



Pacific Northwest
NATIONAL LABORATORY

Proudly Operated by Battelle Since 1965

Geochemical Modeling of ILAW Lysimeter Water Extracts

December 2014

KJ Cantrell



Prepared for the U.S. Department of Energy
under Contract DE-AC05-76RL01830

DISCLAIMER

This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency thereof, nor Battelle Memorial Institute, nor any of their employees, makes **any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights.** Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof, or Battelle Memorial Institute. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.

PACIFIC NORTHWEST NATIONAL LABORATORY
operated by
BATTELLE
for the
UNITED STATES DEPARTMENT OF ENERGY
under Contract DE-AC05-76RL01830

Printed in the United States of America

Available to DOE and DOE contractors from the
Office of Scientific and Technical Information,
P.O. Box 62, Oak Ridge, TN 37831-0062;
ph: (865) 576-8401
fax: (865) 576-5728
email: reports@adonis.osti.gov

Available to the public from the National Technical Information Service
5301 Shawnee Rd., Alexandria, VA 22312
ph: (800) 553-NTIS (6847)
email: orders@ntis.gov <<http://www.ntis.gov/about/form.aspx>>
Online ordering: <http://www.ntis.gov>



This document was printed on recycled paper.

(8/2010)

Geochemical Modeling of ILAW Lysimeter Water Extracts

KJ Cantrell

December 2014

Prepared for
the U.S. Department of Energy
under Contract DE-AC05-76RL01830

Pacific Northwest National Laboratory
Richland, Washington 99352

Executive Summary

Geochemical modeling results of water extracts from simulated immobilized low-activity waste (ILAW) glasses, placed in lysimeters for eight years suggest that the secondary phase reaction network developed using product consistency test (PCT) results at 90 °C may need to be modified for field conditions. For sediment samples that had been collected from near the glass samples, the impact of glass corrosion could be readily observed based upon the pH of their water extracts. For unimpacted sediments the pH ranged from 7.88 to 8.11 with an average of 8.04. Sediments that had observable impacts from glass corrosion exhibited elevated pH values (as high as 9.97). For lysimeter sediment samples that appear to have been impacted by glass corrosion to the greatest extent, saturation indices determined for analcime, calcite, and chalcedony in the 1:1 water extracts were near equilibrium and were consistent with the secondary phase reaction network developed using PCT results at 90 °C. $\text{Fe}(\text{OH})_3(\text{s})$ also appears to be essentially at equilibrium in extracts impacted by glass corrosion, but with a solubility product ($\log K_{\text{sp}}$) that is approximately 2.13 units lower than that used in the secondary phase reaction network developed using PCT results at 90 °C. The solubilities of $\text{TiO}_2(\text{am})$ and $\text{ZrO}_2(\text{am})$ [(am) indicates an amorphous phase] also appear to be much lower than that assumed in the secondary phase reaction network developed using PCT results at 90 °C. The extent that the solubility of $\text{TiO}_2(\text{am})$ and $\text{ZrO}_2(\text{am})$ were reduced relative to that assumed in the secondary phase reaction network developed using PCT results at 90°C could not be quantified because the concentrations of Ti and Zr in the extracts were below the estimated quantification limit. Gibbsite was consistently highly oversaturated in the extract while dawsonite was at or near equilibrium. This suggests that dawsonite might be a more suitable phase for the secondary phase reaction network than gibbsite under field conditions. This may be due to the availability of carbonate that exists in the Hanford sediments as calcite. A significant source of carbonate was not available in the PCTs and this may account for why this phase did not appear in the PCTs. Sepiolite was consistently highly undersaturated, suggesting that another phase controls the solubility of magnesium. For samples that were most impacted by the effects of glass corrosion, magnesite appears to control glass corrosion. For samples that show less impact from glass corrosion, clinocllore-7A or saponite-Mg appears to control the magnesium concentrations. For zinc, it appears that zincite is a better candidate than $\text{Zn}(\text{OH})_2\text{-}\gamma$ for controlling zinc concentrations in the extracts; however, in some samples all zinc phases considered were highly oversaturated. As a result the phase that controls zinc concentrations in the lysimeter extracts remains uncertain.

