	41.28	MnO2:H2O
Quartz	0.55	-3.43	-3.97	SiO2
Rhodochrosite	-0.64	-11.77	-11.13	MnCO3
Sepiolite	-6.10	9.64	15.74	Mg2Si3O7.5OH:3H2O
Sepiolite(d)	-9.02	9.64	18.66	Mg2Si3O7.5OH:3H2O
Siderite	-2.26	-13.15	-10.89	FeCO3
SiO2(a)	-0.72	-3.43	-2.71	SiO2
Smithsonite	-3.78	-13.79	-10.01	ZnCO3
Sylvite	-7.15	-6.25	0.90	KCl
Talc	-5.15	16.18	21.33	Mg3Si4O10(OH)2
Vivianite	-8.33	-44.33	-36.00	Fe3(PO4)2:8H2O
Willemite	-6.05	9.23	15.28	Zn2SiO4
Witherite	-3.93	-12.49	-8.56	BaCO3
Zn(OH)2(e)	-5.17	6.33	11.50	Zn(OH)2

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
For ideal gases, phi = 1.

Initial solution 39.

-----------------------------Solution composition------------------------------

Elements	Molality	Moles
Al	2.976e-07	2.976e-07
B	6.791e-05	6.791e-05
Ba	5.097e-07	5.097e-07
Br	3.619e-34	3.619e-34
Cd	5.961e-09	5.961e-09
Cu	7.459e-08	7.459e-08
F	3.421e-05	3.421e-05
Fe	6.267e-06	6.267e-06
Mn	6.553e-06	6.553e-06
N(-3)	1.149e-05	1.149e-05
N(3)	9.995e-07	9.995e-07
N(5)	9.995e-07	9.995e-07
P	1.550e-06	1.550e-06
Pb	1.125e-08	1.125e-08
Si	2.413e-04	2.413e-04
Zn	1.820e-07	1.820e-07

----------Description of solution----------

pH	= 7.000
pe	= 4.000
Specific Conductance (µS/cm, 25°C)	= 4
Density (g/cm³)	= 0.99706
Volume (L)	= 1.00298
Activity of water	= 1.000
Ionic strength (mol/kgw)	= 4.966e-05
Mass of water (kg)	= 1.000e+00
Total alkalinity (eq/kg)	= 3.761e-06
Temperature (°C)	= 25.00
Electrical balance (eq)	= -3.885e-06
Percent error, 100*(Cat-|An|)/(Cat+|An|)	= -5.18
Iterations	= 10 (417 overall)
Total H	= 1.110137e+02
Total O	= 5.550740e+01

----------Redox couples----------

Redox couple	pe	Eh (volts)
N(-3)/N(3)	5.5748	0.3298
N(-3)/N(5)	6.0023	0.3551
N(3)/N(5)	7.2850	0.4310

----------Distribution of species----------

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma	mole V cm³/mol
OH-	1.020e-07	1.012e-07	-6.991	-6.995	-0.004	-4.13
H+	1.008e-07	1.000e-07	-6.996	-7.000	-0.004	0.00
H2O	5.551e+01	1.000e+00	1.744	-0.000	0.000	18.07
Al	2.976e-07					
Al(OH)4-	2.637e-07	2.615e-07	-6.579	-6.583	-0.004	(0)
Al(OH)3	1.387e-08	1.388e-08	-7.858	-7.858	0.000	(0)
Al(OH)2+	9.494e-09	9.417e-09	-8.023	-8.026	-0.004	(0)
AlF2+	7.025e-09	6.968e-09	-8.153	-8.157	-0.004	(0)
AlF3	2.974e-09	2.974e-09	-8.527	-8.527	0.000	(0)
AlF+2	4.237e-10	4.101e-10	-9.373	-9.387	-0.014	(0)
AlOH+2	1.241e-10	1.202e-10	-9.906	-9.920	-0.014	-27.85
AlF4-	4.047e-11	4.014e-11	-10.393	-10.396	-0.004	(0)
Al+3	1.301e-12	1.210e-12	-11.886	-11.917	-0.032	-42.48
B	6.791e-05					
H3BO3	6.752e-05	6.752e-05	-4.171	-4.171	0.000	39.23
H2BO3-	3.917e-07	3.885e-07	-6.407	-6.411	-0.004	(0)
BF(OH)3-	9.188e-10	9.113e-10	-9.037	-9.040	-0.004	(0)
BF2(OH)2-	3.338e-13	3.310e-13	-12.477	-12.480	-0.004	(0)

BF3OH-	1.241e-18	1.231e-18	-17.906	-17.910	-0.004	(0)
BF4-	1.714e-23	1.700e-23	-22.766	-22.770	-0.004	(0)
Ba	5.097e-07					
Ba+2	5.097e-07	4.933e-07	-6.293	-6.307	-0.014	-12.84
BaOH+	1.685e-13	1.671e-13	-12.773	-12.777	-0.004	(0)
BaNO3+	6.207e-14	6.156e-14	-13.207	-13.211	-0.004	(0)
Br	3.619e-34					
Br-	3.619e-34	3.590e-34	-33.441	-33.445	-0.004	24.54
CdBr+	3.084e-40	3.059e-40	-39.511	-39.514	-0.004	(0)
PbBr+	1.946e-40	1.931e-40	-39.711	-39.714	-0.004	(0)
ZnBr+	0.000e+00	0.000e+00	-40.781	-40.784	-0.004	(0)
CdBr2	0.000e+00	0.000e+00	-72.229	-72.229	0.000	(0)
PbBr2	0.000e+00	0.000e+00	-73.489	-73.489	0.000	(0)
ZnBr2	0.000e+00	0.000e+00	-74.629	-74.629	0.000	(0)
Cd	5.961e-09					
Cd+2	5.954e-09	5.761e-09	-8.225	-8.239	-0.014	-18.84
CdOH+	4.832e-12	4.792e-12	-11.316	-11.319	-0.004	(0)
CdF+	2.479e-12	2.459e-12	-11.606	-11.609	-0.004	(0)
CdNO3+	1.447e-14	1.435e-14	-13.840	-13.843	-0.004	17.50
Cd(OH)2	2.574e-15	2.574e-15	-14.589	-14.589	0.000	(0)
CdF2	2.094e-16	2.094e-16	-15.679	-15.679	0.000	(0)
Cd2OH+3	1.456e-19	1.352e-19	-18.837	-18.869	-0.032	(0)
Cd(OH)3-	2.911e-21	2.888e-21	-20.536	-20.539	-0.004	(0)
Cd(OH)4-2	2.659e-28	2.574e-28	-27.575	-27.589	-0.014	(0)
CdBr+	3.084e-40	3.059e-40	-39.511	-39.514	-0.004	(0)
CdBr2	0.000e+00	0.000e+00	-72.229	-72.229	0.000	(0)
Cu(1)	1.204e-09					
Cu+	1.204e-09	1.195e-09	-8.919	-8.923	-0.004	(0)
Cu(2)	7.339e-08					
Cu(OH)2	4.756e-08	4.756e-08	-7.323	-7.323	0.000	(0)
Cu+2	2.352e-08	2.276e-08	-7.629	-7.643	-0.014	-26.70
CuOH+	2.295e-09	2.276e-09	-8.639	-8.643	-0.004	(0)
CuF+	1.416e-11	1.404e-11	-10.849	-10.853	-0.004	(0)
Cu2(OH)2+2	2.343e-12	2.267e-12	-11.630	-11.645	-0.014	(0)
Cu(OH)3-	2.889e-14	2.866e-14	-13.539	-13.543	-0.004	(0)
Cu(OH)4-2	5.908e-20	5.718e-20	-19.229	-19.243	-0.014	(0)
F	3.421e-05					
F-	3.418e-05	3.390e-05	-4.466	-4.470	-0.004	-1.34
AlF2+	7.025e-09	6.968e-09	-8.153	-8.157	-0.004	(0)
HF	5.084e-09	5.084e-09	-8.294	-8.294	0.000	12.50
AlF3	2.974e-09	2.974e-09	-8.527	-8.527	0.000	(0)
MnF+	1.499e-09	1.487e-09	-8.824	-8.828	-0.004	(0)
FeF+	1.418e-09	1.406e-09	-8.848	-8.852	-0.004	(0)
BF(OH)3-	9.188e-10	9.113e-10	-9.037	-9.040	-0.004	(0)
AlF+2	4.237e-10	4.101e-10	-9.373	-9.387	-0.014	(0)
ZnF+	8.402e-11	8.334e-11	-10.076	-10.079	-0.004	(0)
AlF4-	4.047e-11	4.014e-11	-10.393	-10.396	-0.004	(0)
CuF+	1.416e-11	1.404e-11	-10.849	-10.853	-0.004	(0)
PbF+	5.552e-12	5.506e-12	-11.256	-11.259	-0.004	(0)
CdF+	2.479e-12	2.459e-12	-11.606	-11.609	-0.004	(0)
HF2-	6.668e-13	6.614e-13	-12.176	-12.180	-0.004	22.04
BF2(OH)2-	3.338e-13	3.310e-13	-12.477	-12.480	-0.004	(0)
FeF2+	2.896e-13	2.873e-13	-12.538	-12.542	-0.004	(0)
FeF+2	2.199e-13	2.129e-13	-12.658	-12.672	-0.014	(0)
FeF3	1.544e-14	1.544e-14	-13.811	-13.811	0.000	(0)
PbF2	3.811e-15	3.811e-15	-14.419	-14.419	0.000	(0)
CdF2	2.094e-16	2.094e-16	-15.679	-15.679	0.000	(0)
BF3OH-	1.241e-18	1.231e-18	-17.906	-17.910	-0.004	(0)
PbF3-	9.438e-19	9.360e-19	-18.025	-18.029	-0.004	(0)
BF4-	1.714e-23	1.700e-23	-22.766	-22.770	-0.004	(0)
PbF4-2	1.570e-23	1.519e-23	-22.804	-22.818	-0.014	(0)
SiF6-2	5.722e-29	5.538e-29	-28.242	-28.257	-0.014	42.48
Fe(2)	4.312e-06					
Fe+2	4.286e-06	4.148e-06	-5.368	-5.382	-0.014	-22.22
FeOH+	1.323e-08	1.312e-08	-7.879	-7.882	-0.004	(0)
FeHPO4	9.560e-09	9.560e-09	-8.020	-8.020	0.000	(0)
FeH2PO4+	1.954e-09	1.938e-09	-8.709	-8.713	-0.004	(0)
FeF+	1.418e-09	1.406e-09	-8.848	-8.852	-0.004	(0)

Fe(OH)2	1.116e-12	1.116e-12	-11.952	-11.952	0.000	(0)
Fe(OH)3-	4.182e-16	4.148e-16	-15.379	-15.382	-0.004	(0)
Fe(3)	1.955e-06					
Fe(OH)3	1.091e-06	1.091e-06	-5.962	-5.962	0.000	(0)
Fe(OH)2+	8.539e-07	8.469e-07	-6.069	-6.072	-0.004	(0)
Fe(OH)4-	1.003e-08	9.951e-09	-7.999	-8.002	-0.004	(0)
FeOH+2	2.643e-10	2.558e-10	-9.578	-9.592	-0.014	(0)
FeF2+	2.896e-13	2.873e-13	-12.538	-12.542	-0.004	(0)
FeF+2	2.199e-13	2.129e-13	-12.658	-12.672	-0.014	(0)
FeF3	1.544e-14	1.544e-14	-13.811	-13.811	0.000	(0)
Fe+3	4.261e-15	3.961e-15	-14.370	-14.402	-0.032	(0)
FeH2PO4+2	1.027e-15	9.942e-16	-14.988	-15.003	-0.014	(0)
FeHPO4+	6.223e-16	6.172e-16	-15.206	-15.210	-0.004	(0)
Fe2(OH)2+4	2.008e-18	1.761e-18	-17.697	-17.754	-0.057	(0)
Fe3(OH)4+5	3.825e-22	3.116e-22	-21.417	-21.506	-0.089	(0)
H(0)	1.416e-25					
H2	7.079e-26	7.079e-26	-25.150	-25.150	0.000	28.61
Mn(2)	6.553e-06					
Mn+2	6.550e-06	6.339e-06	-5.184	-5.198	-0.014	-22.03
MnOH+	1.643e-09	1.629e-09	-8.784	-8.788	-0.004	(0)
MnF+	1.499e-09	1.487e-09	-8.824	-8.828	-0.004	(0)
Mn(NO3)2	2.480e-17	2.480e-17	-16.605	-16.605	0.000	41.04
Mn(OH)3-	1.013e-19	1.005e-19	-18.994	-18.998	-0.004	(0)
Mn(3)	2.107e-27					
Mn+3	2.107e-27	1.959e-27	-26.676	-26.708	-0.032	(0)
N(-3)	1.149e-05					
NH4+	1.143e-05	1.134e-05	-4.942	-4.946	-0.004	17.94
NH3	6.460e-08	6.460e-08	-7.190	-7.190	0.000	24.42
N(3)	9.995e-07					
NO2-	9.995e-07	9.914e-07	-6.000	-6.004	-0.004	24.94
N(5)	9.995e-07					
NO3-	9.995e-07	9.914e-07	-6.000	-6.004	-0.004	29.47
PbNO3+	1.350e-13	1.339e-13	-12.870	-12.873	-0.004	(0)
BaNO3+	6.207e-14	6.156e-14	-13.207	-13.211	-0.004	(0)
CdNO3+	1.447e-14	1.435e-14	-13.840	-13.843	-0.004	17.50
Mn(NO3)2	2.480e-17	2.480e-17	-16.605	-16.605	0.000	41.04
O(0)	0.000e+00					
O2	0.000e+00	0.000e+00	-42.080	-42.080	0.000	30.40
P	1.550e-06					
H2PO4-	9.400e-07	9.324e-07	-6.027	-6.030	-0.004	33.18
HPO4-2	5.982e-07	5.789e-07	-6.223	-6.237	-0.014	6.62
FeHPO4	9.560e-09	9.560e-09	-8.020	-8.020	0.000	(0)
FeH2PO4+	1.954e-09	1.938e-09	-8.709	-8.713	-0.004	(0)
H3PO4	1.373e-11	1.373e-11	-10.862	-10.862	0.000	47.41
PO4-3	2.810e-12	2.610e-12	-11.551	-11.583	-0.032	-23.45
FeH2PO4+2	1.027e-15	9.942e-16	-14.988	-15.003	-0.014	(0)
FeHPO4+	6.223e-16	6.172e-16	-15.206	-15.210	-0.004	(0)
Pb	1.125e-08					
Pb+2	9.438e-09	9.133e-09	-8.025	-8.039	-0.014	-15.63
PbOH+	1.795e-09	1.781e-09	-8.746	-8.749	-0.004	(0)
Pb(OH)2	6.928e-12	6.928e-12	-11.159	-11.159	0.000	(0)
PbF+	5.552e-12	5.506e-12	-11.256	-11.259	-0.004	(0)
PbNO3+	1.350e-13	1.339e-13	-12.870	-12.873	-0.004	(0)
PbF2	3.811e-15	3.811e-15	-14.419	-14.419	0.000	(0)
Pb(OH)3-	8.020e-16	7.955e-16	-15.096	-15.099	-0.004	(0)
Pb2OH+3	3.920e-16	3.641e-16	-15.407	-15.439	-0.032	(0)
PbF3-	9.438e-19	9.360e-19	-18.025	-18.029	-0.004	(0)
Pb(OH)4-2	1.883e-20	1.822e-20	-19.725	-19.739	-0.014	(0)
Pb3(OH)4+2	1.038e-20	1.004e-20	-19.984	-19.998	-0.014	(0)
PbF4-2	1.570e-23	1.519e-23	-22.804	-22.818	-0.014	(0)
PbBr+	1.946e-40	1.931e-40	-39.711	-39.714	-0.004	(0)
PbBr2	0.000e+00	0.000e+00	-73.489	-73.489	0.000	(0)
Si	2.413e-04					
H4SiO4	2.410e-04	2.410e-04	-3.618	-3.618	0.000	52.08
H3SiO4-	3.582e-07	3.553e-07	-6.446	-6.449	-0.004	27.95
H2SiO4-2	2.497e-13	2.417e-13	-12.603	-12.617	-0.014	(0)
SiF6-2	5.722e-29	5.538e-29	-28.242	-28.257	-0.014	42.48
Zn	1.820e-07					

Zn+2	1.798e-07	1.740e-07	-6.745	-6.759	-0.014	-25.45
ZnOH+	1.924e-09	1.908e-09	-8.716	-8.719	-0.004	(0)
Zn(OH)2	2.191e-10	2.191e-10	-9.659	-9.659	0.000	(0)
ZnF+	8.402e-11	8.334e-11	-10.076	-10.079	-0.004	(0)
Zn(OH)3-	6.985e-15	6.928e-15	-14.156	-14.159	-0.004	(0)
Zn(OH)4-2	1.135e-20	1.098e-20	-19.945	-19.959	-0.014	(0)
ZnBr+	0.000e+00	0.000e+00	-40.781	-40.784	-0.004	(0)
ZnBr2	0.000e+00	0.000e+00	-74.629	-74.629	0.000	(0)