Acronyms and Abbreviations

DOE	U.S. Department of Energy
EQL	estimated quantification limit
FIB	focused ion beam
FLTF	Field Lysimeter Test Facility
FY	fiscal year (October 1 through September 30; e.g., FY 2010 spans October 1, 2009 through September 30, 2010)
ICP-OES	inductively coupled plasma optical emission spectroscopy
IDF	Integrated Disposal Facility
IDF-PA	Integrated Disposal Facility performance assessment
ILAW	immobilized low-activity waste
LAW	low-activity waste
PA	performance assessment
PCT	product consistency test
PVC	polyvinyl chloride
PNNL	Pacific Northwest National Laboratory
QA	quality assurance
R&D	research and development
RTL	Research Technology Laboratory
SEM	scanning electron microscopy
SEM-EDS	scanning electron microscopy-energy dispersive spectroscopy
SI	saturation index
STOMP	Subsurface Transport Over Multiple Phases
TEM-SAED	transmission electron microscopy-selected area electron diffraction
WRPS	Washington River Protection Solutions
WWFTP	WRPS Waste Form Testing Program
XRD	X-ray diffraction

Contents

Executive Summary	iii
Acronyms and Abbreviations	v
1.0 Introduction	1
1.1 Quality Assurance	1
2.0 Background and Methods	3
2.1 ILAW Glass Lysimeter Experiments	3
2.2 Lysimeter Sampling and Characterization	4
2.3 Geochemical Modeling	8
3.0 Modeling Results and Discussion	13
3.1 Saturation Indices of 1:1 Water Extracts.....	13
4.0 Conclusions	18
5.0 References	19
Appendix A – Geochemist’s Workbench Output	A.1

Figures

1.	Surface of Field Lysimeter Test Facility Showing Several Lysimeters and a Side View Diagram of ILAW Glass Test Lysimeters Showing that Each Consisted of Two Groups of Three Glass Cylinders at Upper and Lower Levels	3
2.	Glass Cylinders Being Buried in a Lysimeter at the Hanford Site.....	4
3.	Side View Diagram of ILAW Glass Test Lysimeters Showing that Each Consisted of Two Groups of Three Glass Cylinders at Upper and Lower Levels	5
4.	Plan View of Glass Cylinder Arrays in Lysimeters.	6
5.	Field Photo of Lysimeter D-14 Showing Locations of Large-Diameter Cores Outside Cylinder Array and the Channel of a Small-Diameter Core between Cylinders	7
6.	Photograph of Part of a Glass Cylinder from Lysimeter D-14 Showing the Process of Collection of Glass with Attached Sediment	8
7.	Lysimeter D-10 Glass and Sediment Core Locations	9
8.	Lysimeter D-11 Glass and Sediment Core Locations	10
9.	Lysimeter D-14 Glass and Sediment Core Locations	11

Tables

1.	Thermodynamic Solubility Constants for the Secondary Phase Reaction Network Developed for LAWA44 Glass and Used to Calculate Saturation Indices of Lysimeter Extracts.....	12
2.	Saturation Indices Calculated for Noteworthy Phases in 1:1 Water Extracts of Background Samples and Outer Top Samples from Lysimeter D-14; Also Included are pH Values of the Water Extracts.....	14
3.	Saturation Indices Calculated for Noteworthy Phases in 1:1 Water Extracts of Center Samples from Lysimeters D-10 and D-11; Also Included are pH Values of the Extracts	15
4.	Saturation Indices Calculated for Noteworthy Phases in 1:1 Water Extracts of Center Samples from Lysimeter D-14; Also Included are pH Values of the Extracts	17

1.0 Introduction

Performance assessment calculations for immobilized low-activity waste (ILAW) glass to be disposed at the Hanford Site depend on simulations of long-term glass corrosion behavior and contaminant transport that are being performed via reactive chemical transport modeling (e.g., STOMP simulations). Confidence in the underlying physical and geochemical processes that are included in conceptual models and are being simulated by computer codes can be significantly enhanced through the use of carefully controlled field testing. Field-testing allows the Integrated Disposal Facility performance assessment (IDF-PA) program to obtain independent and site-relevant data on glass corrosion at a length scale more relevant to the actual disposal system. As a result, these field test data can be used to validate the models used to forecast the long-term behavior of the glass waste form and the resulting environmental impacts.

Although lysimeters have several disadvantages, they are the logical choice for field-testing glass corrosion and contaminant transport for IDF-PA model validation. The lysimeter system provides an approach to combine the low-activity waste (LAW) glass, Hanford soil, and other engineered materials in a well-controlled test at a length-scale that is not practical in the laboratory. The walls of the lysimeter: 1) form a physical boundary in the system being studied that defines a fixed volume for calculating water storage and tracer mass balance, and 2) restrict the geometry of flow within the lysimeter to essentially one dimension. Interpretation of complex temporal variations in tracer release and transport is much simpler in one spatial dimension. The field-scale affords the opportunity to monitor contaminant release and transport in time and space that is not possible in laboratory experiments.

In 2002 and 2003 a set of lysimeter field studies was initiated to field-test glass corrosion and contaminant transport for IDF-PA model validation (Meyer et al. 2001; McGrail et al. 2003). The lysimeter field studies were conducted in existing lysimeters at the Field Lysimeter Test Facility (FLTF) at Hanford. In fiscal year 2010 (FY 2010) after approximately eight years of testing, all three of the lysimeters were excavated and soil samples and glass cylinders retrieved. Portions of the solids from all three lysimeters were archived for potential future solids and solution characterization. In FY 2013 experimental data were collected to determine the elemental concentration profiles of samples obtained from lysimeters to determine the flux of elements from the glass samples as a function of depth. This was accomplished with 1:1 water extracts on sediment samples collected from sediment cores taken from the lysimeters (Pierce et al. 2013). Mineralogical and surface analysis of a select number of glass samples collected from the lysimeter facility was also completed. This work included X-ray diffraction (XRD) and scanning electron microscopy (SEM) analyses. In FY 2014 geochemical modeling of the water extracts was conducted to assess the applicability of the currently used suite of secondary phases. This work consisted of conducting saturation index (SI) calculations on the 1:1 water extracts of sediment samples collected from sediment cores taken from the lysimeters. These results are reported here along with a discussion regarding the implications of the results.

1.1 Quality Assurance

This work was conducted with funding from Washington River Protection Solutions (WRPS) under contract 36437-161, ILAW Glass Testing for Disposal at IDF. The work was conducted as part of Pacific Northwest National Laboratory (PNNL) Project 66309, ILAW Glass Testing for Disposal at IDF.

All research and development (R&D) work at PNNL is performed in accordance with PNNL's Laboratory-level Quality Management Program, which is based on a graded application of NQA-1-2000, *Quality Assurance Requirements for Nuclear Facility Applications*, to R&D activities. To ensure that all client quality assurance (QA) expectations were addressed, the QA controls of the WRPS Waste Form Testing Program (WWFTP) QA program were also implemented for this work. The WWFTP QA program consists of the WWFTP Quality Assurance Plan (QA-WWFTP-001) and associated QA-NSLW-numbered procedures that provide detailed instructions for implementing NQA-1 requirements for R&D work.

The work described in this report was assigned the technology level "Applied Research" and was planned, performed, documented, and reported in accordance with Procedure QA-NSLW-1102, *Scientific Investigation for Applied Research*. All staff members contributing to the work received proper technical and quality assurance training prior to performing quality-affecting work.

2.0 Background and Methods

2.1 ILAW Glass Lysimeter Experiments

The ILAW glass lysimeter field studies experiments were conducted in existing lysimeters at the Field Lysimeter Test Facility (FLTF) at Hanford. The FLTF consists of 14 non-weighing lysimeters and four weighing lysimeters installed within a subsurface concrete vault. The size of the lysimeters was 2-m diameter by 3-m deep. Power and water are available at the site. Use of the existing FLTF infrastructure reduced the overall cost of the ILAW glass corrosion field experiments, while satisfying the scientific requirements of the study. Figure 1 shows the surface of the FLTF along with a schematic of how the glass cylinders were arranged in each lysimeter. Three FLTF lysimeters, designated as D-10, D-11, and D-14, were selected and modified for these experiments.

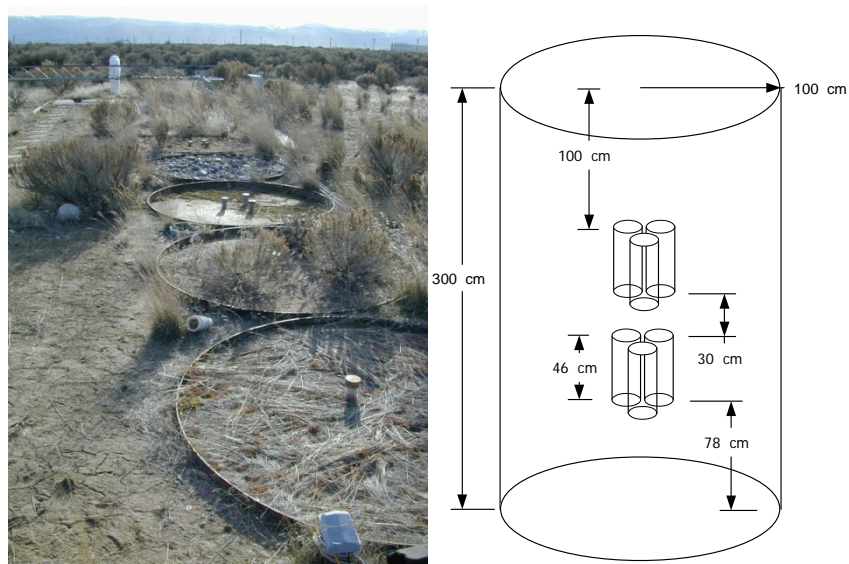


Figure 1. Surface of Field Lysimeter Test Facility (left) Showing Several Lysimeters and a Side View Diagram of ILAW Glass Test Lysimeters Showing that Each Consisted of Two Groups of Three Glass Cylinders at Upper and Lower Levels