----------Distribution of alkalinity----------

Total alkalinity (eq/kgw) = 3.761e-06

Species	Alkalinity	Molality	Alk/Mol
Fe(OH)3	1.091e-06	1.091e-06	1.00
Al(OH)4-	1.055e-06	2.637e-07	4.00
HPO4-2	5.982e-07	5.982e-07	1.00
H2BO3-	3.917e-07	3.917e-07	1.00
H3SiO4-	3.582e-07	3.582e-07	1.00
OH-	1.020e-07	1.020e-07	1.00
H+	-1.008e-07	1.008e-07	-1.00
Cu(OH)2	9.511e-08	4.756e-08	2.00
NH3	6.460e-08	6.460e-08	1.00
Al(OH)3	4.162e-08	1.387e-08	3.00
Fe(OH)4-	2.006e-08	1.003e-08	2.00
Al(OH)2+	1.899e-08	9.494e-09	2.00
FeOH+	1.323e-08	1.323e-08	1.00
FeHPO4	9.560e-09	9.560e-09	1.00
HF	-5.084e-09	5.084e-09	-1.00
CuOH+	2.295e-09	2.295e-09	1.00
ZnOH+	1.924e-09	1.924e-09	1.00
PbOH+	1.795e-09	1.795e-09	1.00
MnOH+	1.643e-09	1.643e-09	1.00
Zn(OH)2	4.382e-10	2.191e-10	2.00
FeOH+2	-2.643e-10	2.643e-10	-1.00
AlOH+2	1.241e-10	1.241e-10	1.00
Pb(OH)2	1.386e-11	6.928e-12	2.00
H3PO4	-1.373e-11	1.373e-11	-1.00
PO4-3	5.619e-12	2.810e-12	2.00
CdOH+	4.832e-12	4.832e-12	1.00
Cu2(OH)2+2	4.686e-12	2.343e-12	2.00
Fe(OH)2	2.233e-12	1.116e-12	2.00
HF2-	-6.668e-13	6.668e-13	-1.00
FeF2+	-5.793e-13	2.896e-13	-2.00
H2SiO4-2	4.995e-13	2.497e-13	2.00
FeF+2	-4.399e-13	2.199e-13	-2.00
BF2(OH)2-	-3.338e-13	3.338e-13	-1.00
BaOH+	1.685e-13	1.685e-13	1.00
Cu(OH)3-	8.668e-14	2.889e-14	3.00
FeF3	-3.087e-14	1.544e-14	-2.00
Zn(OH)3-	2.096e-14	6.985e-15	3.00
Fe+3	-8.523e-15	4.261e-15	-2.00
Cd(OH)2	5.147e-15	2.574e-15	2.00
Pb(OH)3-	2.406e-15	8.020e-16	3.00
FeH2PO4+2	-2.054e-15	1.027e-15	-2.00
Fe(OH)3-	1.255e-15	4.182e-16	3.00
FeHPO4+	-6.223e-16	6.223e-16	-1.00
Pb2OH+3	3.920e-16	3.920e-16	1.00
Fe2(OH)2+4	-4.015e-18	2.008e-18	-2.00
BF3OH-	-2.481e-18	1.241e-18	-2.00
Mn(OH)3-	3.039e-19	1.013e-19	3.00
Cu(OH)4-2	2.363e-19	5.908e-20	4.00
Cd2OH+3	1.456e-19	1.456e-19	1.00
Pb(OH)4-2	7.532e-20	1.883e-20	4.00
Zn(OH)4-2	4.539e-20	1.135e-20	4.00
Pb3(OH)4+2	4.151e-20	1.038e-20	4.00
Cd(OH)3-	8.734e-21	2.911e-21	3.00

Fe3(OH)4+5	-7.649e-22	3.825e-22	-2.00
BF4-	-5.141e-23	1.714e-23	-3.00
Cd(OH)4-2	1.064e-27	2.659e-28	4.00
SiF6-2	-2.289e-28	5.722e-29	-4.00

-----Saturation indices-----

Phase	SI**	log IAP	log K(298 K, 1 atm)	
Al(OH)3(a)	-1.72	9.08	10.80	Al(OH)3
Cd(OH)2	-7.89	5.76	13.65	Cd(OH)2
CdSiO3	-6.92	2.14	9.06	CdSiO3
Chalcedony	-0.07	-3.62	-3.55	SiO2
Fe(OH)3(a)	1.71	6.60	4.89	Fe(OH)3
Gibbsite	0.97	9.08	8.11	Al(OH)3
Goethite	7.60	6.60	-1.00	FeOOH
H2(g)	-22.05	-25.15	-3.10	H2
H2O(g)	-1.50	-0.00	1.50	H2O
Hausmannite	-12.62	48.41	61.03	Mn3O4
Hematite	17.20	13.20	-4.01	Fe2O3
Kaolinite	3.49	10.93	7.43	Al2Si2O5(OH)4
Manganite	-5.54	19.80	25.34	MnOOH
NH3(g)	-8.99	-7.19	1.80	NH3
O2(g)	-39.19	-42.08	-2.89	O2
Pb(OH)2	-2.19	5.96	8.15	Pb(OH)2
Pyrochroite	-6.40	8.80	15.20	Mn(OH)2
Pyrolusite	-10.58	30.80	41.38	MnO2:H2O
Quartz	0.36	-3.62	-3.98	SiO2
SiO2(a)	-0.91	-3.62	-2.71	SiO2
Vivianite	-3.31	-39.31	-36.00	Fe3(PO4)2:8H2O
Willemite	-4.47	10.86	15.33	Zn2SiO4
Zn(OH)2(e)	-4.26	7.24	11.50	Zn(OH)2

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
For ideal gases, phi = 1.

Initial solution 40.

-----Solution composition-----

Elements	Molality	Moles
Alkalinity	3.299e-03	3.299e-03
Ba	3.052e-06	3.052e-06
Ca	1.098e-03	1.098e-03
Cl	2.314e-04	2.314e-04
F	1.474e-05	1.474e-05
K	1.637e-04	1.637e-04
Mg	8.641e-04	8.641e-04
N(5)	2.857e-03	2.857e-03
Na	3.655e-04	3.655e-04
O(0)	5.002e-05	5.002e-05
S(6)	2.812e-06	2.812e-06
Si	1.092e-03	1.092e-03
Sr	6.279e-06	6.279e-06
Zn	1.530e-07	1.530e-07

-----Description of solution-----

pH	=	7.470
pe	=	7.037
Specific Conductance (µS/cm, 26°C)	=	568
Density (g/cm³)	=	0.99711
Volume (L)	=	1.00348
Activity of water	=	1.000
Ionic strength (mol/kgw)	=	7.285e-03
Mass of water (kg)	=	1.000e+00
Total carbon (mol/kg)	=	3.500e-03

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                    Total CO2 (mol/kg)  =   3.500e-03
                      Temperature (°C)  =  26.20
                Electrical balance (eq) =  -1.935e-03
 Percent error, 100*(Cat-|An|)/(Cat+|An|) = -18.02
                             Iterations  =   9 (426 overall)
                                Total H  = 1.110201e+02
                                Total O  = 5.552950e+01
```

----------Redox couples----------

Redox couple	pe	Eh (volts)
O(-2)/O(0)	12.8007	0.7603

----------Distribution of species----------

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma	mole V cm³/mol
OH-	3.584e-07	3.271e-07	-6.446	-6.485	-0.040	-4.01
H+	3.671e-08	3.388e-08	-7.435	-7.470	-0.035	0.00
H2O	5.551e+01	9.998e-01	1.744	-0.000	0.000	18.08
Ba	3.052e-06					
Ba+2	2.977e-06	2.080e-06	-5.526	-5.682	-0.156	-12.51
BaHCO3+	6.666e-08	6.092e-08	-7.176	-7.215	-0.039	(0)
BaCO3	4.583e-09	4.591e-09	-8.339	-8.338	0.001	-10.69
BaSO4	1.715e-09	1.718e-09	-8.766	-8.765	0.001	(0)
BaCl+	1.537e-09	1.405e-09	-8.813	-8.852	-0.039	(0)
BaNO3+	7.459e-10	6.817e-10	-9.127	-9.166	-0.039	(0)
BaOH+	2.271e-12	2.079e-12	-11.644	-11.682	-0.038	(0)
C(4)	3.500e-03					
HCO3-	3.211e-03	2.943e-03	-2.493	-2.531	-0.038	24.83
CO2	2.207e-04	2.210e-04	-3.656	-3.656	0.001	34.49
CaHCO3+	3.117e-05	2.860e-05	-4.506	-4.544	-0.037	9.76
MgHCO3+	2.251e-05	2.056e-05	-4.648	-4.687	-0.039	5.55
CO3-2	5.913e-06	4.171e-06	-5.228	-5.380	-0.152	-4.98
CaCO3	5.365e-06	5.374e-06	-5.270	-5.270	0.001	-14.59
MgCO3	2.404e-06	2.408e-06	-5.619	-5.618	0.001	-17.09
NaHCO3	5.474e-07	5.483e-07	-6.262	-6.261	0.001	1.80
SrHCO3+	2.185e-07	2.003e-07	-6.660	-6.698	-0.038	(0)
BaHCO3+	6.666e-08	6.092e-08	-7.176	-7.215	-0.039	(0)
ZnCO3	4.515e-08	4.523e-08	-7.345	-7.345	0.001	(0)
NaCO3-	3.011e-08	2.752e-08	-7.521	-7.560	-0.039	-0.84
ZnHCO3+	2.203e-08	2.013e-08	-7.657	-7.696	-0.039	(0)
SrCO3	1.176e-08	1.178e-08	-7.930	-7.929	0.001	-14.12
Zn(CO3)2-2	5.781e-09	4.033e-09	-8.238	-8.394	-0.156	(0)
BaCO3	4.583e-09	4.591e-09	-8.339	-8.338	0.001	-10.69
(CO2)2	9.313e-10	9.329e-10	-9.031	-9.030	0.001	68.98
Ca	1.098e-03					
Ca+2	1.061e-03	7.483e-04	-2.974	-3.126	-0.152	-17.96
CaHCO3+	3.117e-05	2.860e-05	-4.506	-4.544	-0.037	9.76
CaCO3	5.365e-06	5.374e-06	-5.270	-5.270	0.001	-14.59
CaSO4	2.210e-07	2.213e-07	-6.656	-6.655	0.001	7.54
CaOH+	4.009e-09	3.664e-09	-8.397	-8.436	-0.039	(0)
CaHSO4+	5.488e-14	5.016e-14	-13.261	-13.300	-0.039	(0)
Cl	2.314e-04					
Cl-	2.310e-04	2.109e-04	-3.636	-3.676	-0.039	18.16
NaCl	4.238e-07	4.245e-07	-6.373	-6.372	0.001	(0)
BaCl+	1.537e-09	1.405e-09	-8.813	-8.852	-0.039	(0)
ZnCl+	3.559e-11	3.251e-11	-10.449	-10.488	-0.039	-12.73
ZnOHCl	1.118e-11	1.120e-11	-10.952	-10.951	0.001	(0)
ZnCl2	7.202e-15	7.214e-15	-14.143	-14.142	0.001	99.72
ZnCl3-	1.882e-18	1.719e-18	-17.725	-17.765	-0.039	17.09
ZnCl4-2	2.609e-22	1.835e-22	-21.583	-21.736	-0.153	145.54
F	1.474e-05					
F-	1.417e-05	1.293e-05	-4.849	-4.888	-0.040	-1.25
MgF+	5.670e-07	5.186e-07	-6.246	-6.285	-0.039	-10.53
NaF	2.478e-09	2.483e-09	-8.606	-8.605	0.001	7.31

HF	6.706e-10	6.717e-10	-9.174	-9.173	0.001	12.55
ZnF+	1.103e-11	1.008e-11	-10.958	-10.997	-0.039	(0)
HF2-	3.681e-14	3.364e-14	-13.434	-13.473	-0.039	22.16
SiF6-2	1.297e-32	9.118e-33	-31.887	-32.040	-0.153	42.84
H(0)	1.352e-32					
H2	6.762e-33	6.774e-33	-32.170	-32.169	0.001	28.60
K	1.637e-04					
K+	1.637e-04	1.495e-04	-3.786	-3.825	-0.040	9.09
KSO4-	1.929e-09	1.768e-09	-8.715	-8.753	-0.038	34.18
Mg	8.641e-04					
Mg+2	8.383e-04	5.939e-04	-3.077	-3.226	-0.150	-21.70
MgHCO3+	2.251e-05	2.056e-05	-4.648	-4.687	-0.039	5.55
MgCO3	2.404e-06	2.408e-06	-5.619	-5.618	0.001	-17.09
MgF+	5.670e-07	5.186e-07	-6.246	-6.285	-0.039	-10.53
MgSO4	2.363e-07	2.367e-07	-6.627	-6.626	0.001	5.88
MgOH+	7.716e-08	7.087e-08	-7.113	-7.150	-0.037	(0)
N(5)	2.857e-03					
NO3-	2.857e-03	2.604e-03	-2.544	-2.584	-0.040	29.65
BaNO3+	7.459e-10	6.817e-10	-9.127	-9.166	-0.039	(0)
Na	3.655e-04					
Na+	3.645e-04	3.335e-04	-3.438	-3.477	-0.039	-1.34
NaHCO3	5.474e-07	5.483e-07	-6.262	-6.261	0.001	1.80
NaCl	4.238e-07	4.245e-07	-6.373	-6.372	0.001	(0)
NaCO3-	3.011e-08	2.752e-08	-7.521	-7.560	-0.039	-0.84
NaSO4-	3.030e-09	2.777e-09	-8.519	-8.556	-0.038	14.16
NaF	2.478e-09	2.483e-09	-8.606	-8.605	0.001	7.31
NaOH	1.089e-20	1.091e-20	-19.963	-19.962	0.001	(0)
O(0)	5.002e-05					
O2	2.501e-05	2.505e-05	-4.602	-4.601	0.001	30.49
S(6)	2.812e-06					
SO4-2	2.346e-06	1.648e-06	-5.630	-5.783	-0.153	14.86
MgSO4	2.363e-07	2.367e-07	-6.627	-6.626	0.001	5.88
CaSO4	2.210e-07	2.213e-07	-6.656	-6.655	0.001	7.54
NaSO4-	3.030e-09	2.777e-09	-8.519	-8.556	-0.038	14.16
KSO4-	1.929e-09	1.768e-09	-8.715	-8.753	-0.038	34.18
BaSO4	1.715e-09	1.718e-09	-8.766	-8.765	0.001	(0)
SrSO4	1.390e-09	1.392e-09	-8.857	-8.856	0.001	24.28
ZnSO4	2.116e-11	2.119e-11	-10.675	-10.674	0.001	21.53
HSO4-	6.100e-12	5.575e-12	-11.215	-11.254	-0.039	40.41
CaHSO4+	5.488e-14	5.016e-14	-13.261	-13.300	-0.039	(0)
Zn(SO4)2-2	4.032e-16	2.814e-16	-15.394	-15.551	-0.156	-11.89
Si	1.092e-03					
H4SiO4	1.087e-03	1.089e-03	-2.964	-2.963	0.001	51.98
H3SiO4-	5.404e-06	4.937e-06	-5.267	-5.306	-0.039	28.05
H2SiO4-2	1.518e-11	1.071e-11	-10.819	-10.970	-0.152	(0)
SiF6-2	1.297e-32	9.118e-33	-31.887	-32.040	-0.153	42.84
Sr	6.279e-06					
Sr+2	6.048e-06	4.270e-06	-5.218	-5.370	-0.151	-17.65
SrHCO3+	2.185e-07	2.003e-07	-6.660	-6.698	-0.038	(0)
SrCO3	1.176e-08	1.178e-08	-7.930	-7.929	0.001	-14.12
SrSO4	1.390e-09	1.392e-09	-8.857	-8.856	0.001	24.28
SrOH+	7.057e-12	6.462e-12	-11.151	-11.190	-0.038	(0)
Zn	1.530e-07					
Zn+2	7.729e-08	5.434e-08	-7.112	-7.265	-0.153	-25.27
ZnCO3	4.515e-08	4.523e-08	-7.345	-7.345	0.001	(0)
ZnHCO3+	2.203e-08	2.013e-08	-7.657	-7.696	-0.039	(0)
Zn(CO3)2-2	5.781e-09	4.033e-09	-8.238	-8.394	-0.156	(0)
ZnOH+	2.106e-09	1.925e-09	-8.677	-8.716	-0.039	(0)
Zn(OH)2	5.946e-10	5.956e-10	-9.226	-9.225	0.001	(0)
ZnCl+	3.559e-11	3.251e-11	-10.449	-10.488	-0.039	-12.73
ZnSO4	2.116e-11	2.119e-11	-10.675	-10.674	0.001	21.53
ZnOHCl	1.118e-11	1.120e-11	-10.952	-10.951	0.001	(0)
ZnF+	1.103e-11	1.008e-11	-10.958	-10.997	-0.039	(0)
Zn(OH)3-	6.081e-14	5.558e-14	-13.216	-13.255	-0.039	(0)
ZnCl2	7.202e-15	7.214e-15	-14.143	-14.142	0.001	99.72
Zn(SO4)2-2	4.032e-16	2.814e-16	-15.394	-15.551	-0.156	-11.89
ZnCl3-	1.882e-18	1.719e-18	-17.725	-17.765	-0.039	17.09
Zn(OH)4-2	3.725e-19	2.599e-19	-18.429	-18.585	-0.156	(0)

ZnCl4-2	2.609e-22	1.835e-22	-21.583	-21.736	-0.153	145.54

----------Distribution of alkalinity----------

Total alkalinity (eq/kgw) = 3.299e-03

Species	Alkalinity	Molality	Alk/Mol
HCO3-	3.211e-03	3.211e-03	1.00
CaHCO3+	3.117e-05	3.117e-05	1.00
MgHCO3+	2.251e-05	2.251e-05	1.00
CO3-2	1.183e-05	5.913e-06	2.00
CaCO3	1.073e-05	5.365e-06	2.00
H3SiO4-	5.404e-06	5.404e-06	1.00
MgCO3	4.808e-06	2.404e-06	2.00
NaHCO3	5.474e-07	5.474e-07	1.00
OH-	3.584e-07	3.584e-07	1.00
SrHCO3+	2.185e-07	2.185e-07	1.00
ZnCO3	9.030e-08	4.515e-08	2.00
MgOH+	7.716e-08	7.716e-08	1.00
BaHCO3+	6.666e-08	6.666e-08	1.00
NaCO3-	6.022e-08	3.011e-08	2.00
H+	-3.671e-08	3.671e-08	-1.00
SrCO3	2.352e-08	1.176e-08	2.00
Zn(CO3)2-2	2.312e-08	5.781e-09	4.00
ZnHCO3+	2.203e-08	2.203e-08	1.00
BaCO3	9.166e-09	4.583e-09	2.00
CaOH+	4.009e-09	4.009e-09	1.00
ZnOH+	2.106e-09	2.106e-09	1.00
Zn(OH)2	1.189e-09	5.946e-10	2.00
HF	-6.706e-10	6.706e-10	-1.00
H2SiO4-2	3.037e-11	1.518e-11	2.00
ZnOHCl	1.118e-11	1.118e-11	1.00
SrOH+	7.057e-12	7.057e-12	1.00
HSO4-	-6.100e-12	6.100e-12	-1.00
BaOH+	2.271e-12	2.271e-12	1.00
Zn(OH)3-	1.824e-13	6.081e-14	3.00
CaHSO4+	-5.488e-14	5.488e-14	-1.00
HF2-	-3.681e-14	3.681e-14	-1.00
Zn(OH)4-2	1.490e-18	3.725e-19	4.00
NaOH	1.089e-20	1.089e-20	1.00
SiF6-2	-5.188e-32	1.297e-32	-4.00

----------Saturation indices----------

Phase	SI**	log IAP	log K(299 K, 1 atm)	
Anhydrite	-4.62	-8.91	-4.29	CaSO4
Aragonite	-0.16	-8.51	-8.34	CaCO3
BaCl2	-15.25	-13.03	2.22	BaCl2
BaCl2:2H2O	-13.25	-13.03	0.22	BaCl2:2H2O
BaCl2:H2O	-13.86	-13.03	0.83	BaCl2:H2O
Barite	-1.63	-11.46	-9.83	BaSO4
Calcite	-0.02	-8.51	-8.49	CaCO3
Celestite	-4.49	-11.15	-6.66	SrSO4
Chalcedony	0.57	-2.96	-3.54	SiO2
Chrysotile	-2.84	29.21	32.05	Mg3Si2O5(OH)4
CO2(g)	-2.17	-3.66	-1.48	CO2
Dolomite	0.01	-17.11	-17.12	CaMg(CO3)2
Fluorite	-2.32	-12.90	-10.59	CaF2
Gypsum	-4.33	-8.91	-4.58	CaSO4:2H2O
H2(g)	-29.07	-32.17	-3.10	H2
H2O(g)	-1.47	-0.00	1.47	H2O
Halite	-8.72	-7.15	1.57	NaCl
O2(g)	-1.70	-4.60	-2.90	O2
Quartz	1.00	-2.96	-3.96	SiO2
Sepiolite	-1.19	14.54	15.73	Mg2Si3O7.5OH:3H2O
Sepiolite(d)	-4.12	14.54	18.66	Mg2Si3O7.5OH:3H2O

SiO2(a)	-0.26	-2.96	-2.70	SiO2
Smithsonite	-2.63	-12.64	-10.01	ZnCO3
Strontianite	-1.48	-10.75	-9.27	SrCO3
Sylvite	-8.41	-7.50	0.91	KCl
Talc	2.03	23.29	21.26	Mg3Si4O10(OH)2
Willemite	-2.84	12.39	15.23	Zn2SiO4
Witherite	-2.50	-11.06	-8.56	BaCO3
Zn(OH)2(e)	-3.83	7.67	11.50	Zn(OH)2

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
For ideal gases, phi = 1.

Initial solution 41.

-----------------------------Solution composition-----------------------------

Elements	Molality	Moles
Al	1.853e-06	1.853e-06
Alkalinity	1.957e-03	1.957e-03
Ba	1.238e-07	1.238e-07
Ca	4.741e-05	4.741e-05
Cl	3.385e-05	3.385e-05
F	1.685e-05	1.685e-05
Fe	5.373e-08	5.373e-08
K	9.208e-05	9.208e-05
Mg	8.228e-06	8.228e-06
N(5)	1.642e-05	1.642e-05
Na	1.958e-03	1.958e-03
O(0)	2.063e-04	2.063e-04
P	7.750e-06	7.750e-06
S(6)	1.770e-05	1.770e-05
Si	2.913e-04	2.913e-04
Sr	1.027e-06	1.027e-06
Zn	1.530e-07	1.530e-07

----------------------------Description of solution----------------------------

pH	= 9.170
pe	= 6.483
Specific Conductance (µS/cm, 27°C)	= 211
Density (g/cm³)	= 0.99668
Volume (L)	= 1.00353
Activity of water	= 1.000
Ionic strength (mol/kgw)	= 2.295e-03
Mass of water (kg)	= 1.000e+00
Total carbon (mol/kg)	= 1.724e-03
Total CO2 (mol/kg)	= 1.724e-03
Temperature (°C)	= 26.90
Electrical balance (eq)	= 1.023e-04
Percent error, 100*(Cat-|An|)/(Cat+|An|)	= 2.45
Iterations	= 7 (433 overall)
Total H	= 1.110152e+02
Total O	= 5.551293e+01

---------------------------------Redox couples---------------------------------

Redox couple	pe	Eh (volts)
O(-2)/O(0)	11.1970	0.6666

----------------------------Distribution of species----------------------------

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma	mole V cm³/mol
OH-	1.823e-05	1.728e-05	-4.739	-4.762	-0.023	-4.02
H+	7.103e-10	6.761e-10	-9.149	-9.170	-0.021	0.00

H2O	5.551e+01	9.999e-01	1.744	-0.000	0.000	18.08
Al	1.853e-06					
Al(OH)4-	1.853e-06	1.758e-06	-5.732	-5.755	-0.023	(0)
Al(OH)3	6.135e-10	6.138e-10	-9.212	-9.212	0.000	(0)
Al(OH)2+	2.585e-12	2.454e-12	-11.588	-11.610	-0.023	(0)
AlOH+2	2.213e-16	1.797e-16	-15.655	-15.745	-0.090	-27.78
AlF2+	1.483e-17	1.408e-17	-16.829	-16.851	-0.023	(0)
AlF3	2.830e-18	2.831e-18	-17.548	-17.548	0.000	(0)
AlF+2	2.148e-18	1.744e-18	-17.668	-17.758	-0.090	(0)
AlF4-	1.896e-20	1.798e-20	-19.722	-19.745	-0.023	(0)
Al+3	1.688e-20	1.081e-20	-19.773	-19.966	-0.193	-42.31
AlSO4+	5.226e-22	4.958e-22	-21.282	-21.305	-0.023	(0)
Al(SO4)2-	2.358e-25	2.237e-25	-24.627	-24.650	-0.023	(0)
AlHSO4+2	3.739e-32	3.024e-32	-31.427	-31.519	-0.092	(0)
Ba	1.238e-07					
Ba+2	1.162e-07	9.402e-08	-6.935	-7.027	-0.092	-12.59
BaCO3	5.431e-09	5.433e-09	-8.265	-8.265	0.000	-10.68
BaHCO3+	1.509e-09	1.431e-09	-8.821	-8.844	-0.023	(0)
BaSO4	6.663e-10	6.666e-10	-9.176	-9.176	0.000	(0)
BaCl+	1.019e-11	9.664e-12	-10.992	-11.015	-0.023	(0)
BaOH+	4.965e-12	4.712e-12	-11.304	-11.327	-0.023	(0)
BaNO3+	1.942e-13	1.842e-13	-12.712	-12.735	-0.023	(0)
C(4)	1.724e-03					
HCO3-	1.575e-03	1.495e-03	-2.803	-2.825	-0.023	24.83
CO3-2	1.326e-04	1.077e-04	-3.878	-3.968	-0.090	-5.08
CaCO3	6.111e-06	6.115e-06	-5.214	-5.214	0.000	-14.59
NaCO3-	4.305e-06	4.083e-06	-5.366	-5.389	-0.023	-0.85
CO2	2.222e-06	2.223e-06	-5.653	-5.653	0.000	34.53
NaHCO3	1.539e-06	1.540e-06	-5.813	-5.812	0.000	1.80
CaHCO3+	6.713e-07	6.375e-07	-6.173	-6.196	-0.022	9.75
MgCO3	6.275e-07	6.278e-07	-6.202	-6.202	0.000	-17.09
MgHCO3+	1.105e-07	1.048e-07	-6.957	-6.980	-0.023	5.54
Zn(CO3)2-2	8.229e-08	6.656e-08	-7.085	-7.177	-0.092	(0)
SrCO3	5.603e-08	5.606e-08	-7.252	-7.251	0.000	-14.12
ZnCO3	2.890e-08	2.891e-08	-7.539	-7.539	0.000	(0)