The actual glass waste packages to be produced for the IDF will be 213-cm-high cylinders, 122-cm in diameter; however, because of the cost to produce and handle full-size glass cylinders, smaller samples (46 cm high and 20 cm in diameter) were used in the field experiments. These glass samples' dimensions represent a balance between the cost to produce the glass and the desire to represent the key aspects of the flow and transport characteristics of the full-scale facility. Innovatech Services, Inc. prepared twelve HAN28F glass cylinders and six LAWA44 (or equivalent) glass cylinders in 2002 and 2003, respectively (Meyer et al. 2001; McGrail et al. 2003). The glasses were prepared in graphite crucibles, but were transferred to the field in polyvinyl chloride (PVC) containers, which were removed as the glass was buried. The glasses did not include the steel canister of the planned ILAW waste form. A photograph (Figure 2) taken prior to glass burial, illustrates the degree of glass fracturing, which extended throughout the volume of the glass. The fracturing increased the glass surface area and made handling and burial more difficult.



Figure 2. Glass Cylinders Being Buried in a Lysimeter at the Hanford Site

The lysimeter experiments were conducted on the irrigated side of the FLTF; therefore, the experiments received untreated Columbia River water in addition to natural precipitation. The track-mounted overhead irrigation system was set to increase the applied water to three times the average natural precipitation for each month. Irrigation water was typically applied at a rate of 4-mm/hr in increments ranging from 3 to 344-mm per application (Fayer et al. 1999). The lysimeters were watered at 36 cm/year in addition to natural precipitation.

At the time this experiment was set up (FY 2002 and FY 2003), it was expected that the glass waste packages would be placed in the IDF using a hexagonal packing arrangement. The hexagonal packing produces two distinct regions within a layer of the glass cylinders: 1) a central region formed by three adjacent cylinders, and 2) the region along the edge of the layer (or row). Because of the differences in the hydraulic properties of the glass and backfill material, it is anticipated that more water will flow between the glass cylinders than through them. As a consequence, the water content in the region between the cylinders is expected to be higher than the water content outside the row(s) of waste packages. Results from Bacon and McGrail (2001) suggest that the chemistry and transport will also be different in these two regions. To represent both regions in the experimental facility, three glass cylinders were arranged as an equilateral triangle, as shown in Figure 1. The glass cylinders were buried in typical Hanford sandy loam or sandy gravel soils in sets of three per level, two levels in each lysimeter, at depths of 1.0 and 1.76 meters to the tops of the logs. Glass weathering and leachate transport simulation results also suggested that the multiple layers of waste packages will affect the chemistry and transport within the IDF. To investigate these effects in this field experiment, two layers of three glass cylinders are included in the experimental design.

2.2 Lysimeter Sampling and Characterization

After approximately eight years of testing, all three of the lysimeters were excavated and soil and glass cylinders retrieved in FY 2010. The glass samples in one lysimeter (D-14 with LAWA44 glass) were largely intact when dismantled, as compared with the glass samples in lysimeters D-10 and D-11 (HAN28F glass), which were only found in fragments. Portions of the solids from all three lysimeters

were archived for potential future solids and solution characterization. The soil and weathered glass samples were stored in refrigerated storage in the Research Technology Laboratory (RTL) Building at PNNL, and later moved to similar storage in the 331 Building.

During excavation and sampling, large-diameter sediment cores were taken approximately 30 cm from the glass cylinders and small-diameter (19 mm) cores were collected in the volume between the cylinders approximately 1 cm from the glass. These soil samples were collected both for the upper and lower glass cylinder arrays (see Figure 3, Figure 4, Figure 5, and Figure 6). Detailed schematics of the locations, diameters, and lengths of the soil cores obtained from the three lysimeters are found in Figure 7, Figure 8, and Figure 9 for lysimeters D-10 and D-11 with HAN28F glass, and D-14 with LAWA44 glass.