SrHCO3+	1.983e-08	1.882e-08	-7.703	-7.725	-0.023	(0)
BaCO3	5.431e-09	5.433e-09	-8.265	-8.265	0.000	-10.68
BaHCO3+	1.509e-09	1.431e-09	-8.821	-8.844	-0.023	(0)
ZnHCO3+	2.671e-10	2.533e-10	-9.573	-9.596	-0.023	(0)
(CO2)2	9.644e-14	9.650e-14	-13.016	-13.015	0.000	69.05
FeCO3	1.461e-16	1.462e-16	-15.835	-15.835	0.000	(0)
FeHCO3+	8.925e-18	8.464e-18	-17.049	-17.072	-0.023	(0)
Ca	4.741e-05					
Ca+2	4.003e-05	3.250e-05	-4.398	-4.488	-0.091	-18.07
CaCO3	6.111e-06	6.115e-06	-5.214	-5.214	0.000	-14.59
CaHCO3+	6.713e-07	6.375e-07	-6.173	-6.196	-0.022	9.75
CaPO4-	4.017e-07	3.814e-07	-6.396	-6.419	-0.023	(0)
CaHPO4	1.051e-07	1.052e-07	-6.978	-6.978	0.000	(0)
CaSO4	8.288e-08	8.292e-08	-7.082	-7.081	0.000	7.57
CaOH+	8.412e-09	7.977e-09	-8.075	-8.098	-0.023	(0)
CaH2PO4+	5.577e-11	5.294e-11	-10.254	-10.276	-0.023	(0)
CaHSO4+	3.995e-16	3.788e-16	-15.399	-15.422	-0.023	(0)
Cl	3.385e-05					
Cl-	3.350e-05	3.176e-05	-4.475	-4.498	-0.023	18.14
NaCl	3.564e-07	3.566e-07	-6.448	-6.448	0.000	(0)
BaCl+	1.019e-11	9.664e-12	-10.992	-11.015	-0.023	(0)
ZnOHCl	2.092e-12	2.093e-12	-11.679	-11.679	0.000	(0)
ZnCl+	1.318e-13	1.250e-13	-12.880	-12.903	-0.023	-12.08
ZnCl2	4.187e-18	4.189e-18	-17.378	-17.378	0.000	98.42
FeCl+	2.617e-21	2.481e-21	-20.582	-20.605	-0.023	(0)
ZnCl3-	1.592e-22	1.510e-22	-21.798	-21.821	-0.023	17.16
FeCl+2	2.288e-26	1.856e-26	-25.640	-25.731	-0.091	(0)
ZnCl4-2	3.007e-27	2.439e-27	-26.522	-26.613	-0.091	145.47
FeCl2+	2.613e-30	2.480e-30	-29.583	-29.606	-0.023	(0)
FeCl3	7.873e-36	7.877e-36	-35.104	-35.104	0.000	(0)
F	1.685e-05					
F-	1.682e-05	1.595e-05	-4.774	-4.797	-0.023	-1.28
NaF	1.698e-08	1.699e-08	-7.770	-7.770	0.000	7.33

MgF+	6.820e-09	6.470e-09	-8.166	-8.189	-0.023	-10.57
HF	1.672e-11	1.673e-11	-10.777	-10.776	0.000	12.58
ZnF+	3.273e-13	3.104e-13	-12.485	-12.508	-0.023	(0)
HF2-	1.095e-15	1.039e-15	-14.961	-14.984	-0.023	22.16
AlF2+	1.483e-17	1.408e-17	-16.829	-16.851	-0.023	(0)
AlF3	2.830e-18	2.831e-18	-17.548	-17.548	0.000	(0)
AlF+2	2.148e-18	1.744e-18	-17.668	-17.758	-0.090	(0)
AlF4-	1.896e-20	1.798e-20	-19.722	-19.745	-0.023	(0)
FeF+	9.518e-21	9.026e-21	-20.021	-20.044	-0.023	(0)
FeF+2	5.846e-22	4.742e-22	-21.233	-21.324	-0.091	(0)
FeF2+	3.244e-22	3.079e-22	-21.489	-21.512	-0.023	(0)
FeF3	7.827e-24	7.831e-24	-23.106	-23.106	0.000	(0)
SiF6-2	1.261e-39	1.023e-39	-38.899	-38.990	-0.091	42.74
Fe(2)	2.587e-16					
FeCO3	1.461e-16	1.462e-16	-15.835	-15.835	0.000	(0)
Fe+2	6.957e-17	5.660e-17	-16.158	-16.247	-0.090	-21.97
FeOH+	3.212e-17	3.049e-17	-16.493	-16.516	-0.023	(0)
FeHCO3+	8.925e-18	8.464e-18	-17.049	-17.072	-0.023	(0)
FeHPO4	1.283e-18	1.284e-18	-17.892	-17.891	0.000	(0)
Fe(OH)2	4.520e-19	4.522e-19	-18.345	-18.345	0.000	(0)
FeSO4	1.473e-19	1.474e-19	-18.832	-18.832	0.000	17.04
Fe(OH)3-	2.668e-20	2.532e-20	-19.574	-19.597	-0.023	(0)
FeF+	9.518e-21	9.026e-21	-20.021	-20.044	-0.023	(0)
FeCl+	2.617e-21	2.481e-21	-20.582	-20.605	-0.023	(0)
FeH2PO4+	1.835e-21	1.742e-21	-20.736	-20.759	-0.023	(0)
FeHSO4+	6.958e-28	6.598e-28	-27.158	-27.181	-0.023	(0)
Fe(3)	5.373e-08					
Fe(OH)4-	3.246e-08	3.081e-08	-7.489	-7.511	-0.023	(0)
Fe(OH)3	2.116e-08	2.117e-08	-7.674	-7.674	0.000	(0)
Fe(OH)2+	1.078e-10	1.023e-10	-9.967	-9.990	-0.023	(0)
FeOH+2	2.398e-16	1.945e-16	-15.620	-15.711	-0.091	(0)
FeF+2	5.846e-22	4.742e-22	-21.233	-21.324	-0.091	(0)
FeF2+	3.244e-22	3.079e-22	-21.489	-21.512	-0.023	(0)
FeHPO4+	3.133e-23	2.973e-23	-22.504	-22.527	-0.023	(0)
Fe+3	2.845e-23	1.823e-23	-22.546	-22.739	-0.193	(0)
FeF3	7.827e-24	7.831e-24	-23.106	-23.106	0.000	(0)
FeSO4+	3.107e-24	2.948e-24	-23.508	-23.530	-0.023	(0)
FeH2PO4+2	3.709e-25	3.012e-25	-24.431	-24.521	-0.090	(0)
FeCl+2	2.288e-26	1.856e-26	-25.640	-25.731	-0.091	(0)
Fe(SO4)2-	9.693e-28	9.192e-28	-27.014	-27.037	-0.023	(0)
FeCl2+	2.613e-30	2.480e-30	-29.583	-29.606	-0.023	(0)
Fe2(OH)2+4	2.202e-30	9.422e-31	-29.657	-30.026	-0.369	(0)
FeHSO4+2	6.600e-33	5.338e-33	-32.180	-32.273	-0.092	(0)
FeCl3	7.873e-36	7.877e-36	-35.104	-35.104	0.000	(0)
Fe3(OH)4+5	6.378e-38	1.693e-38	-37.195	-37.771	-0.576	(0)
H(0)	6.865e-35					
H2	3.432e-35	3.434e-35	-34.464	-34.464	0.000	28.60
K	9.208e-05					
K+	9.207e-05	8.728e-05	-4.036	-4.059	-0.023	9.08
KSO4-	9.445e-09	8.966e-09	-8.025	-8.047	-0.023	34.16
KHPO4-	1.021e-09	9.697e-10	-8.991	-9.013	-0.023	38.00
Mg	8.228e-06					
Mg+2	7.298e-06	5.935e-06	-5.137	-5.227	-0.090	-21.84
MgCO3	6.275e-07	6.278e-07	-6.202	-6.202	0.000	-17.09
MgHCO3+	1.105e-07	1.048e-07	-6.957	-6.980	-0.023	5.54
MgPO4-	9.896e-08	9.394e-08	-7.005	-7.027	-0.023	(0)
MgOH+	3.978e-08	3.779e-08	-7.400	-7.423	-0.022	(0)
MgHPO4	2.595e-08	2.597e-08	-7.586	-7.586	0.000	(0)
MgSO4	2.065e-08	2.066e-08	-7.685	-7.685	0.000	5.91
MgF+	6.820e-09	6.470e-09	-8.166	-8.189	-0.023	-10.57
MgH2PO4+	1.297e-11	1.231e-11	-10.887	-10.910	-0.023	(0)
N(5)	1.642e-05					
NO3-	1.642e-05	1.556e-05	-4.785	-4.808	-0.023	29.68
BaNO3+	1.942e-13	1.842e-13	-12.712	-12.735	-0.023	(0)
Na	1.958e-03					
Na+	1.951e-03	1.851e-03	-2.710	-2.733	-0.023	-1.36
NaCO3-	4.305e-06	4.083e-06	-5.366	-5.389	-0.023	-0.85
NaHCO3	1.539e-06	1.540e-06	-5.813	-5.812	0.000	1.80

NaCl	3.564e-07	3.566e-07	-6.448	-6.448	0.000	(0)
NaSO4-	1.399e-07	1.328e-07	-6.854	-6.877	-0.023	13.81
NaHPO4-	2.167e-08	2.057e-08	-7.664	-7.687	-0.023	33.55
NaF	1.698e-08	1.699e-08	-7.770	-7.770	0.000	7.33
NaOH	3.197e-18	3.199e-18	-17.495	-17.495	0.000	(0)
O(0)	2.063e-04					
O2	1.031e-04	1.032e-04	-3.987	-3.986	0.000	30.55
P	7.750e-06					
HPO4-2	7.024e-06	5.698e-06	-5.153	-5.244	-0.091	6.71
CaPO4-	4.017e-07	3.814e-07	-6.396	-6.419	-0.023	(0)
CaHPO4	1.051e-07	1.052e-07	-6.978	-6.978	0.000	(0)
MgPO4-	9.896e-08	9.394e-08	-7.005	-7.027	-0.023	(0)
H2PO4-	6.467e-08	6.139e-08	-7.189	-7.212	-0.023	33.18
MgHPO4	2.595e-08	2.597e-08	-7.586	-7.586	0.000	(0)
NaHPO4-	2.167e-08	2.057e-08	-7.664	-7.687	-0.023	33.55
PO4-3	6.363e-09	3.945e-09	-8.196	-8.404	-0.208	-23.28
KHPO4-	1.021e-09	9.697e-10	-8.991	-9.013	-0.023	38.00
CaH2PO4+	5.577e-11	5.294e-11	-10.254	-10.276	-0.023	(0)
MgH2PO4+	1.297e-11	1.231e-11	-10.887	-10.910	-0.023	(0)
H3PO4	6.247e-15	6.250e-15	-14.204	-14.204	0.000	47.51
FeHPO4	1.283e-18	1.284e-18	-17.892	-17.891	0.000	(0)
FeH2PO4+	1.835e-21	1.742e-21	-20.736	-20.759	-0.023	(0)
FeHPO4+	3.133e-23	2.973e-23	-22.504	-22.527	-0.023	(0)
FeH2PO4+2	3.709e-25	3.012e-25	-24.431	-24.521	-0.090	(0)
S(6)	1.770e-05					
SO4-2	1.744e-05	1.415e-05	-4.758	-4.849	-0.091	14.80
NaSO4-	1.399e-07	1.328e-07	-6.854	-6.877	-0.023	13.81
CaSO4	8.288e-08	8.292e-08	-7.082	-7.081	0.000	7.57
MgSO4	2.065e-08	2.066e-08	-7.685	-7.685	0.000	5.91
KSO4-	9.445e-09	8.966e-09	-8.025	-8.047	-0.023	34.16
SrSO4	2.174e-09	2.175e-09	-8.663	-8.663	0.000	24.31
BaSO4	6.663e-10	6.666e-10	-9.176	-9.176	0.000	(0)
ZnSO4	4.526e-12	4.528e-12	-11.344	-11.344	0.000	21.42
HSO4-	1.022e-12	9.695e-13	-11.990	-12.013	-0.023	40.41
Zn(SO4)2-2	6.345e-16	5.132e-16	-15.198	-15.290	-0.092	-11.51
CaHSO4+	3.995e-16	3.788e-16	-15.399	-15.422	-0.023	(0)
FeSO4	1.473e-19	1.474e-19	-18.832	-18.832	0.000	17.04
AlSO4+	5.226e-22	4.958e-22	-21.282	-21.305	-0.023	(0)
FeSO4+	3.107e-24	2.948e-24	-23.508	-23.530	-0.023	(0)
Al(SO4)2-	2.358e-25	2.237e-25	-24.627	-24.650	-0.023	(0)
Fe(SO4)2-	9.693e-28	9.192e-28	-27.014	-27.037	-0.023	(0)
FeHSO4+	6.958e-28	6.598e-28	-27.158	-27.181	-0.023	(0)
AlHSO4+2	3.739e-32	3.024e-32	-31.427	-31.519	-0.092	(0)
FeHSO4+2	6.600e-33	5.338e-33	-32.180	-32.273	-0.092	(0)
Si	2.913e-04					
H4SiO4	2.339e-04	2.340e-04	-3.631	-3.631	0.000	51.92
H3SiO4-	5.744e-05	5.447e-05	-4.241	-4.264	-0.023	28.03
H2SiO4-2	7.627e-09	6.194e-09	-8.118	-8.208	-0.090	(0)
SiF6-2	1.261e-39	1.023e-39	-38.899	-38.990	-0.091	42.74
Sr	1.027e-06					
Sr+2	9.492e-07	7.711e-07	-6.023	-6.113	-0.090	-17.78
SrCO3	5.603e-08	5.606e-08	-7.252	-7.251	0.000	-14.12
SrHCO3+	1.983e-08	1.882e-08	-7.703	-7.725	-0.023	(0)
SrSO4	2.174e-09	2.175e-09	-8.663	-8.663	0.000	24.31
SrOH+	6.163e-11	5.849e-11	-10.210	-10.233	-0.023	(0)
Zn	1.530e-07					
Zn(CO3)2-2	8.229e-08	6.656e-08	-7.085	-7.177	-0.092	(0)
Zn(OH)2	3.704e-08	3.706e-08	-7.431	-7.431	0.000	(0)
ZnCO3	2.890e-08	2.891e-08	-7.539	-7.539	0.000	(0)
ZnOH+	2.656e-09	2.519e-09	-8.576	-8.599	-0.023	(0)
Zn+2	1.659e-09	1.346e-09	-8.780	-8.871	-0.091	-25.43
ZnHCO3+	2.671e-10	2.533e-10	-9.573	-9.596	-0.023	(0)
Zn(OH)3-	1.828e-10	1.733e-10	-9.738	-9.761	-0.023	(0)
ZnSO4	4.526e-12	4.528e-12	-11.344	-11.344	0.000	21.42
ZnOHCl	2.092e-12	2.093e-12	-11.679	-11.679	0.000	(0)
ZnF+	3.273e-13	3.104e-13	-12.485	-12.508	-0.023	(0)
ZnCl+	1.318e-13	1.250e-13	-12.880	-12.903	-0.023	-12.08
Zn(OH)4-2	5.024e-14	4.063e-14	-13.299	-13.391	-0.092	(0)

Zn(SO4)2-2	6.345e-16	5.132e-16	-15.198	-15.290	-0.092	-11.51
ZnCl2	4.187e-18	4.189e-18	-17.378	-17.378	0.000	98.42
ZnCl3-	1.592e-22	1.510e-22	-21.798	-21.821	-0.023	17.16
ZnCl4-2	3.007e-27	2.439e-27	-26.522	-26.613	-0.091	145.47

----------Distribution of alkalinity----------

Total alkalinity (eq/kgw) = 1.957e-03

Species	Alkalinity	Molality	Alk/Mol
HCO3-	1.575e-03	1.575e-03	1.00
CO3-2	2.652e-04	1.326e-04	2.00
H3SiO4-	5.744e-05	5.744e-05	1.00
OH-	1.823e-05	1.823e-05	1.00
CaCO3	1.222e-05	6.111e-06	2.00
NaCO3-	8.610e-06	4.305e-06	2.00
Al(OH)4-	7.411e-06	1.853e-06	4.00
HPO4-2	7.024e-06	7.024e-06	1.00
NaHCO3	1.539e-06	1.539e-06	1.00
MgCO3	1.255e-06	6.275e-07	2.00
CaPO4-	8.035e-07	4.017e-07	2.00
CaHCO3+	6.713e-07	6.713e-07	1.00
Zn(CO3)2-2	3.292e-07	8.229e-08	4.00
MgPO4-	1.979e-07	9.896e-08	2.00
SrCO3	1.121e-07	5.603e-08	2.00
MgHCO3+	1.105e-07	1.105e-07	1.00
CaHPO4	1.051e-07	1.051e-07	1.00
Zn(OH)2	7.408e-08	3.704e-08	2.00
Fe(OH)4-	6.491e-08	3.246e-08	2.00
ZnCO3	5.779e-08	2.890e-08	2.00
MgOH+	3.978e-08	3.978e-08	1.00
MgHPO4	2.595e-08	2.595e-08	1.00
NaHPO4-	2.167e-08	2.167e-08	1.00
Fe(OH)3	2.116e-08	2.116e-08	1.00
SrHCO3+	1.983e-08	1.983e-08	1.00
H2SiO4-2	1.525e-08	7.627e-09	2.00
PO4-3	1.273e-08	6.363e-09	2.00
BaCO3	1.086e-08	5.431e-09	2.00
CaOH+	8.412e-09	8.412e-09	1.00
ZnOH+	2.656e-09	2.656e-09	1.00
Al(OH)3	1.840e-09	6.135e-10	3.00
BaHCO3+	1.509e-09	1.509e-09	1.00
KHPO4-	1.021e-09	1.021e-09	1.00
H+	-7.103e-10	7.103e-10	-1.00
Zn(OH)3-	5.483e-10	1.828e-10	3.00
ZnHCO3+	2.671e-10	2.671e-10	1.00
SrOH+	6.163e-11	6.163e-11	1.00
HF	-1.672e-11	1.672e-11	-1.00
Al(OH)2+	5.170e-12	2.585e-12	2.00
BaOH+	4.965e-12	4.965e-12	1.00
ZnOHCl	2.092e-12	2.092e-12	1.00
HSO4-	-1.022e-12	1.022e-12	-1.00
Zn(OH)4-2	2.009e-13	5.024e-14	4.00
H3PO4	-6.247e-15	6.247e-15	-1.00
HF2-	-1.095e-15	1.095e-15	-1.00
CaHSO4+	-3.995e-16	3.995e-16	-1.00
FeCO3	2.922e-16	1.461e-16	2.00
FeOH+2	-2.398e-16	2.398e-16	-1.00
AlOH+2	2.213e-16	2.213e-16	1.00
FeOH+	3.212e-17	3.212e-17	1.00
FeHCO3+	8.925e-18	8.925e-18	1.00
NaOH	3.197e-18	3.197e-18	1.00
FeHPO4	1.283e-18	1.283e-18	1.00
Fe(OH)2	9.040e-19	4.520e-19	2.00
Fe(OH)3-	8.003e-20	2.668e-20	3.00
FeF+2	-1.169e-21	5.846e-22	-2.00
FeF2+	-6.488e-22	3.244e-22	-2.00

Fe+3	-5.689e-23	2.845e-23	-2.00
FeHPO4+	-3.133e-23	3.133e-23	-1.00
FeF3	-1.565e-23	7.827e-24	-2.00
FeSO4+	-6.213e-24	3.107e-24	-2.00
FeH2PO4+2	-7.418e-25	3.709e-25	-2.00
FeCl+2	-4.577e-26	2.288e-26	-2.00
Fe(SO4)2-	-1.939e-27	9.693e-28	-2.00
FeHSO4+	-6.958e-28	6.958e-28	-1.00
FeCl2+	-5.227e-30	2.613e-30	-2.00
Fe2(OH)2+4	-4.404e-30	2.202e-30	-2.00
AlHSO4+2	-3.739e-32	3.739e-32	-1.00
FeHSO4+2	-1.980e-32	6.600e-33	-3.00
FeCl3	-1.575e-35	7.873e-36	-2.00
Fe3(OH)4+5	-1.276e-37	6.378e-38	-2.00
SiF6-2	-5.044e-39	1.261e-39	-4.00

----------Saturation indices----------

Phase	SI**	log IAP	log K(300 K, 1 atm)	
Al(OH)3(a)	-3.13	7.54	10.68	Al(OH)3
Albite	-1.50	-19.38	-17.88	NaAlSi3O8
Alunite	-17.00	-18.64	-1.63	KAl3(SO4)2(OH)6
Anhydrite	-5.04	-9.34	-4.30	CaSO4
Anorthite	-3.60	-23.26	-19.66	CaAl2Si2O8
Aragonite	-0.11	-8.46	-8.35	CaCO3
BaCl2	-18.24	-16.02	2.21	BaCl2
BaCl2:2H2O	-16.25	-16.02	0.22	BaCl2:2H2O
BaCl2:H2O	-16.85	-16.02	0.83	BaCl2:H2O
Barite	-2.05	-11.88	-9.83	BaSO4
Ca-Montmorillonite	-1.06	-45.81	-44.76	Ca0.165Al2.33Si3.67O10(OH)2
Calcite	0.03	-8.46	-8.49	CaCO3
Celestite	-4.29	-10.96	-6.67	SrSO4
Chalcedony	-0.10	-3.63	-3.53	SiO2
Chlorite(14A)	2.09	69.76	67.68	Mg5Al2Si3O10(OH)8
Chrysotile	0.11	32.08	31.97	Mg3Si2O5(OH)4
CO2(g)	-4.16	-5.65	-1.49	CO2
Dolomite	-0.52	-17.65	-17.13	CaMg(CO3)2
Fe(OH)3(a)	-0.12	4.77	4.89	Fe(OH)3
Fluorite	-3.50	-14.08	-10.58	CaF2
Gibbsite	-0.46	7.54	8.00	Al(OH)3
Goethite	5.84	4.77	-1.07	FeOOH
Gypsum	-4.75	-9.34	-4.58	CaSO4:2H2O
H2(g)	-31.36	-34.46	-3.11	H2
H2O(g)	-1.45	-0.00	1.45	H2O
Halite	-8.80	-7.23	1.57	NaCl
Hematite	13.69	9.54	-4.15	Fe2O3
Hydroxyapatite	2.10	-1.49	-3.59	Ca5(PO4)3OH
Illite	-0.68	-40.69	-40.01	K0.6Mg0.25Al2.3Si3.5O10(OH)2
Jarosite-K	-17.60	-26.96	-9.36	KFe3(SO4)2(OH)6
K-feldspar	-0.28	-20.71	-20.43	KAlSi3O8
K-mica	4.42	16.85	12.43	KAl3Si3O10(OH)2
Kaolinite	0.56	7.83	7.27	Al2Si2O5(OH)4
Melanterite	-18.91	-21.10	-2.19	FeSO4:7H2O
O2(g)	-1.08	-3.99	-2.91	O2
Quartz	0.32	-3.63	-3.95	SiO2
Sepiolite	-0.38	15.33	15.71	Mg2Si3O7.5OH:3H2O
Sepiolite(d)	-3.33	15.33	18.66	Mg2Si3O7.5OH:3H2O
Siderite	-9.31	-20.22	-10.90	FeCO3
SiO2(a)	-0.93	-3.63	-2.70	SiO2
Smithsonite	-2.82	-12.84	-10.02	ZnCO3
Strontianite	-0.81	-10.08	-9.27	SrCO3
Sylvite	-9.47	-8.56	0.91	KCl
Talc	3.63	24.82	21.18	Mg3Si4O10(OH)2
Vivianite	-29.55	-65.55	-36.00	Fe3(PO4)2:8H2O
Willemite	0.13	15.31	15.18	Zn2SiO4
Witherite	-2.44	-10.99	-8.56	BaCO3
Zn(OH)2(e)	-2.03	9.47	11.50	Zn(OH)2

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
  For ideal gases, phi = 1.

Initial solution 42.

-----------------------------Solution composition------------------------------

Elements	Molality	Moles
Alkalinity	1.303e-03	1.303e-03
Ba	1.580e-06	1.580e-06
Ca	3.743e-04	3.743e-04
Cl	8.463e-05	8.463e-05
F	7.370e-06	7.370e-06
K	1.100e-04	1.100e-04
Mg	2.345e-04	2.345e-04
Mn	3.641e-07	3.641e-07
N(5)	7.855e-04	7.855e-04
Na	4.002e-04	4.002e-04
O(0)	2.625e-04	2.625e-04
P	3.229e-06	3.229e-06
S(6)	2.915e-06	2.915e-06
Si	4.378e-04	4.378e-04
Sr	1.370e-06	1.370e-06
Zn	6.120e-07	6.120e-07

----------------------------Description of solution----------------------------

pH	= 6.330
pe	= 8.149
Specific Conductance (µS/cm, 31°C)	= 229
Density (g/cm³)	= 0.99564
Volume (L)	= 1.00464
Activity of water	= 1.000
Ionic strength (mol/kgw)	= 2.560e-03
Mass of water (kg)	= 1.000e+00
Total carbon (mol/kg)	= 2.515e-03
Total CO2 (mol/kg)	= 2.515e-03
Temperature (°C)	= 30.50
Electrical balance (eq)	= -4.537e-04
Percent error, 100*(Cat-|An|)/(Cat+|An|)	= -11.61
Iterations	= 11 (444 overall)
Total H	= 1.110155e+02
Total O	= 5.551694e+01

---------------------------------Redox couples---------------------------------

Redox couple	pe	Eh (volts)
O(-2)/O(0)	13.7722	0.8297

----------------------------Distribution of species----------------------------

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma	mole V cm³/mol
H+	4.928e-07	4.677e-07	-6.307	-6.330	-0.023	0.00
OH-	3.444e-08	3.254e-08	-7.463	-7.488	-0.025	-3.92
H2O	5.551e+01	9.999e-01	1.744	-0.000	0.000	18.10
Ba	1.580e-06					
Ba+2	1.560e-06	1.247e-06	-5.807	-5.904	-0.097	-12.41
BaHCO3+	1.840e-08	1.739e-08	-7.735	-7.760	-0.024	(0)
BaSO4	1.342e-09	1.342e-09	-8.872	-8.872	0.000	(0)
BaCl+	3.592e-10	3.395e-10	-9.445	-9.469	-0.024	(0)
BaNO3+	1.232e-10	1.164e-10	-9.910	-9.934	-0.024	(0)
BaCO3	9.782e-11	9.787e-11	-10.010	-10.009	0.000	-10.65
BaOH+	9.545e-14	9.031e-14	-13.020	-13.044	-0.024	(0)

C(4)	2.515e-03					
HCO3-	1.293e-03	1.224e-03	-2.888	-2.912	-0.024	25.06
CO2	1.213e-03	1.213e-03	-2.916	-2.916	0.000	34.70
CaHCO3+	5.256e-06	4.977e-06	-5.279	-5.303	-0.024	9.87
MgHCO3+	2.895e-06	2.736e-06	-5.538	-5.563	-0.024	5.62
NaHCO3	2.523e-07	2.525e-07	-6.598	-6.598	0.000	1.80
CO3-2	1.696e-07	1.361e-07	-6.771	-6.866	-0.096	-4.89
CaCO3	7.621e-08	7.626e-08	-7.118	-7.118	0.000	-14.58
ZnHCO3+	6.914e-08	6.536e-08	-7.160	-7.185	-0.024	(0)
(CO2)2	3.220e-08	3.222e-08	-7.492	-7.492	0.000	69.40
MnHCO3+	3.063e-08	2.898e-08	-7.514	-7.538	-0.024	(0)
MgCO3	2.624e-08	2.626e-08	-7.581	-7.581	0.000	-17.09
SrHCO3+	2.575e-08	2.437e-08	-7.589	-7.613	-0.024	(0)
BaHCO3+	1.840e-08	1.739e-08	-7.735	-7.760	-0.024	(0)
ZnCO3	1.151e-08	1.151e-08	-7.939	-7.939	0.000	(0)
MnCO3	2.869e-09	2.871e-09	-8.542	-8.542	0.000	(0)
NaCO3-	1.331e-09	1.258e-09	-8.876	-8.900	-0.024	-0.58
SrCO3	1.101e-10	1.102e-10	-9.958	-9.958	0.000	-14.11
BaCO3	9.782e-11	9.787e-11	-10.010	-10.009	0.000	-10.65
Zn(CO3)2-2	4.194e-11	3.350e-11	-10.377	-10.475	-0.098	(0)
Ca	3.743e-04					
Ca+2	3.688e-04	2.958e-04	-3.433	-3.529	-0.096	-18.04
CaHCO3+	5.256e-06	4.977e-06	-5.279	-5.303	-0.024	9.87
CaSO4	1.176e-07	1.177e-07	-6.930	-6.929	0.000	7.69
CaCO3	7.621e-08	7.626e-08	-7.118	-7.118	0.000	-14.58
CaHPO4	6.144e-08	6.147e-08	-7.212	-7.211	0.000	(0)
CaH2PO4+	2.222e-08	2.103e-08	-7.653	-7.677	-0.024	(0)
CaPO4-	3.638e-10	3.443e-10	-9.439	-9.463	-0.024	(0)
CaOH+	1.110e-10	1.049e-10	-9.955	-9.979	-0.024	(0)
CaHSO4+	4.154e-13	3.927e-13	-12.382	-12.406	-0.024	(0)
Cl	8.463e-05					
Cl-	8.444e-05	7.981e-05	-4.073	-4.098	-0.025	18.22
NaCl	1.875e-07	1.876e-07	-6.727	-6.727	0.000	(0)
BaCl+	3.592e-10	3.395e-10	-9.445	-9.469	-0.024	(0)
ZnCl+	1.223e-10	1.156e-10	-9.913	-9.937	-0.024	-8.89
MnCl+	9.127e-11	8.635e-11	-10.040	-10.064	-0.024	-1.88
ZnOHCl	2.395e-12	2.396e-12	-11.621	-11.621	0.000	(0)
ZnCl2	9.866e-15	9.872e-15	-14.006	-14.006	0.000	92.07
MnCl2	3.006e-15	3.008e-15	-14.522	-14.522	0.000	79.64
ZnCl3-	9.660e-19	9.131e-19	-18.015	-18.039	-0.024	17.46
MnCl3-	6.989e-20	6.612e-20	-19.156	-19.180	-0.024	43.15
ZnCl4-2	4.757e-23	3.812e-23	-22.323	-22.419	-0.096	145.88
F	7.370e-06					
F-	7.265e-06	6.865e-06	-5.139	-5.163	-0.025	-1.27
MgF+	9.829e-08	9.296e-08	-7.007	-7.032	-0.024	-10.58
HF	5.319e-09	5.322e-09	-8.274	-8.274	0.000	12.73
NaF	1.493e-09	1.494e-09	-8.826	-8.826	0.000	7.45
ZnF+	4.656e-11	4.401e-11	-10.332	-10.356	-0.024	(0)
MnF+	1.333e-11	1.261e-11	-10.875	-10.899	-0.024	(0)
HF2-	1.542e-13	1.458e-13	-12.812	-12.836	-0.024	22.29
SiF6-2	2.521e-30	2.020e-30	-29.599	-29.695	-0.096	42.92
H(0)	1.477e-32					
H2	7.386e-33	7.390e-33	-32.132	-32.131	0.000	28.60
K	1.100e-04					
K+	1.100e-04	1.039e-04	-3.959	-3.983	-0.025	9.19
KSO4-	1.821e-09	1.724e-09	-8.740	-8.764	-0.024	34.24
KHPO4-	7.338e-11	6.945e-11	-10.134	-10.158	-0.024	37.76
Mg	2.345e-04					
Mg+2	2.313e-04	1.859e-04	-3.636	-3.731	-0.095	-21.96
MgHCO3+	2.895e-06	2.736e-06	-5.538	-5.563	-0.024	5.62
MgSO4	1.075e-07	1.076e-07	-6.969	-6.968	0.000	6.03
MgF+	9.829e-08	9.296e-08	-7.007	-7.032	-0.024	-10.58
MgHPO4	5.220e-08	5.223e-08	-7.282	-7.282	0.000	(0)
MgCO3	2.624e-08	2.626e-08	-7.581	-7.581	0.000	-17.09
MgH2PO4+	1.778e-08	1.683e-08	-7.750	-7.774	-0.024	(0)
MgOH+	2.480e-09	2.349e-09	-8.606	-8.629	-0.024	(0)
MgPO4-	3.083e-10	2.918e-10	-9.511	-9.535	-0.024	(0)
Mn(2)	3.641e-07					

Mn+2	3.304e-07	2.656e-07	-6.481	-6.576	-0.095	-20.53
MnHCO3+	3.063e-08	2.898e-08	-7.514	-7.538	-0.024	(0)
MnCO3	2.869e-09	2.871e-09	-8.542	-8.542	0.000	(0)
MnSO4	1.124e-10	1.125e-10	-9.949	-9.949	0.000	20.29
MnCl+	9.127e-11	8.635e-11	-10.040	-10.064	-0.024	-1.88
MnOH+	2.396e-11	2.267e-11	-10.621	-10.645	-0.024	(0)
MnF+	1.333e-11	1.261e-11	-10.875	-10.899	-0.024	(0)
Mn(NO3)2	5.746e-13	5.749e-13	-12.241	-12.240	0.000	39.68
MnCl2	3.006e-15	3.008e-15	-14.522	-14.522	0.000	79.64
MnCl3-	6.989e-20	6.612e-20	-19.156	-19.180	-0.024	43.15
Mn(OH)3-	4.347e-23	4.113e-23	-22.362	-22.386	-0.024	(0)
Mn(3)	4.071e-24					
Mn+3	4.071e-24	2.545e-24	-23.390	-23.594	-0.204	(0)
N(5)	7.855e-04					
NO3-	7.855e-04	7.418e-04	-3.105	-3.130	-0.025	29.99
BaNO3+	1.232e-10	1.164e-10	-9.910	-9.934	-0.024	(0)
Mn(NO3)2	5.746e-13	5.749e-13	-12.241	-12.240	0.000	39.68
Na	4.002e-04					
Na+	3.998e-04	3.781e-04	-3.398	-3.422	-0.024	-1.18
NaHCO3	2.523e-07	2.525e-07	-6.598	-6.598	0.000	1.80
NaCl	1.875e-07	1.876e-07	-6.727	-6.727	0.000	(0)
NaSO4-	4.451e-09	4.213e-09	-8.352	-8.375	-0.024	13.69
NaF	1.493e-09	1.494e-09	-8.826	-8.826	0.000	7.45
NaCO3-	1.331e-09	1.258e-09	-8.876	-8.900	-0.024	-0.58
NaHPO4-	2.670e-10	2.527e-10	-9.574	-9.597	-0.024	33.49
NaOH	1.230e-21	1.230e-21	-20.910	-20.910	0.000	(0)
O(0)	2.625e-04					
O2	1.313e-04	1.313e-04	-3.882	-3.882	0.000	30.80
P	3.229e-06					
H2PO4-	2.646e-06	2.505e-06	-5.577	-5.601	-0.024	33.10
HPO4-2	4.277e-07	3.427e-07	-6.369	-6.465	-0.096	6.58
CaHPO4	6.144e-08	6.147e-08	-7.212	-7.211	0.000	(0)
MgHPO4	5.220e-08	5.223e-08	-7.282	-7.282	0.000	(0)
CaH2PO4+	2.222e-08	2.103e-08	-7.653	-7.677	-0.024	(0)
MgH2PO4+	1.778e-08	1.683e-08	-7.750	-7.774	-0.024	(0)
CaPO4-	3.638e-10	3.443e-10	-9.439	-9.463	-0.024	(0)
MgPO4-	3.083e-10	2.918e-10	-9.511	-9.535	-0.024	(0)
NaHPO4-	2.670e-10	2.527e-10	-9.574	-9.597	-0.024	33.49
H3PO4	1.839e-10	1.840e-10	-9.736	-9.735	0.000	47.68
KHPO4-	7.338e-11	6.945e-11	-10.134	-10.158	-0.024	37.76
PO4-3	6.104e-13	3.679e-13	-12.214	-12.434	-0.220	-23.59
S(6)	2.915e-06					
SO4-2	2.682e-06	2.148e-06	-5.572	-5.668	-0.096	15.19
CaSO4	1.176e-07	1.177e-07	-6.930	-6.929	0.000	7.69
MgSO4	1.075e-07	1.076e-07	-6.969	-6.968	0.000	6.03
NaSO4-	4.451e-09	4.213e-09	-8.352	-8.375	-0.024	13.69
KSO4-	1.821e-09	1.724e-09	-8.740	-8.764	-0.024	34.24
BaSO4	1.342e-09	1.342e-09	-8.872	-8.872	0.000	(0)
SrSO4	4.810e-10	4.813e-10	-9.318	-9.318	0.000	24.43
ZnSO4	2.225e-10	2.226e-10	-9.653	-9.652	0.000	20.90
HSO4-	1.168e-10	1.104e-10	-9.932	-9.957	-0.024	40.62
MnSO4	1.124e-10	1.125e-10	-9.949	-9.949	0.000	20.29
CaHSO4+	4.154e-13	3.927e-13	-12.382	-12.406	-0.024	(0)
Zn(SO4)2-2	4.669e-15	3.729e-15	-14.331	-14.428	-0.098	-8.77
Si	4.378e-04					
H4SiO4	4.376e-04	4.379e-04	-3.359	-3.359	0.000	51.65
H3SiO4-	1.756e-07	1.660e-07	-6.755	-6.780	-0.024	28.09
H2SiO4-2	4.256e-14	3.415e-14	-13.371	-13.467	-0.096	(0)
SiF6-2	2.521e-30	2.020e-30	-29.599	-29.695	-0.096	42.92
Sr	1.370e-06					
Sr+2	1.343e-06	1.078e-06	-5.872	-5.967	-0.096	-17.85
SrHCO3+	2.575e-08	2.437e-08	-7.589	-7.613	-0.024	(0)
SrSO4	4.810e-10	4.813e-10	-9.318	-9.318	0.000	24.43
SrCO3	1.101e-10	1.102e-10	-9.958	-9.958	0.000	-14.11
SrOH+	1.249e-13	1.182e-13	-12.903	-12.927	-0.024	(0)
Zn	6.120e-07					
Zn+2	5.293e-07	4.241e-07	-6.276	-6.373	-0.096	-25.65
ZnHCO3+	6.914e-08	6.536e-08	-7.160	-7.185	-0.024	(0)

ZnCO3	1.151e-08	1.151e-08	-7.939	-7.939	0.000	(0)
ZnOH+	1.584e-09	1.497e-09	-8.800	-8.825	-0.024	(0)
ZnSO4	2.225e-10	2.226e-10	-9.653	-9.652	0.000	20.90
ZnCl+	1.223e-10	1.156e-10	-9.913	-9.937	-0.024	-8.89
ZnF+	4.656e-11	4.401e-11	-10.332	-10.356	-0.024	(0)
Zn(CO3)2-2	4.194e-11	3.350e-11	-10.377	-10.475	-0.098	(0)
Zn(OH)2	2.439e-11	2.440e-11	-10.613	-10.613	0.000	(0)
ZnOHCl	2.395e-12	2.396e-12	-11.621	-11.621	0.000	(0)
ZnCl2	9.866e-15	9.872e-15	-14.006	-14.006	0.000	92.07
Zn(SO4)2-2	4.669e-15	3.729e-15	-14.331	-14.428	-0.098	-8.77
Zn(OH)3-	1.745e-16	1.650e-16	-15.758	-15.783	-0.024	(0)
ZnCl3-	9.660e-19	9.131e-19	-18.015	-18.039	-0.024	17.46
Zn(OH)4-2	6.998e-23	5.589e-23	-22.155	-22.253	-0.098	(0)
ZnCl4-2	4.757e-23	3.812e-23	-22.323	-22.419	-0.096	145.88

----------Distribution of alkalinity----------

Total alkalinity (eq/kgw) = 1.303e-03

Species	Alkalinity	Molality	Alk/Mol
HCO3-	1.293e-03	1.293e-03	1.00
CaHCO3+	5.256e-06	5.256e-06	1.00
MgHCO3+	2.895e-06	2.895e-06	1.00
H+	-4.928e-07	4.928e-07	-1.00
HPO4-2	4.277e-07	4.277e-07	1.00
CO3-2	3.392e-07	1.696e-07	2.00
NaHCO3	2.523e-07	2.523e-07	1.00
H3SiO4-	1.756e-07	1.756e-07	1.00
CaCO3	1.524e-07	7.621e-08	2.00
ZnHCO3+	6.914e-08	6.914e-08	1.00
CaHPO4	6.144e-08	6.144e-08	1.00
MgCO3	5.249e-08	2.624e-08	2.00
MgHPO4	5.220e-08	5.220e-08	1.00
OH-	3.444e-08	3.444e-08	1.00
MnHCO3+	3.063e-08	3.063e-08	1.00
SrHCO3+	2.575e-08	2.575e-08	1.00
ZnCO3	2.302e-08	1.151e-08	2.00
BaHCO3+	1.840e-08	1.840e-08	1.00
MnCO3	5.738e-09	2.869e-09	2.00
HF	-5.319e-09	5.319e-09	-1.00
NaCO3-	2.661e-09	1.331e-09	2.00
MgOH+	2.480e-09	2.480e-09	1.00
ZnOH+	1.584e-09	1.584e-09	1.00
CaPO4-	7.275e-10	3.638e-10	2.00
MgPO4-	6.167e-10	3.083e-10	2.00
NaHPO4-	2.670e-10	2.670e-10	1.00
SrCO3	2.202e-10	1.101e-10	2.00
BaCO3	1.956e-10	9.782e-11	2.00
H3PO4	-1.839e-10	1.839e-10	-1.00
Zn(CO3)2-2	1.678e-10	4.194e-11	4.00
HSO4-	-1.168e-10	1.168e-10	-1.00
CaOH+	1.110e-10	1.110e-10	1.00
KHPO4-	7.338e-11	7.338e-11	1.00
Zn(OH)2	4.877e-11	2.439e-11	2.00
MnOH+	2.396e-11	2.396e-11	1.00
ZnOHCl	2.395e-12	2.395e-12	1.00
PO4-3	1.221e-12	6.104e-13	2.00
CaHSO4+	-4.154e-13	4.154e-13	-1.00
HF2-	-1.542e-13	1.542e-13	-1.00
SrOH+	1.249e-13	1.249e-13	1.00
BaOH+	9.545e-14	9.545e-14	1.00
H2SiO4-2	8.512e-14	4.256e-14	2.00
Zn(OH)3-	5.235e-16	1.745e-16	3.00
NaOH	1.230e-21	1.230e-21	1.00