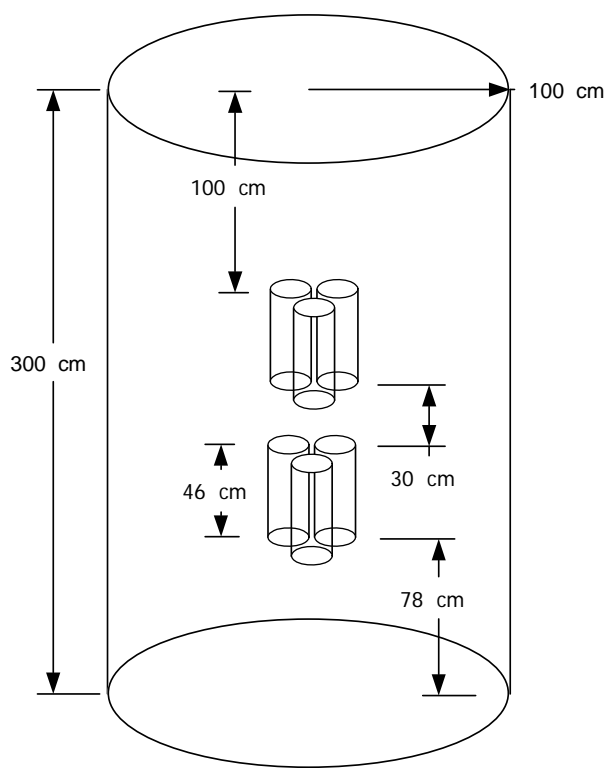


Figure 3. Side View Diagram of ILAW Glass Test Lysimeters Showing that Each Consisted of Two Groups of Three Glass Cylinders at Upper and Lower Levels

For each of the lysimeters, background samples were collected from above the locations of the glass cylinders (indicated as BG in Figure 7, Figure 8, and Figure 9). After the soil cores were brought to the laboratory, 1:1 deionized water extractions were performed. The resulting extracts were analyzed for major and minor cations, anions, pH, and alkalinity. Details of the sample preparation and analysis are available in Pierce et al. (2013). The analytical results of the 1:1 water extracts are also compiled in Pierce et al. (2013).

Selected pieces of glass with sediment attached were subsampled for solid-phase characterization by SEM and XRD. The SEM samples were prepared by first impregnating the sample with epoxy, followed

by cutting with a diamond saw, polishing, and mounting. Samples for XRD analysis were prepared by scraping off sediment attached to the weathered glass samples; the sediment was then powdered and mounted on glass plates.

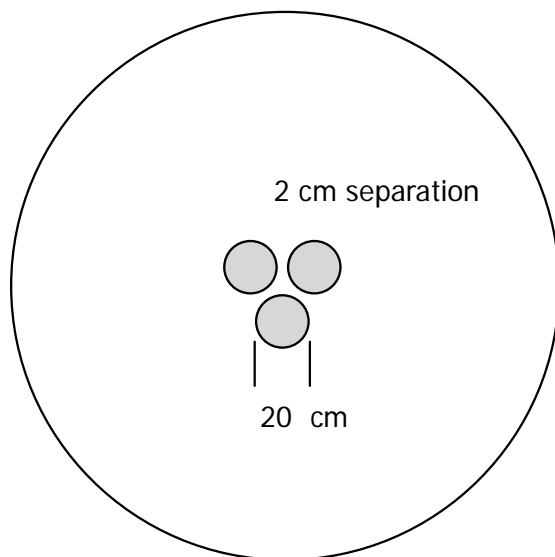


Figure 4. Plan View of Glass Cylinder Arrays in Lysimeters. Sediment samples were collected in two types: large-diameter cores ca. 20–30 cm away from outside of the cylinder array and small-diameter cores between cylinders.



Figure 5. Field Photo of Lysimeter D-14 Showing Locations of Large-Diameter Cores Outside Cylinder Array and the Channel (open hole) of a Small-Diameter Core between Cylinders



Figure 6. Photograph of Part of a Glass Cylinder (LAWA44) from Lysimeter D-14 Showing the Process of Collection of Glass with Attached Sediment

2.3 Geochemical Modeling

Results of the 1:1 water extracts compositions, along with methods used to conduct the extractions, are reported in Piece et al. (2013). Thermodynamic equilibrium modeling was used to calculate mineral saturation indices and to identify solid phases potentially in equilibrium with the 1:1 water extract compositions. For modeling purposes, the redox status of the water extracts was assumed to be approximately in equilibrium with air (an O_2 concentration of 8 mg/L was used in the input). The saturation index is defined as $SI = \log(Q/K_{sp})$, where Q is the activity product and K_{sp} is the mineral solubility product at equilibrium at the temperature of interest. Minerals with SI values near zero (within $\pm \sim 0.5$) are generally considered to be at or near equilibrium, more positive values are considered oversaturated, and more negative values are considered undersaturated with respect to the solution composition. Geochemist's Workbench[®] version 8.09 (Bethke and Yeakel 2010) was used to calculate the mineral SIs for the leachates. The thermodynamic database "thermo.com.V8.R6+.dat" was used for the modeling calculations. Some of the data in the thermodynamic database were modified to better represent the solubility of expected secondary phases (Pierce et al. 2004). Table 1 shows the thermodynamic solubility constants used to model secondary phase formation in the reaction network developed for LAWA44 glass (Pierce et al. 2004). This set of secondary phases was confirmed to be

largely representative of the secondary phases that form during product consistency tests (PCTs) performed with a large number of glass compositions (Pierce et al. 2013).