Zn(OH)4-2	2.799e-22	6.998e-23	4.00
Mn(OH)3-	1.304e-22	4.347e-23	3.00
SiF6-2	-1.008e-29	2.521e-30	-4.00

-----------------------------Saturation indices-------------------------------

Phase	SI**	log IAP	log K(303 K, 1 atm)	
Anhydrite	-4.86	-9.20	-4.34	CaSO4
Aragonite	-2.02	-10.40	-8.37	CaCO3
BaCl2	-16.28	-14.10	2.18	BaCl2
BaCl2:2H2O	-14.36	-14.10	0.26	BaCl2:2H2O
BaCl2:H2O	-14.93	-14.10	0.83	BaCl2:H2O
Barite	-1.78	-11.57	-9.79	BaSO4
Calcite	-1.88	-10.40	-8.51	CaCO3
Celestite	-4.95	-11.64	-6.69	SrSO4
Chalcedony	0.13	-3.36	-3.49	SiO2
Chrysotile	-11.46	20.07	31.53	Mg3Si2O5(OH)4
CO2(g)	-1.39	-2.92	-1.53	CO2
Dolomite	-3.78	-20.99	-17.22	CaMg(CO3)2
Fluorite	-3.32	-13.86	-10.54	CaF2
Gypsum	-4.61	-9.20	-4.58	CaSO4:2H2O
H2(g)	-29.02	-32.13	-3.11	H2
H2O(g)	-1.36	-0.00	1.36	H2O
Halite	-9.09	-7.52	1.57	NaCl
Hausmannite	-12.48	47.21	59.69	Mn3O4
Hydroxyapatite	-7.82	-11.72	-3.90	Ca5(PO4)3OH
Manganite	-4.78	20.56	25.34	MnOOH
O2(g)	-0.95	-3.88	-2.93	O2
Pyrochroite	-9.12	6.08	15.20	Mn(OH)2
Pyrolusite	-5.47	35.04	40.52	MnO2:H2O
Quartz	0.54	-3.36	-3.90	SiO2
Rhodochrosite	-2.29	-13.44	-11.15	MnCO3
Sepiolite	-7.84	7.78	15.62	Mg2Si3O7.5OH:3H2O
Sepiolite(d)	-10.88	7.78	18.66	Mg2Si3O7.5OH:3H2O
SiO2(a)	-0.69	-3.36	-2.67	SiO2
Smithsonite	-3.18	-13.24	-10.06	ZnCO3
Strontianite	-3.55	-12.83	-9.28	SrCO3
Sylvite	-9.01	-8.08	0.93	KCl
Talc	-7.43	13.35	20.78	Mg3Si4O10(OH)2
Willemite	-5.67	9.22	14.89	Zn2SiO4
Witherite	-4.21	-12.77	-8.56	BaCO3
Zn(OH)2(e)	-5.21	6.29	11.50	Zn(OH)2

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
For ideal gases, phi = 1.

Initial solution 43.

-----------------------------Solution composition-------------------------------

Elements	Molality	Moles
Al	3.707e-07	3.707e-07
Alkalinity	2.432e-03	2.432e-03
Ba	8.448e-07	8.448e-07
Ca	5.740e-04	5.740e-04
Cl	7.053e-06	7.053e-06
F	8.950e-06	8.950e-06
K	1.100e-04	1.100e-04
Mg	5.348e-04	5.348e-04
Mn	1.821e-07	1.821e-07
N(5)	4.285e-06	4.285e-06
Na	3.655e-04	3.655e-04
O(0)	1.500e-04	1.500e-04
P	3.875e-07	3.875e-07
S(6)	1.145e-06	1.145e-06
Si	1.042e-03	1.042e-03
Sr	9.475e-06	9.475e-06
Zn	1.530e-07	1.530e-07

----------Description of solution----------

pH	= 7.770
pe	= 7.653
Specific Conductance (µS/cm, 30°C)	= 264
Density (g/cm³)	= 0.99573
Volume (L)	= 1.00459
Activity of water	= 1.000
Ionic strength (mol/kgw)	= 3.635e-03
Mass of water (kg)	= 1.000e+00
Total carbon (mol/kg)	= 2.480e-03
Total CO2 (mol/kg)	= 2.480e-03
Temperature (°C)	= 30.40
Electrical balance (eq)	= 2.604e-04
Percent error, 100*(Cat-|An|)/(Cat+|An|)	= 5.13
Iterations	= 9 (453 overall)
Total H	= 1.110190e+02
Total O	= 5.551792e+01

----------Redox couples----------

Redox couple	pe	Eh (volts)
O(-2)/O(0)	12.2795	0.7396

----------Distribution of species----------

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma	mole V cm³/mol
OH-	9.513e-07	8.898e-07	-6.022	-6.051	-0.029	-3.91
H+	1.804e-08	1.698e-08	-7.744	-7.770	-0.026	0.00
H2O	5.551e+01	9.999e-01	1.744	-0.000	0.000	18.10
Al	3.707e-07					
Al(OH)4-	3.676e-07	3.443e-07	-6.435	-6.463	-0.028	(0)
Al(OH)3	2.857e-09	2.859e-09	-8.544	-8.544	0.000	(0)
Al(OH)2+	2.398e-10	2.248e-10	-9.620	-9.648	-0.028	(0)
AlOH+2	3.997e-13	3.087e-13	-12.398	-12.510	-0.112	-27.87
AlF2+	1.399e-13	1.312e-13	-12.854	-12.882	-0.028	(0)
AlF+2	4.054e-14	3.131e-14	-13.392	-13.504	-0.112	(0)
AlF3	1.349e-14	1.350e-14	-13.870	-13.870	0.000	(0)
Al+3	6.437e-16	3.730e-16	-15.191	-15.428	-0.237	-42.47
AlF4-	4.674e-17	4.377e-17	-16.330	-16.359	-0.028	(0)
AlSO4+	1.037e-18	9.716e-19	-17.984	-18.013	-0.028	(0)
Al(SO4)2-	2.586e-23	2.422e-23	-22.587	-22.616	-0.028	(0)
AlHSO4+2	2.007e-27	1.541e-27	-26.697	-26.812	-0.115	(0)
Ba	8.448e-07					
Ba+2	8.251e-07	6.339e-07	-6.083	-6.198	-0.114	-12.38
BaHCO3+	1.700e-08	1.592e-08	-7.769	-7.798	-0.029	(0)
BaCO3	2.463e-09	2.465e-09	-8.609	-8.608	0.000	-10.65
BaSO4	2.441e-10	2.443e-10	-9.612	-9.612	0.000	(0)
BaCl+	1.520e-11	1.423e-11	-10.818	-10.847	-0.029	(0)
BaOH+	1.350e-12	1.265e-12	-11.870	-11.898	-0.028	(0)
BaNO3+	3.415e-13	3.196e-13	-12.467	-12.495	-0.029	(0)
C(4)	2.480e-03					
HCO3-	2.357e-03	2.210e-03	-2.628	-2.656	-0.028	25.06
CO2	7.953e-05	7.960e-05	-4.099	-4.099	0.000	34.69
CaHCO3+	1.385e-05	1.299e-05	-4.859	-4.886	-0.028	9.88
MgHCO3+	1.143e-05	1.069e-05	-4.942	-4.971	-0.029	5.63
CO3-2	8.743e-06	6.753e-06	-5.058	-5.170	-0.112	-4.86
CaCO3	5.461e-06	5.466e-06	-5.263	-5.262	0.000	-14.58
MgCO3	2.816e-06	2.819e-06	-5.550	-5.550	0.000	-17.09
NaHCO3	4.119e-07	4.123e-07	-6.385	-6.385	0.000	1.80
SrHCO3+	3.061e-07	2.870e-07	-6.514	-6.542	-0.028	(0)
ZnCO3	6.166e-08	6.171e-08	-7.210	-7.210	0.000	(0)
NaCO3-	6.002e-08	5.618e-08	-7.222	-7.250	-0.029	-0.57
MnCO3	4.784e-08	4.788e-08	-7.320	-7.320	0.000	(0)
SrCO3	3.565e-08	3.568e-08	-7.448	-7.448	0.000	-14.11

MnHCO3+	1.876e-08	1.758e-08	-7.727	-7.755	-0.028	(0)
BaHCO3+	1.700e-08	1.592e-08	-7.769	-7.798	-0.029	(0)
ZnHCO3+	1.361e-08	1.274e-08	-7.866	-7.895	-0.029	(0)
Zn(CO3)2-2	1.161e-08	8.910e-09	-7.935	-8.050	-0.115	(0)
BaCO3	2.463e-09	2.465e-09	-8.609	-8.608	0.000	-10.65
(CO2)2	1.381e-10	1.382e-10	-9.860	-9.859	0.000	69.39
Ca	5.740e-04					
Ca+2	5.546e-04	4.281e-04	-3.256	-3.368	-0.112	-18.01
CaHCO3+	1.385e-05	1.299e-05	-4.859	-4.886	-0.028	9.88
CaCO3	5.461e-06	5.466e-06	-5.263	-5.262	0.000	-14.58
CaSO4	6.088e-08	6.093e-08	-7.216	-7.215	0.000	7.69
CaHPO4	4.414e-08	4.418e-08	-7.355	-7.355	0.000	(0)
CaPO4-	7.255e-09	6.802e-09	-8.139	-8.167	-0.028	(0)
CaOH+	4.470e-09	4.184e-09	-8.350	-8.378	-0.029	(0)
CaH2PO4+	5.857e-10	5.490e-10	-9.232	-9.260	-0.028	(0)
CaHSO4+	7.876e-15	7.372e-15	-14.104	-14.132	-0.029	(0)
Cl	7.053e-06					
Cl-	7.039e-06	6.586e-06	-5.152	-5.181	-0.029	18.22
NaCl	1.398e-08	1.399e-08	-7.855	-7.854	0.000	(0)
BaCl+	1.520e-11	1.423e-11	-10.818	-10.847	-0.029	(0)
MnCl+	2.556e-12	2.395e-12	-11.593	-11.621	-0.028	-1.89
ZnCl+	1.096e-12	1.026e-12	-11.960	-11.989	-0.029	-8.97
ZnOHCl	5.876e-13	5.881e-13	-12.231	-12.231	0.000	(0)
ZnCl2	7.220e-18	7.226e-18	-17.141	-17.141	0.000	92.24
MnCl2	6.879e-18	6.884e-18	-17.162	-17.162	0.000	79.75
ZnCl3-	5.890e-23	5.513e-23	-22.230	-22.259	-0.029	17.45
MnCl3-	1.333e-23	1.249e-23	-22.875	-22.903	-0.028	43.16
ZnCl4-2	2.462e-28	1.898e-28	-27.609	-27.722	-0.113	145.91
F	8.950e-06					
F-	8.694e-06	8.132e-06	-5.061	-5.090	-0.029	-1.26
MgF+	2.542e-07	2.381e-07	-6.595	-6.623	-0.028	-10.57
NaF	1.598e-09	1.600e-09	-8.796	-8.796	0.000	7.45
HF	2.283e-10	2.285e-10	-9.641	-9.641	0.000	12.73
ZnF+	6.007e-12	5.623e-12	-11.221	-11.250	-0.029	(0)
MnF+	5.359e-12	5.021e-12	-11.271	-11.299	-0.028	(0)
AlF2+	1.399e-13	1.312e-13	-12.854	-12.882	-0.028	(0)
AlF+2	4.054e-14	3.131e-14	-13.392	-13.504	-0.112	(0)
AlF3	1.349e-14	1.350e-14	-13.870	-13.870	0.000	(0)
HF2-	7.915e-15	7.409e-15	-14.102	-14.130	-0.029	22.30
AlF4-	4.674e-17	4.377e-17	-16.330	-16.359	-0.028	(0)
SiF6-2	2.991e-35	2.306e-35	-34.524	-34.637	-0.113	42.95
H(0)	1.913e-34					
H2	9.565e-35	9.573e-35	-34.019	-34.019	0.000	28.60
K	1.100e-04					
K+	1.100e-04	1.029e-04	-3.959	-3.988	-0.029	9.19
KSO4-	6.506e-10	6.099e-10	-9.187	-9.215	-0.028	34.24
KHPO4-	3.648e-11	3.420e-11	-10.438	-10.466	-0.028	37.78
Mg	5.348e-04					
Mg+2	5.200e-04	4.026e-04	-3.284	-3.395	-0.111	-21.93
MgHCO3+	1.143e-05	1.069e-05	-4.942	-4.971	-0.029	5.63
MgCO3	2.816e-06	2.819e-06	-5.550	-5.550	0.000	-17.09
MgF+	2.542e-07	2.381e-07	-6.595	-6.623	-0.028	-10.57
MgOH+	1.480e-07	1.389e-07	-6.830	-6.857	-0.027	(0)
MgSO4	8.313e-08	8.320e-08	-7.080	-7.080	0.000	6.03
MgHPO4	5.611e-08	5.616e-08	-7.251	-7.251	0.000	(0)
MgPO4-	9.202e-09	8.627e-09	-8.036	-8.064	-0.028	(0)
MgH2PO4+	7.012e-10	6.574e-10	-9.154	-9.182	-0.028	(0)
Mn(2)	1.821e-07					
Mn+2	1.152e-07	8.925e-08	-6.938	-7.049	-0.111	-20.35
MnCO3	4.784e-08	4.788e-08	-7.320	-7.320	0.000	(0)
MnHCO3+	1.876e-08	1.758e-08	-7.727	-7.755	-0.028	(0)
MnOH+	2.221e-10	2.081e-10	-9.653	-9.682	-0.028	(0)
MnSO4	1.349e-11	1.351e-11	-10.870	-10.869	0.000	20.33
MnF+	5.359e-12	5.021e-12	-11.271	-11.299	-0.028	(0)
MnCl+	2.556e-12	2.395e-12	-11.593	-11.621	-0.028	-1.89
MnCl2	6.879e-18	6.884e-18	-17.162	-17.162	0.000	79.75
Mn(NO3)2	5.628e-18	5.632e-18	-17.250	-17.249	0.000	39.70
Mn(OH)3-	3.081e-19	2.887e-19	-18.511	-18.540	-0.028	(0)

MnCl3-	1.333e-23	1.249e-23	-22.875	-22.903	-0.028	43.16
Mn(3)	4.646e-25					
Mn+3	4.646e-25	2.692e-25	-24.333	-24.570	-0.237	(0)
N(5)	4.285e-06					
NO3-	4.285e-06	4.005e-06	-5.368	-5.397	-0.029	29.99
BaNO3+	3.415e-13	3.196e-13	-12.467	-12.495	-0.029	(0)
Mn(NO3)2	5.628e-18	5.632e-18	-17.250	-17.249	0.000	39.70
Na	3.655e-04					
Na+	3.650e-04	3.419e-04	-3.438	-3.466	-0.028	-1.17
NaHCO3	4.119e-07	4.123e-07	-6.385	-6.385	0.000	1.80
NaCO3-	6.002e-08	5.618e-08	-7.222	-7.250	-0.029	-0.57
NaCl	1.398e-08	1.399e-08	-7.855	-7.854	0.000	(0)
NaF	1.598e-09	1.600e-09	-8.796	-8.796	0.000	7.45
NaSO4-	1.454e-09	1.363e-09	-8.838	-8.866	-0.028	13.78
NaHPO4-	1.212e-10	1.136e-10	-9.917	-9.945	-0.028	33.58
NaOH	3.039e-20	3.042e-20	-19.517	-19.517	0.000	(0)
O(0)	1.500e-04					
O2	7.502e-05	7.508e-05	-4.125	-4.124	0.000	30.80
P	3.875e-07					
HPO4-2	2.211e-07	1.704e-07	-6.655	-6.768	-0.113	6.62
MgHPO4	5.611e-08	5.616e-08	-7.251	-7.251	0.000	(0)
H2PO4-	4.827e-08	4.526e-08	-7.316	-7.344	-0.028	33.11
CaHPO4	4.414e-08	4.418e-08	-7.355	-7.355	0.000	(0)
MgPO4-	9.202e-09	8.627e-09	-8.036	-8.064	-0.028	(0)
CaPO4-	7.255e-09	6.802e-09	-8.139	-8.167	-0.028	(0)
MgH2PO4+	7.012e-10	6.574e-10	-9.154	-9.182	-0.028	(0)
CaH2PO4+	5.857e-10	5.490e-10	-9.232	-9.260	-0.028	(0)
NaHPO4-	1.212e-10	1.136e-10	-9.917	-9.945	-0.028	33.58
KHPO4-	3.648e-11	3.420e-11	-10.438	-10.466	-0.028	37.78
PO4-3	9.129e-12	5.031e-12	-11.040	-11.298	-0.259	-23.50
H3PO4	1.204e-13	1.205e-13	-12.919	-12.919	0.000	47.68
S(6)	1.145e-06					
SO4-2	9.978e-07	7.691e-07	-6.001	-6.114	-0.113	15.22
MgSO4	8.313e-08	8.320e-08	-7.080	-7.080	0.000	6.03
CaSO4	6.088e-08	6.093e-08	-7.216	-7.215	0.000	7.69
NaSO4-	1.454e-09	1.363e-09	-8.838	-8.866	-0.028	13.78
SrSO4	1.125e-09	1.126e-09	-8.949	-8.948	0.000	24.42
KSO4-	6.506e-10	6.099e-10	-9.187	-9.215	-0.028	34.24
BaSO4	2.441e-10	2.443e-10	-9.612	-9.612	0.000	(0)
MnSO4	1.349e-11	1.351e-11	-10.870	-10.869	0.000	20.33
ZnSO4	8.593e-12	8.600e-12	-11.066	-11.065	0.000	20.91
HSO4-	1.530e-12	1.432e-12	-11.815	-11.844	-0.029	40.63
CaHSO4+	7.876e-15	7.372e-15	-14.104	-14.132	-0.029	(0)
Zn(SO4)2-2	6.724e-17	5.161e-17	-16.172	-16.287	-0.115	-8.79
AlSO4+	1.037e-18	9.716e-19	-17.984	-18.013	-0.028	(0)
Al(SO4)2-	2.586e-23	2.422e-23	-22.587	-22.616	-0.028	(0)
AlHSO4+2	2.007e-27	1.541e-27	-26.697	-26.812	-0.115	(0)
Si	1.042e-03					
H4SiO4	1.031e-03	1.032e-03	-2.987	-2.987	0.000	51.66
H3SiO4-	1.147e-05	1.074e-05	-4.940	-4.969	-0.029	28.10
H2SiO4-2	7.827e-11	6.046e-11	-10.106	-10.219	-0.112	(0)
SiF6-2	2.991e-35	2.306e-35	-34.524	-34.637	-0.113	42.95
Sr	9.475e-06					
Sr+2	9.132e-06	7.056e-06	-5.039	-5.151	-0.112	-17.81
SrHCO3+	3.061e-07	2.870e-07	-6.514	-6.542	-0.028	(0)
SrCO3	3.565e-08	3.568e-08	-7.448	-7.448	0.000	-14.11
SrSO4	1.125e-09	1.126e-09	-8.949	-8.948	0.000	24.42
SrOH+	2.274e-11	2.131e-11	-10.643	-10.671	-0.028	(0)
Zn	1.530e-07					
ZnCO3	6.166e-08	6.171e-08	-7.210	-7.210	0.000	(0)
Zn+2	5.940e-08	4.580e-08	-7.226	-7.339	-0.113	-25.62
ZnHCO3+	1.361e-08	1.274e-08	-7.866	-7.895	-0.029	(0)
Zn(CO3)2-2	1.161e-08	8.910e-09	-7.935	-8.050	-0.115	(0)
ZnOH+	4.723e-09	4.421e-09	-8.326	-8.354	-0.029	(0)
Zn(OH)2	1.997e-09	1.999e-09	-8.700	-8.699	0.000	(0)
ZnSO4	8.593e-12	8.600e-12	-11.066	-11.065	0.000	20.91
ZnF+	6.007e-12	5.623e-12	-11.221	-11.250	-0.029	(0)
ZnCl+	1.096e-12	1.026e-12	-11.960	-11.989	-0.029	-8.97

ZnOHCl	5.876e-13	5.881e-13	-12.231	-12.231	0.000	(0)
Zn(OH)3-	3.976e-13	3.721e-13	-12.401	-12.429	-0.029	(0)
Zn(SO4)2-2	6.724e-17	5.161e-17	-16.172	-16.287	-0.115	-8.79
ZnCl2	7.220e-18	7.226e-18	-17.141	-17.141	0.000	92.24
Zn(OH)4-2	4.524e-18	3.473e-18	-17.344	-17.459	-0.115	(0)
ZnCl3-	5.890e-23	5.513e-23	-22.230	-22.259	-0.029	17.45
ZnCl4-2	2.462e-28	1.898e-28	-27.609	-27.722	-0.113	145.91

----------Distribution of alkalinity----------

Total alkalinity (eq/kgw) = 2.432e-03

Species	Alkalinity	Molality	Alk/Mol
HCO3-	2.357e-03	2.357e-03	1.00
CO3-2	1.749e-05	8.743e-06	2.00
CaHCO3+	1.385e-05	1.385e-05	1.00