Lysimeter D-10

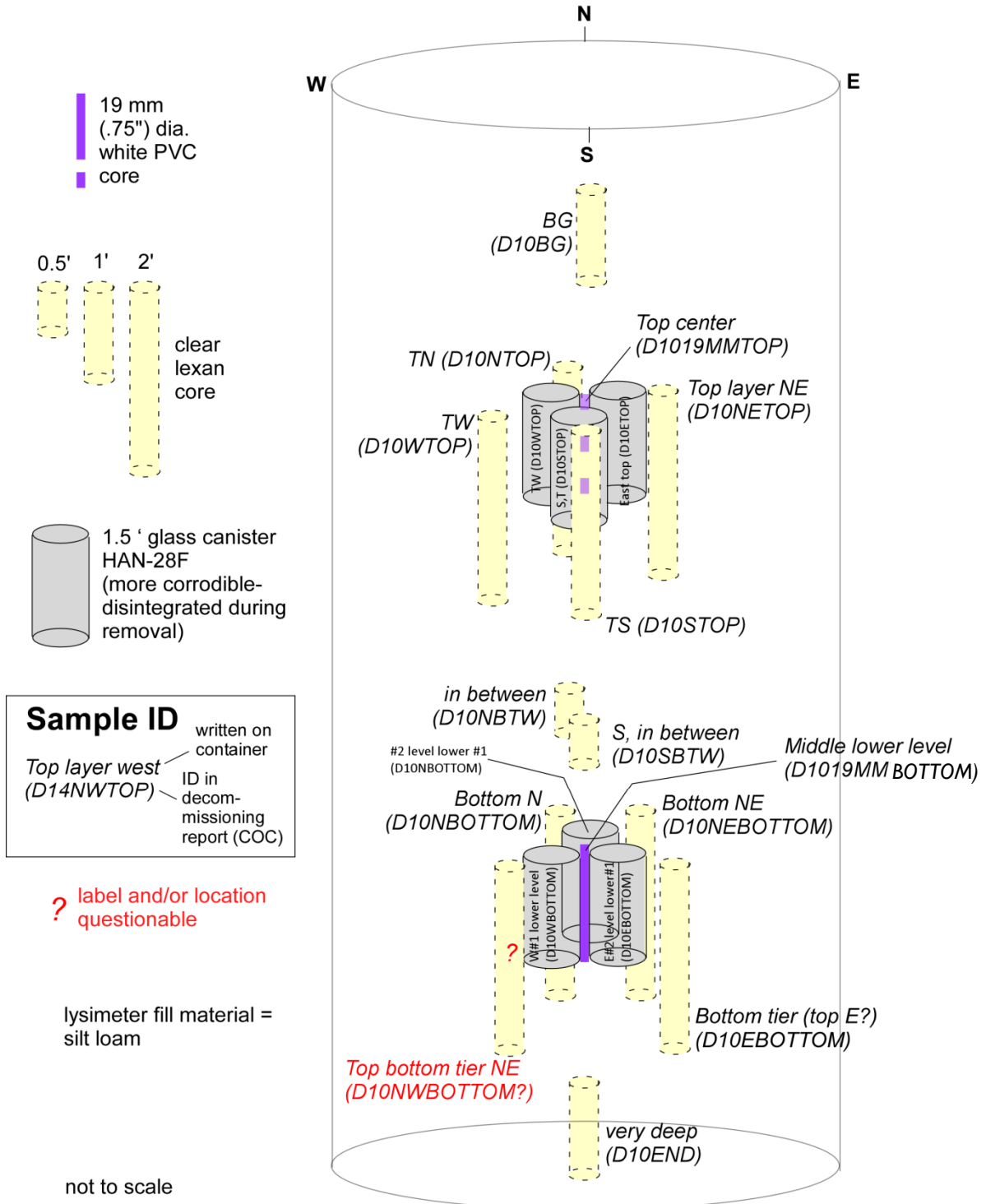


Figure 7. Lysimeter D-10 Glass and Sediment Core Locations

Lysimeter D-11

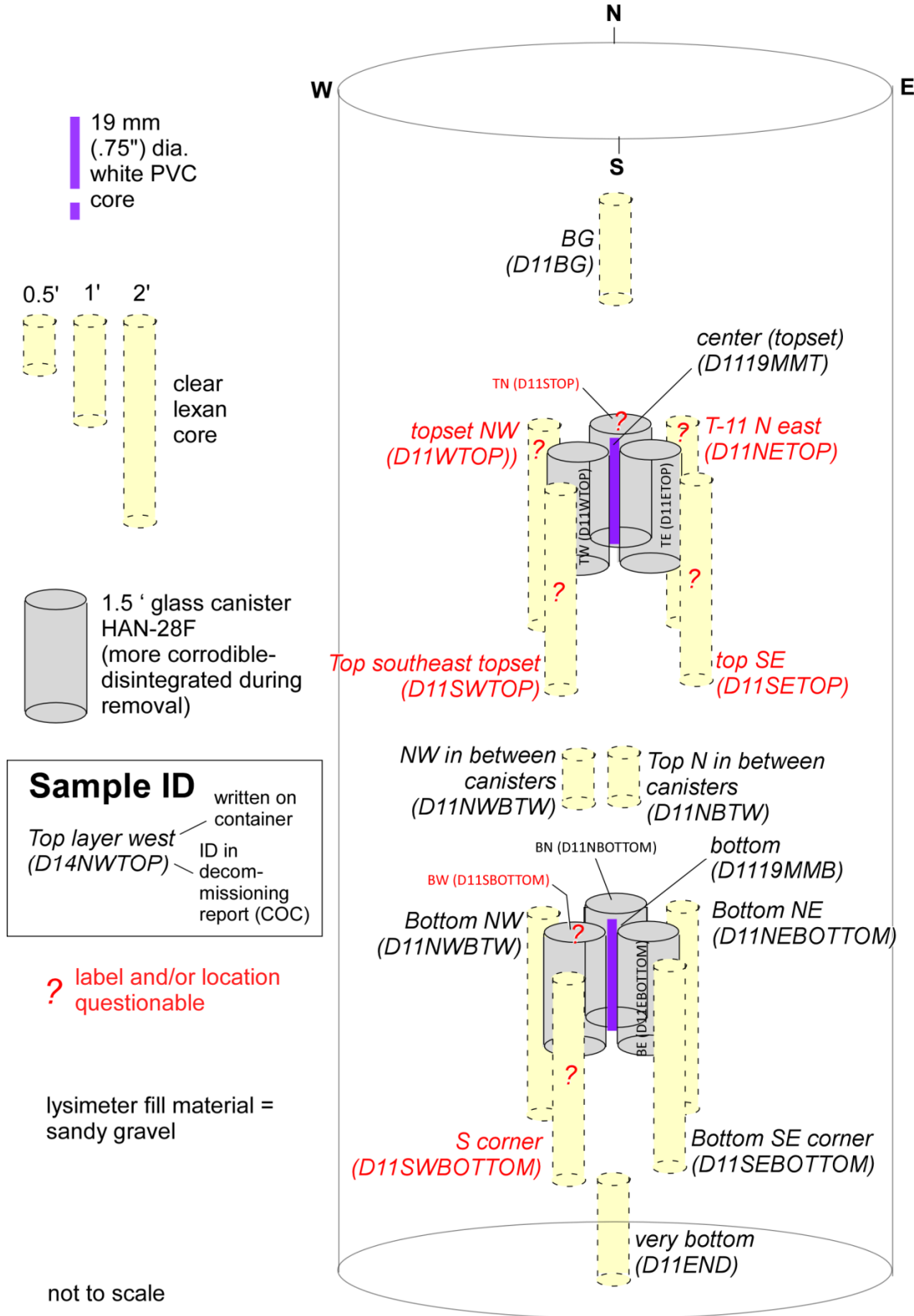


Figure 8. Lysimeter D-11 Glass and Sediment Core Locations

Lysimeter D-14

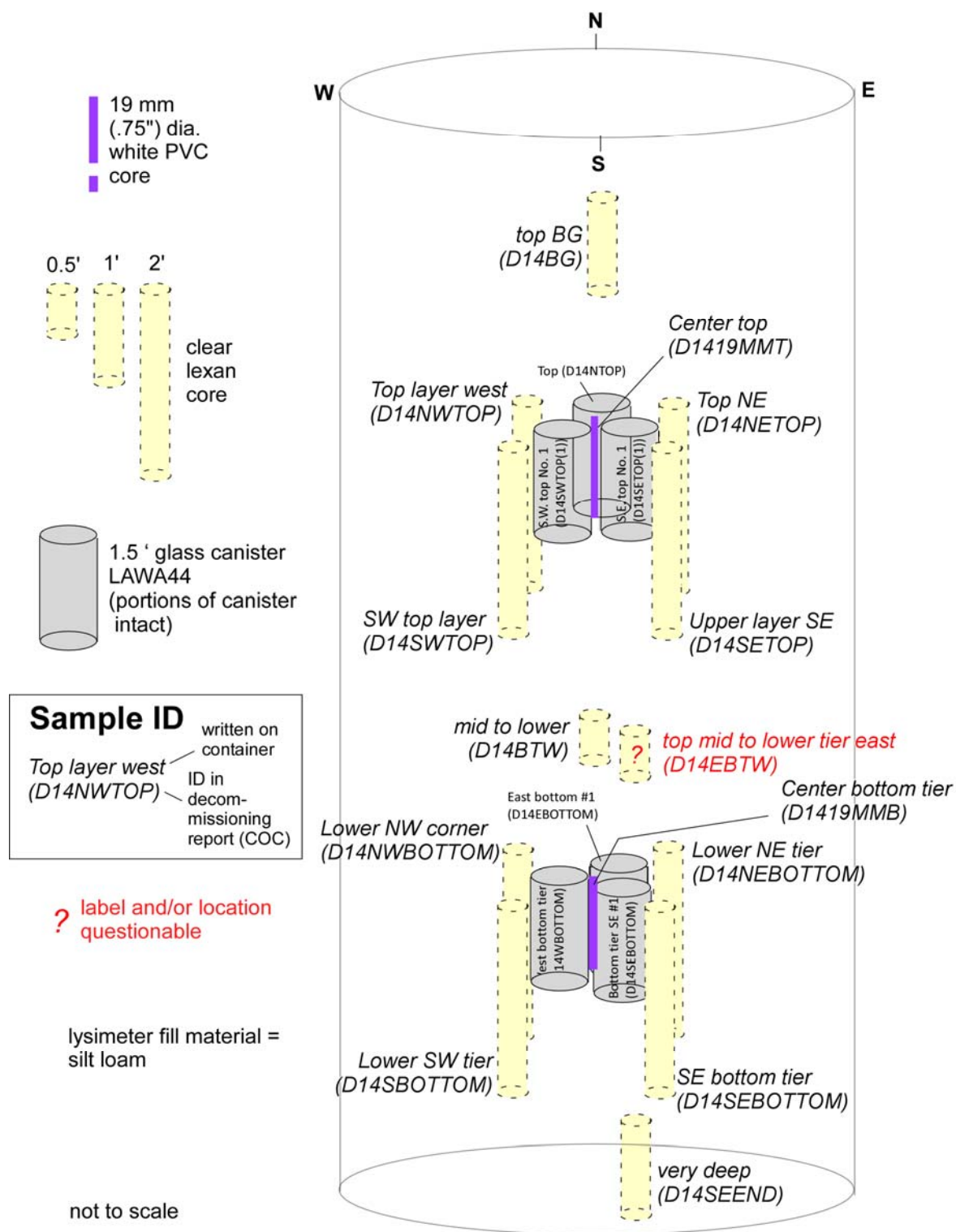


Figure 9. Lysimeter D-14 Glass and Sediment Core Locations

Table 1. Thermodynamic Solubility Constants for the Secondary Phase Reaction Network Developed for LAWA44 Glass and Used to Calculate Saturation Indices of Lysimeter Extracts (Pierce et al. 2004)