H3SiO4-	1.147e-05	1.147e-05	1.00
MgHCO3+	1.143e-05	1.143e-05	1.00
CaCO3	1.092e-05	5.461e-06	2.00
MgCO3	5.632e-06	2.816e-06	2.00
Al(OH)4-	1.470e-06	3.676e-07	4.00
OH-	9.513e-07	9.513e-07	1.00
NaHCO3	4.119e-07	4.119e-07	1.00
SrHCO3+	3.061e-07	3.061e-07	1.00
HPO4-2	2.211e-07	2.211e-07	1.00
MgOH+	1.480e-07	1.480e-07	1.00
ZnCO3	1.233e-07	6.166e-08	2.00
NaCO3-	1.200e-07	6.002e-08	2.00
MnCO3	9.567e-08	4.784e-08	2.00
SrCO3	7.130e-08	3.565e-08	2.00
MgHPO4	5.611e-08	5.611e-08	1.00
Zn(CO3)2-2	4.643e-08	1.161e-08	4.00
CaHPO4	4.414e-08	4.414e-08	1.00
MnHCO3+	1.876e-08	1.876e-08	1.00
MgPO4-	1.840e-08	9.202e-09	2.00
H+	-1.804e-08	1.804e-08	-1.00
BaHCO3+	1.700e-08	1.700e-08	1.00
CaPO4-	1.451e-08	7.255e-09	2.00
ZnHCO3+	1.361e-08	1.361e-08	1.00
Al(OH)3	8.570e-09	2.857e-09	3.00
BaCO3	4.926e-09	2.463e-09	2.00
ZnOH+	4.723e-09	4.723e-09	1.00
CaOH+	4.470e-09	4.470e-09	1.00
Zn(OH)2	3.994e-09	1.997e-09	2.00
Al(OH)2+	4.796e-10	2.398e-10	2.00
HF	-2.283e-10	2.283e-10	-1.00
MnOH+	2.221e-10	2.221e-10	1.00
H2SiO4-2	1.565e-10	7.827e-11	2.00
NaHPO4-	1.212e-10	1.212e-10	1.00
KHPO4-	3.648e-11	3.648e-11	1.00
SrOH+	2.274e-11	2.274e-11	1.00
PO4-3	1.826e-11	9.129e-12	2.00
HSO4-	-1.530e-12	1.530e-12	-1.00
BaOH+	1.350e-12	1.350e-12	1.00
Zn(OH)3-	1.193e-12	3.976e-13	3.00
ZnOHCl	5.876e-13	5.876e-13	1.00
AlOH+2	3.997e-13	3.997e-13	1.00
H3PO4	-1.204e-13	1.204e-13	-1.00
HF2-	-7.915e-15	7.915e-15	-1.00
CaHSO4+	-7.876e-15	7.876e-15	-1.00
Zn(OH)4-2	1.810e-17	4.524e-18	4.00
Mn(OH)3-	9.244e-19	3.081e-19	3.00
NaOH	3.039e-20	3.039e-20	1.00
AlHSO4+2	-2.007e-27	2.007e-27	-1.00
SiF6-2	-1.196e-34	2.991e-35	-4.00

----------Saturation indices----------

Phase	SI**	log IAP	log K(303 K, 1 atm)	
Al(OH)3(a)	-2.57	7.88	10.45	Al(OH)3
Albite	-1.22	-18.89	-17.66	NaAlSi3O8
Alunite	-13.83	-15.88	-2.06	KAl3(SO4)2(OH)6
Anhydrite	-5.14	-9.48	-4.34	CaSO4
Anorthite	-2.70	-22.27	-19.56	CaAl2Si2O8
Aragonite	-0.17	-8.54	-8.37	CaCO3
BaCl2	-18.74	-16.56	2.18	BaCl2
BaCl2:2H2O	-16.82	-16.56	0.25	BaCl2:2H2O
BaCl2:H2O	-17.39	-16.56	0.83	BaCl2:H2O
Barite	-2.52	-12.31	-9.79	BaSO4
Ca-Montmorillonite	2.15	-42.11	-44.27	Ca0.165Al2.33Si3.67O10(OH)2
Calcite	-0.03	-8.54	-8.51	CaCO3
Celestite	-4.58	-11.27	-6.69	SrSO4
Chalcedony	0.50	-2.99	-3.49	SiO2
Chlorite(14A)	1.12	67.53	66.40	Mg5Al2Si3O10(OH)8
Chrysotile	-1.08	30.46	31.54	Mg3Si2O5(OH)4
CO2(g)	-2.57	-4.10	-1.53	CO2
Dolomite	0.11	-17.10	-17.21	CaMg(CO3)2
Fluorite	-3.01	-13.55	-10.54	CaF2
Gibbsite	0.07	7.88	7.81	Al(OH)3
Gypsum	-4.90	-9.48	-4.58	CaSO4:2H2O
H2(g)	-30.91	-34.02	-3.11	H2
H2O(g)	-1.37	-0.00	1.37	H2O
Halite	-10.22	-8.65	1.57	NaCl
Hausmannite	-3.40	56.32	59.72	Mn3O4
Hydroxyapatite	-2.17	-6.07	-3.89	Ca5(PO4)3OH
Illite	1.67	-37.88	-39.55	K0.6Mg0.25Al2.3Si3.5O10(OH)2
K-feldspar	0.76	-19.41	-20.17	KAlSi3O8
K-mica	6.54	18.47	11.93	KAl3Si3O10(OH)2
Kaolinite	2.82	9.79	6.97	Al2Si2O5(OH)4
Manganite	-1.43	23.91	25.34	MnOOH
O2(g)	-1.20	-4.12	-2.93	O2
Pyrochroite	-6.71	8.49	15.20	Mn(OH)2
Pyrolusite	-1.19	39.34	40.53	MnO2:H2O
Quartz	0.92	-2.99	-3.90	SiO2
Rhodochrosite	-1.07	-12.22	-11.15	MnCO3
Sepiolite	-0.29	15.33	15.62	Mg2Si3O7.5OH:3H2O
Sepiolite(d)	-3.33	15.33	18.66	Mg2Si3O7.5OH:3H2O
SiO2(a)	-0.32	-2.99	-2.67	SiO2
Smithsonite	-2.45	-12.51	-10.06	ZnCO3
Strontianite	-1.04	-10.32	-9.28	SrCO3
Sylvite	-10.10	-9.17	0.93	KCl
Talc	3.69	24.49	20.79	Mg3Si4O10(OH)2
Willemite	-1.48	13.42	14.89	Zn2SiO4
Witherite	-2.81	-11.37	-8.56	BaCO3
Zn(OH)2(e)	-3.30	8.20	11.50	Zn(OH)2

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
For ideal gases, phi = 1.

Initial solution 44.

pH will be adjusted to obtain desired alkalinity.

----------Solution composition----------

Elements	Molality	Moles
Al	7.452e-05	7.452e-05
Alkalinity	2.796e-03	2.796e-03
Ba	4.006e-07	4.006e-07
C	1.227e-03	1.227e-03
Ca	9.734e-04	9.734e-04
Cl	9.311e-05	9.311e-05

F	2.317e-05	2.317e-05
K	2.737e-04	2.737e-04
N(3)	1.643e-05	1.643e-05
N(5)	1.785e-05	1.785e-05
Na	1.001e-03	1.001e-03
O(0)	6.252e-05	6.252e-05
P	1.615e-06	1.615e-06
S(6)	1.458e-04	1.458e-04
Si	1.682e-04	1.682e-04
Sr	1.027e-05	1.027e-05

----------Description of solution----------

pH	= 10.331	Adjust alkalinity
pe	= 4.349	
Specific Conductance (µS/cm, 28°C)	= 322	
Density (g/cm³)	= 0.99640	
Volume (L)	= 1.00381	
Activity of water	= 1.000	
Ionic strength (mol/kgw)	= 3.694e-03	
Mass of water (kg)	= 1.000e+00	
Total CO2 (mol/kg)	= 1.227e-03	
Temperature (°C)	= 28.10	
Electrical balance (eq)	= 2.264e-04	
Percent error, 100*(Cat-|An|)/(Cat+|An|)	= 4.67	
Iterations	= 12 (465 overall)	
Total H	= 1.110140e+02	
Total O	= 5.551190e+01	

----------Redox couples----------

Redox couple	pe	Eh (volts)
N(3)/N(5)	3.8070	0.2275
O(-2)/O(0)	9.8086	0.5863

----------Distribution of species----------

Species	Molality	Activity	Log Molality	Log Activity	Log Gamma	mole V cm³/mol
OH-	2.928e-04	2.738e-04	-3.533	-3.563	-0.029	-3.97
H+	4.958e-11	4.666e-11	-10.305	-10.331	-0.026	0.00
H2O	5.551e+01	9.999e-01	1.744	-0.000	0.000	18.08
Al	7.452e-05					
Al(OH)4-	7.452e-05	6.977e-05	-4.128	-4.156	-0.029	(0)
Al(OH)3	1.650e-09	1.651e-09	-8.783	-8.782	0.000	(0)
Al(OH)2+	4.464e-13	4.184e-13	-12.350	-12.378	-0.028	(0)
AlOH+2	2.475e-18	1.910e-18	-17.606	-17.719	-0.113	-27.78
AlF2+	1.906e-20	1.786e-20	-19.720	-19.748	-0.028	(0)
AlF3	4.880e-21	4.884e-21	-20.312	-20.311	0.000	(0)
AlF+2	2.099e-21	1.620e-21	-20.678	-20.791	-0.113	(0)
AlF4-	4.500e-23	4.213e-23	-22.347	-22.375	-0.029	(0)
Al+3	1.269e-23	7.343e-24	-22.896	-23.134	-0.238	-42.31
AlSO4+	2.697e-24	2.525e-24	-23.569	-23.598	-0.029	(0)
Al(SO4)2-	9.042e-27	8.466e-27	-26.044	-26.072	-0.029	(0)
AlHSO4+2	1.402e-35	1.075e-35	-34.853	-34.969	-0.115	(0)
Ba	4.006e-07					
Ba+2	3.321e-07	2.550e-07	-6.479	-6.594	-0.115	-12.49
BaCO3	5.380e-08	5.384e-08	-7.269	-7.269	0.000	-10.67
BaSO4	1.334e-08	1.335e-08	-7.875	-7.874	0.000	(0)
BaHCO3+	1.036e-09	9.697e-10	-8.985	-9.013	-0.029	(0)
BaOH+	1.976e-10	1.851e-10	-9.704	-9.732	-0.028	(0)
BaCl+	7.776e-11	7.277e-11	-10.109	-10.138	-0.029	(0)
BaNO3+	5.723e-13	5.356e-13	-12.242	-12.271	-0.029	(0)
C(-4)	0.000e+00					
CH4	0.000e+00	0.000e+00	-100.908	-100.908	0.000	35.71
C(4)	1.227e-03					

CO3-2	4.977e-04	3.841e-04	-3.303	-3.416	-0.113	-4.96
HCO3-	3.840e-04	3.599e-04	-3.416	-3.444	-0.028	24.93
CaCO3	3.324e-04	3.327e-04	-3.478	-3.478	0.000	-14.59
NaCO3-	8.282e-06	7.751e-06	-5.082	-5.111	-0.029	-0.73
CaHCO3+	2.471e-06	2.318e-06	-5.607	-5.635	-0.028	9.81
SrCO3	1.732e-06	1.734e-06	-5.761	-5.761	0.000	-14.12
NaHCO3	1.845e-07	1.846e-07	-6.734	-6.734	0.000	1.80
BaCO3	5.380e-08	5.384e-08	-7.269	-7.269	0.000	-10.67
SrHCO3+	4.214e-08	3.950e-08	-7.375	-7.403	-0.028	(0)
CO2	3.641e-08	3.644e-08	-7.439	-7.438	0.000	34.58
BaHCO3+	1.036e-09	9.697e-10	-8.985	-9.013	-0.029	(0)
(CO2)2	2.693e-17	2.695e-17	-16.570	-16.569	0.000	69.17
Ca	9.734e-04					
Ca+2	6.260e-04	4.829e-04	-3.203	-3.316	-0.113	-18.02
CaCO3	3.324e-04	3.327e-04	-3.478	-3.478	0.000	-14.59
CaSO4	9.175e-06	9.183e-06	-5.037	-5.037	0.000	7.61
CaHCO3+	2.471e-06	2.318e-06	-5.607	-5.635	-0.028	9.81
CaOH+	1.835e-06	1.718e-06	-5.736	-5.765	-0.029	(0)
CaPO4-	1.469e-06	1.376e-06	-5.833	-5.861	-0.028	(0)
CaHPO4	2.560e-08	2.562e-08	-7.592	-7.591	0.000	(0)
CaH2PO4+	9.438e-13	8.846e-13	-12.025	-12.053	-0.028	(0)
CaHSO4+	3.150e-15	2.947e-15	-14.502	-14.531	-0.029	(0)
Cl	9.311e-05					
Cl-	9.262e-05	8.664e-05	-4.033	-4.062	-0.029	18.18
NaCl	4.914e-07	4.918e-07	-6.309	-6.308	0.000	(0)
BaCl+	7.776e-11	7.277e-11	-10.109	-10.138	-0.029	(0)
F	2.317e-05					
F-	2.316e-05	2.165e-05	-4.635	-4.664	-0.029	-1.27
NaF	1.156e-08	1.157e-08	-7.937	-7.937	0.000	7.37
HF	1.601e-12	1.603e-12	-11.796	-11.795	0.000	12.63
HF2-	1.456e-16	1.362e-16	-15.837	-15.866	-0.029	22.22
AlF2+	1.906e-20	1.786e-20	-19.720	-19.748	-0.028	(0)
AlF3	4.880e-21	4.884e-21	-20.312	-20.311	0.000	(0)
AlF+2	2.099e-21	1.620e-21	-20.678	-20.791	-0.113	(0)
AlF4-	4.500e-23	4.213e-23	-22.347	-22.375	-0.029	(0)
SiF6-2	0.000e+00	0.000e+00	-43.592	-43.706	-0.113	42.85
H(0)	5.987e-33					
H2	2.994e-33	2.996e-33	-32.524	-32.523	0.000	28.60
K	2.737e-04					
K+	2.735e-04	2.558e-04	-3.563	-3.592	-0.029	9.13
KSO4-	2.114e-07	1.982e-07	-6.675	-6.703	-0.028	34.20
KHPO4-	4.863e-11	4.558e-11	-10.313	-10.341	-0.028	37.93
N(3)	1.643e-05					
NO2-	1.643e-05	1.535e-05	-4.784	-4.814	-0.029	25.14
N(5)	1.785e-05					
NO3-	1.785e-05	1.669e-05	-4.748	-4.778	-0.029	29.80
BaNO3+	5.723e-13	5.356e-13	-12.242	-12.271	-0.029	(0)
Na	1.001e-03					
Na+	9.913e-04	9.283e-04	-3.004	-3.032	-0.029	-1.28
NaCO3-	8.282e-06	7.751e-06	-5.082	-5.111	-0.029	-0.73
NaSO4-	5.289e-07	4.958e-07	-6.277	-6.305	-0.028	13.88
NaCl	4.914e-07	4.918e-07	-6.309	-6.308	0.000	(0)
NaHCO3	1.845e-07	1.846e-07	-6.734	-6.734	0.000	1.80
NaF	1.156e-08	1.157e-08	-7.937	-7.937	0.000	7.37
NaHPO4-	1.765e-10	1.654e-10	-9.753	-9.781	-0.028	33.64
NaOH	2.539e-17	2.541e-17	-16.595	-16.595	0.000	(0)
O(0)	6.252e-05					
O2	3.126e-05	3.129e-05	-4.505	-4.505	0.000	30.64
P	1.615e-06					
CaPO4-	1.469e-06	1.376e-06	-5.833	-5.861	-0.028	(0)
HPO4-2	1.186e-07	9.138e-08	-6.926	-7.039	-0.113	6.71
CaHPO4	2.560e-08	2.562e-08	-7.592	-7.591	0.000	(0)
PO4-3	1.707e-09	9.387e-10	-8.768	-9.027	-0.260	-23.28
NaHPO4-	1.765e-10	1.654e-10	-9.753	-9.781	-0.028	33.64
H2PO4-	7.201e-11	6.750e-11	-10.143	-10.171	-0.028	33.17
KHPO4-	4.863e-11	4.558e-11	-10.313	-10.341	-0.028	37.93
CaH2PO4+	9.438e-13	8.846e-13	-12.025	-12.053	-0.028	(0)
H3PO4	4.805e-19	4.809e-19	-18.318	-18.318	0.000	47.57

S(6)	1.458e-04					
SO4-2	1.357e-04	1.045e-04	-3.867	-3.981	-0.113	14.99
CaSO4	9.175e-06	9.183e-06	-5.037	-5.037	0.000	7.61
NaSO4-	5.289e-07	4.958e-07	-6.277	-6.305	-0.028	13.88
KSO4-	2.114e-07	1.982e-07	-6.675	-6.703	-0.028	34.20
SrSO4	1.362e-07	1.363e-07	-6.866	-6.865	0.000	24.35
BaSO4	1.334e-08	1.335e-08	-7.875	-7.874	0.000	(0)
HSO4-	5.425e-13	5.077e-13	-12.266	-12.294	-0.029	40.50
CaHSO4+	3.150e-15	2.947e-15	-14.502	-14.531	-0.029	(0)
AlSO4+	2.697e-24	2.525e-24	-23.569	-23.598	-0.029	(0)
Al(SO4)2-	9.042e-27	8.466e-27	-26.044	-26.072	-0.029	(0)
AlHSO4+2	1.402e-35	1.075e-35	-34.853	-34.969	-0.115	(0)
Si	1.682e-04					
H3SiO4-	1.326e-04	1.241e-04	-3.878	-3.906	-0.029	28.07
H4SiO4	3.529e-05	3.532e-05	-4.452	-4.452	0.000	51.83
H2SiO4-2	2.857e-07	2.205e-07	-6.544	-6.657	-0.113	(0)
SiF6-2	0.000e+00	0.000e+00	-43.592	-43.706	-0.113	42.85
Sr	1.027e-05					
Sr+2	8.357e-06	6.452e-06	-5.078	-5.190	-0.112	-17.76
SrCO3	1.732e-06	1.734e-06	-5.761	-5.761	0.000	-14.12
SrSO4	1.362e-07	1.363e-07	-6.866	-6.865	0.000	24.35
SrHCO3+	4.214e-08	3.950e-08	-7.375	-7.403	-0.028	(0)
SrOH+	7.570e-09	7.092e-09	-8.121	-8.149	-0.028	(0)

----------Distribution of alkalinity----------

Total alkalinity (eq/kgw) = 2.796e-03

Species	Alkalinity	Molality	Alk/Mol
CO3-2	9.954e-04	4.977e-04	2.00
CaCO3	6.648e-04	3.324e-04	2.00
HCO3-	3.840e-04	3.840e-04	1.00
Al(OH)4-	2.981e-04	7.452e-05	4.00
OH-	2.928e-04	2.928e-04	1.00
H3SiO4-	1.326e-04	1.326e-04	1.00
NaCO3-	1.656e-05	8.282e-06	2.00
SrCO3	3.465e-06	1.732e-06	2.00
CaPO4-	2.937e-06	1.469e-06	2.00
CaHCO3+	2.471e-06	2.471e-06	1.00
CaOH+	1.835e-06	1.835e-06	1.00
H2SiO4-2	5.714e-07	2.857e-07	2.00
NaHCO3	1.845e-07	1.845e-07	1.00
HPO4-2	1.186e-07	1.186e-07	1.00
BaCO3	1.076e-07	5.380e-08	2.00
SrHCO3+	4.214e-08	4.214e-08	1.00
CaHPO4	2.560e-08	2.560e-08	1.00
SrOH+	7.570e-09	7.570e-09	1.00
Al(OH)3	4.950e-09	1.650e-09	3.00
PO4-3	3.414e-09	1.707e-09	2.00
BaHCO3+	1.036e-09	1.036e-09	1.00
BaOH+	1.976e-10	1.976e-10	1.00
NaHPO4-	1.765e-10	1.765e-10	1.00
H+	-4.958e-11	4.958e-11	-1.00
KHPO4-	4.863e-11	4.863e-11	1.00
HF	-1.601e-12	1.601e-12	-1.00
Al(OH)2+	8.928e-13	4.464e-13	2.00
HSO4-	-5.425e-13	5.425e-13	-1.00
CaHSO4+	-3.150e-15	3.150e-15	-1.00
HF2-	-1.456e-16	1.456e-16	-1.00
NaOH	2.539e-17	2.539e-17	1.00
AlOH+2	2.475e-18	2.475e-18	1.00
H3PO4	-4.805e-19	4.805e-19	-1.00
AlHSO4+2	-1.402e-35	1.402e-35	-1.00
SiF6-2	-0.000e+00	0.000e+00	-4.00

----------Saturation indices----------

Phase	SI**	log IAP	log K(301 K, 1 atm)	
Al(OH)3(a)	-2.74	7.86	10.60	Al(OH)3
Albite	-2.74	-20.54	-17.81	NaAlSi3O8
Alunite	-17.19	-18.97	-1.78	KAl3(SO4)2(OH)6
Anhydrite	-2.98	-7.30	-4.31	CaSO4
Anorthite	-0.91	-20.53	-19.63	CaAl2Si2O8
Aragonite	1.62	-6.73	-8.36	CaCO3
BaCl2	-16.92	-14.72	2.20	BaCl2
BaCl2:2H2O	-14.95	-14.72	0.24	BaCl2:2H2O
BaCl2:H2O	-15.55	-14.72	0.83	BaCl2:H2O
Barite	-0.76	-10.57	-9.81	BaSO4
Ca-Montmorillonite	-2.65	-47.23	-44.59	Ca0.165Al2.33Si3.67O10(OH)2
Calcite	1.77	-6.73	-8.50	CaCO3
Celestite	-2.50	-9.17	-6.67	SrSO4
CH4(g)	-98.08	-100.91	-2.83	CH4
Chalcedony	-0.94	-4.45	-3.52	SiO2
CO2(g)	-5.93	-7.44	-1.50	CO2
Fluorite	-2.08	-12.65	-10.56	CaF2
Gibbsite	-0.08	7.86	7.94	Al(OH)3
Gypsum	-2.71	-7.30	-4.58	CaSO4:2H2O
H2(g)	-29.42	-32.52	-3.11	H2
H2O(g)	-1.42	-0.00	1.42	H2O
Halite	-8.67	-7.09	1.57	NaCl
Hydroxyapatite	7.32	3.63	-3.69	Ca5(PO4)3OH
K-feldspar	-0.76	-21.10	-20.34	KAlSi3O8
K-mica	4.71	16.96	12.26	KAl3Si3O10(OH)2
Kaolinite	-0.35	6.81	7.17	Al2Si2O5(OH)4
O2(g)	-1.59	-4.50	-2.91	O2
Quartz	-0.52	-4.45	-3.94	SiO2
SiO2(a)	-1.77	-4.45	-2.69	SiO2
Strontianite	0.67	-8.61	-9.27	SrCO3
Sylvite	-8.57	-7.65	0.92	KCl
Witherite	-1.45	-10.01	-8.56	BaCO3

**For a gas, SI = log10(fugacity). Fugacity = pressure * phi / 1 atm.
For ideal gases, phi = 1.

End of simulation.

Reading input data for simulation 2.

End of Run after 0.6 Seconds.

Anexo D

Valores de Índice de Perigo (IP) calculados com as Planilhas de Avaliação de Risco da CETESB

Tabela D.1 – Valores de Índice de Perigo (IP) calculados com as planilhas de avaliação de risco da CETESB para amostras de águas subterrâneas coletadas em poços de municípios no estado de São Paulo (Urânia, Gália e Salto de Pirapora). (Uso das concentrações de bário detectadas).

Poço	Valores de IP (Acima de 1 indicados em vermelho)			
	Residente Rural Criança	Residente Rural Adulto	Residente Urbano Criança	Residente Urbano Adulto
Marcolan (2009) - Poços de Urânia/SP				
PM-1	0,13	0,06	0,13	0,06
PM-2	0,01	0,00	0,01	0,00
PM-3A	0,07	0,03	0,07	0,03
PM-3B	0,04	0,02	0,04	0,02
PM-3C	0,02	0,01	0,02	0,01
Tavares (2013) - Poços de Gália/SP e Salto de Pirapora/SP				
G PM-03	0,09	0,04	0,09	0,04
G PM-02	0,49	0,23	0,49	0,21
G PM-01	0,11	0,05	0,11	0,05
PM01	0,02	0,01	0,02	0,01
PM07	0,07	0,03	0,07	0,03
PM03	0,24	0,11	0,24	0,10
PM04	0,47	0,23	0,47	0,20
PM19	0,61	0,29	0,61	0,26
PM24/45	0,19	0,09	0,19	0,08
PM25	0,29	0,14	0,29	0,12
PM27	**2,59**	**1,23**	**2,59**	**1,11**

Tabela D.2 – Valores de Índice de Perigo (IP) calculados com as planilhas de avaliação de risco da CETESB para amostras de águas subterrâneas coletadas em poços de município no estado do Rio de Janeiro (Itaboraí).
(Uso das concentrações de bário detectadas).

Poço	Valores de IP			
	Residente Rural Criança	Residente Rural Adulto	Residente Urbano Criança	Residente Urbano Adulto
Gomes (2012) - Poços de Itaboraí/RJ				
P-01A (08/09)	0,34	0,16	0,34	0,14
P-01B (08/09)	0,12	0,06	0,12	0,05
P-01C (08/09)	0,56	0,27	0,56	0,24
P-02A (08/09)	0,19	0,09	0,19	0,08
P-02B (08/09)	0,03	0,01	0,03	0,01
P-02C (08/09)	0,05	0,03	0,05	0,02
P-03A (08/09)	0,14	0,07	0,14	0,06
P-03B (08/09)	0,06	0,03	0,06	0,03
P-04A (08/09)	0,08	0,04	0,08	0,04
P-04B (08/09)	0,07	0,03	0,07	0,03
P-05 (08/09)	0,02	0,01	0,02	0,01

Tabela D.3 – Valores de Índice de Perigo (IP) calculados com as planilhas de avaliação de risco da CETESB para amostras de águas subterrâneas coletadas em poços de município no estado do Rio de Janeiro (Itaboraí).
(Uso das concentrações de bário detectadas).

Poço	Valores de IP			
	Residente Rural Criança	Residente Rural Adulto	Residente Urbano Criança	Residente Urbano Adulto
Sanches (2015) - Poços de Itaboraí/RJ				
P-01 (06/13)	-	-	-	-
P-02 (06/13)	0,37	0,18	0,37	0,16
P-03 (06/13)	0,20	0,09	0,20	0,08
P-04 (06/13)	0,44	0,21	0,44	0,19
P-05 (10/13)	0,90	0,43	0,90	0,38
P-06 (10/13)	0,58	0,27	0,58	0,25
P-07 (10/13)	0,48	0,23	0,48	0,21
P-08 (10/13)	0,26	0,12	0,26	0,11
P-09 (10/13)	0,38	0,18	0,38	0,16
P-10 (10/13)	0,57	0,27	0,57	0,25
P-11 (10/13)	0,24	0,11	0,24	0,10
P-12 (10/13)	0,81	0,38	0,81	0,35
P-13 (10/13)	0,63	0,30	0,63	0,27
P-14 (10/13)	0,31	0,15	0,31	0,13
P-15 (10/13)	-	-	-	-
P-16 (10/13)	0,51	0,25	0,51	0,22
P-17 (10/13)	0,74	0,35	0,74	0,32

Tabela D.4 – Valores de Índice de Perigo (IP) calculados com as planilhas de avaliação de risco da CETESB para amostras de águas subterrâneas coletadas em poços de municípios no estado de São Paulo (Urânia, Gália e Salto de Pirapora). (Uso das concentrações de bário detectadas subtraídas de BaSO4 da especiação do modelo hidrogeoquímico quando IS_{Barita} >0).

Poço	Valores de IP			
	Residente Rural Criança	Residente Rural Adulto	Residente Urbano Criança	Residente Urbano Adulto
Marcolan (2009) - Poços de Urânia/SP				
PM-1	-	-	-	-
PM-2	-	-	-	-
PM-3A	-	-	-	-
PM-3B	-	-	-	-
PM-3C	-	-	-	-
Tavares (2013) - Poços de Gália/SP e Salto de Pirapora/SP				
G PM-03	-	-	-	-
G PM-02	-	-	-	-
G PM-01	-	-	-	-
PM01	-	-	-	-
PM07	-	-	-	-
PM03	-	-	-	-
PM04	-	-	-	-
PM19	0,60	0,29	0,60	0,26
PM24/45	-	-	-	-
PM25	-	-	-	-
PM27	-	-	-	-

Tabela D.5 – Valores de Índice de Perigo (IP) calculados com as planilhas de avaliação de risco da CETESB para amostras de águas subterrâneas coletadas em poços de município no estado do Rio de Janeiro (Itaboraí).
(Uso das concentrações de bário detectadas subtraídas de BaSO4 da especiação do modelo hidrogeoquímico quando IS_{Barita} >0).

Poço	Valores de IP			
	Residente Rural Criança	Residente Rural Adulto	Residente Urbano Criança	Residente Urbano Adulto
Gomes (2012) - Poços de Itaboraí/RJ				
P-01A (08/09)	-	-	-	-
P-01B (08/09)	0,11	0,05	0,11	0,05
P-01C (08/09)	0,56	0,27	0,56	0,24
P-02A (08/09)	-	-	-	-
P-02B (08/09)	0,03	0,01	0,03	0,01
P-02C (08/09)	0,05	0,03	0,05	0,02
P-03A (08/09)	0,14	0,07	0,14	0,06
P-03B (08/09)	-	-	-	-
P-04A (08/09)	0,08	0,04	0,08	0,03
P-04B (08/09)	-	-	-	-
P-05 (08/09)	0,02	0,01	0,02	0,01

Tabela D.6 – Valores de Índice de Perigo (IP) calculados com as planilhas de avaliação de risco da CETESB para amostras de águas subterrâneas coletadas em poços de município no estado do Rio de Janeiro (Itaboraí).
(Uso das concentrações de bário detectadas subtraídas de BaSO4 da especiação do modelo hidrogeoquímico quando IS_{Barita} >0).

Poço	Valores de IP			
	Residente Rural Criança	Residente Rural Adulto	Residente Urbano Criança	Residente Urbano Adulto
Sanches (2015) - Poços de Itaboraí/RJ				
P-01 (06/13)	-	-	-	-
P-02 (06/13)	0,36	0,17	0,36	0,15
P-03 (06/13)	0,18	0,09	0,18	0,08
P-04 (06/13)	0,42	0,20	0,42	0,18
P-05 (10/13)	0,89	0,42	0,89	0,38
P-06 (10/13)	0,57	0,27	0,57	0,24
P-07 (10/13)	0,48	0,23	0,48	0,21
P-08 (10/13)	0,25	0,12	0,25	0,11
P-09 (10/13)	0,37	0,18	0,37	0,16
P-10 (10/13)	0,57	0,27	0,57	0,24
P-11 (10/13)	-	-	-	-
P-12 (10/13)	0,80	0,38	0,80	0,34
P-13 (10/13)	0,63	0,30	0,63	0,27
P-14 (10/13)	0,30	0,14	0,30	0,13
P-15 (10/13)	-	-	-	-
P-16 (10/13)	0,51	0,24	0,51	0,22
P-17 (10/13)	0,73	0,35	0,73	0,31

Tabela D.7 – Valores de Índice de Perigo (IP) calculados com as planilhas de avaliação de risco da CETESB para amostras de águas subterrâneas coletadas em poços de município no estado do Rio de Janeiro (Itaboraí).
(Uso das concentrações de cádmio detectadas).

Poço	Valores de IP			
	Residente Rural Criança	Residente Rural Adulto	Residente Urbano Criança	Residente Urbano Adulto
Gomes (2012) - Poços de Itaboraí/RJ				
P-01A (08/09)	0,09	0,04	0,09	0,04
P-01B (08/09)	0,08	0,04	0,08	0,04
P-01C (08/09)	0,09	0,04	0,09	0,04
P-02A (08/09)	0,09	0,04	0,09	0,04
P-02B (08/09)	0,10	0,05	0,10	0,04
P-02C (08/09)	0,13	0,06	0,13	0,05
P-03A (08/09)	0,12	0,06	0,12	0,05
P-03B (08/09)	0,11	0,05	0,11	0,05
P-04A (08/09)	0,09	0,04	0,09	0,04
P-04B (08/09)	0,09	0,04	0,09	0,04
P-05 (08/09)	0,09	0,04	0,09	0,04

Tabela D.8 – Valores de Índice de Perigo (IP) calculados com as planilhas de avaliação de risco da CETESB para amostras de águas subterrâneas coletadas em poços de município no estado do Rio de Janeiro (Itaboraí).
(Uso das concentrações de cádmio detectadas).

Poço	Valores de IP			
	Residente Rural Criança	Residente Rural Adulto	Residente Urbano Criança	Residente Urbano Adulto
Sanches (2015) - Poços de Itaboraí/RJ				
P-01 (06/13)	-	-	-	-
P-02 (06/13)	-	-	-	-
P-03 (06/13)	-	-	-	-
P-04 (06/13)	-	-	-	-
P-05 (10/13)	0,12	0,06	0,12	0,05
P-06 (10/13)	0,17	0,08	0,17	0,07
P-07 (10/13)	0,11	0,05	0,11	0,05
P-08 (10/13)	0,11	0,05	0,11	0,05
P-09 (10/13)	0,13	0,06	0,13	0,06
P-10 (10/13)	0,08	0,04	0,08	0,03
P-11 (10/13)	0,12	0,06	0,12	0,05
P-12 (10/13)	0,08	0,04	0,08	0,04
P-13 (10/13)	0,11	0,05	0,11	0,05
P-14 (10/13)	0,10	0,05	0,10	0,04
P-15 (10/13)	0,09	0,04	0,09	0,04
P-16 (10/13)	0,13	0,06	0,13	0,05
P-17 (10/13)	0,13	0,06	0,13	0,06

Tabela D.9 – Valores de Índice de Perigo (IP) calculados com as planilhas de avaliação de risco da CETESB para amostras de águas subterrâneas coletadas em poços de município no estado do Rio de Janeiro (Itaboraí).
(Uso das concentrações de bário e de cádmio detectadas).

Poço	Valores de IP			
	Residente Rural Criança	Residente Rural Adulto	Residente Urbano Criança	Residente Urbano Adulto
Gomes (2012) - Poços de Itaboraí/RJ				
P-01A (08/09)	0,43	0,20	0,43	0,18
P-01B (08/09)	0,20	0,10	0,20	0,09
P-01C (08/09)	0,65	0,31	0,65	0,28
P-02A (08/09)	0,27	0,13	0,27	0,12
P-02B (08/09)	0,13	0,06	0,13	0,05
P-02C (08/09)	0,18	0,09	0,18	0,08
P-03A (08/09)	0,26	0,12	0,26	0,11
P-03B (08/09)	0,17	0,08	0,17	0,07
P-04A (08/09)	0,17	0,08	0,17	0,07
P-04B (08/09)	0,16	0,07	0,16	0,07
P-05 (08/09)	0,11	0,05	0,11	0,05

Tabela D.10 – Valores de Índice de Perigo (IP) calculados com as planilhas de avaliação de risco da CETESB para amostras de águas subterrâneas coletadas em poços de município no estado do Rio de Janeiro (Itaboraí).
(Uso das concentrações de bário e de cádmio detectadas.

Poço	Valores de IP (Acima de 1 indicados em vermelho)			
	Residente Rural Criança	Residente Rural Adulto	Residente Urbano Criança	Residente Urbano Adulto
Sanches (2015) - Poços de Itaboraí/RJ				
P-01 (06/13)	-	-	-	-
P-02 (06/13)	-	-	-	-
P-03 (06/13)	-	-	-	-
P-04 (06/13)	-	-	-	-
P-05 (10/13)	**1,02**	0,48	**1,02**	0,44
P-06 (10/13)	0,74	0,35	0,74	0,32
P-07 (10/13)	0,59	0,28	0,59	0,25
P-08 (10/13)	0,37	0,18	0,37	0,16
P-09 (10/13)	0,51	0,24	0,51	0,22
P-10 (10/13)	0,65	0,31	0,65	0,28
P-11 (10/13)	0,36	0,17	0,36	0,15
P-12 (10/13)	0,89	0,42	0,89	0,38
P-13 (10/13)	0,74	0,35	0,74	0,32
P-14 (10/13)	0,41	0,20	0,41	0,18
P-15 (10/13)	-	-	-	-
P-16 (10/13)	0,64	0,30	0,64	0,27
P-17 (10/13)	0,87	0,41	0,87	0,37

Tabela D.11 – Valores de Índice de Perigo (IP) calculados com as planilhas de avaliação de risco da CETESB para amostras de águas subterrâneas coletadas em poços de município no estado do Rio de Janeiro (Itaboraí).
(Uso das concentrações de bário e de cádmio detectadas subtraídas de BaSO4 da especiação do modelo hidrogeoquímico quando IS_{Barita} >0).

Poço	Valores de IP			
	Residente Rural Criança	Residente Rural Adulto	Residente Urbano Criança	Residente Urbano Adulto
Gomes (2012) - Poços de Itaboraí/RJ				
P-01A (08/09)	-	-	-	-
P-01B (08/09)	0,20	0,09	0,20	0,08
P-01C (08/09)	0,65	0,31	0,65	0,28
P-02A (08/09)	-	-	-	-
P-02B (08/09)	0,13	0,06	0,13	0,05
P-02C (08/09)	0,18	0,09	0,18	0,08
P-03A (08/09)	0,26	0,12	0,26	0,11
P-03B (08/09)	-	-	-	-
P-04A (08/09)	0,17	0,08	0,17	0,07
P-04B (08/09)	-	-	-	-
P-05 (08/09)	0,11	0,05	0,11	0,05

Tabela D.12 – Valores de Índice de Perigo (IP) calculados com as planilhas de avaliação de risco da CETESB para amostras de águas subterrâneas coletadas em poços de município no estado do Rio de Janeiro (Itaboraí).
(Uso das concentrações de bário e de cádmio detectadas subtraídas de BaSO4 da especiação do modelo hidrogeoquímico quando IS_{Barita} >0).

Poço	Valores de IP (Acima de 1 indicados em vermelho)			
	Residente Rural Criança	Residente Rural Adulto	Residente Urbano Criança	Residente Urbano Adulto
Sanches (2015) - Poços de Itaboraí/RJ				
P-01 (06/13)	-	-	-	-
P-02 (06/13)	-	-	-	-
P-03 (06/13)	-	-	-	-
P-04 (06/13)	-	-	-	-
P-05 (10/13)	**1,00**	0,48	**1,00**	0,43
P-06 (10/13)	0,74	0,35	0,74	0,32
P-07 (10/13)	0,59	0,28	0,59	0,25
P-08 (10/13)	0,36	0,17	0,36	0,15
P-09 (10/13)	0,50	0,24	0,50	0,21
P-10 (10/13)	0,65	0,31	0,65	0,28
P-11 (10/13)	-	-	-	-
P-12 (10/13)	0,88	0,42	0,88	0,38
P-13 (10/13)	0,74	0,35	0,74	0,32
P-14 (10/13)	0,40	0,19	0,40	0,17
P-15 (10/13)	-	-	-	-
P-16 (10/13)	0,63	0,30	0,63	0,27
P-17 (10/13)	0,86	0,41	0,86	0,37