Phase	Reaction	Log K (20 °C)
Analcime ($\text{Na}_{0.96}\text{Al}_{0.96}\text{Si}_{2.04}\text{O}_6 \cdot \text{H}_2\text{O}$)	$\text{analcime} + 3.84\text{H}^+ \leftrightarrow 0.96\text{Al}^{3+} + 0.96\text{Na}^+ + 2.04\text{SiO}_2(\text{aq}) + 2.92\text{H}_2\text{O}$	9.34
$\text{TiO}_2(\text{am})$	$\text{TiO}_2 + 2\text{H}_2\text{O} \leftrightarrow \text{Ti}(\text{OH})_4(\text{aq})$	-6.56
$\text{ZrO}_2(\text{am})$	$\text{ZrO}_2 + 2\text{H}^+ \leftrightarrow \text{Zr}(\text{OH})_2^{2+}$	-5.47
Calcite (CaCO_3)	$\text{CaCO}_3 + \text{H}^+ \leftrightarrow \text{Ca}^{2+} + \text{HCO}_3^-$	1.92
Chalcedony (SiO_2)	$\text{SiO}_2 \leftrightarrow \text{SiO}_2(\text{aq})$	-3.55
$\text{Fe}(\text{OH})_3(\text{s})$	$\text{Fe}(\text{OH})_3(\text{am}) + 3\text{H}^+ \leftrightarrow \text{Fe}^{3+} + 3\text{H}_2\text{O}$	9.42
Gibbsite [$\text{Al}(\text{OH})_3$]	$\text{Al}(\text{OH})_3 + 3\text{H}^+ \leftrightarrow \text{Al}^{3+} + 3\text{H}_2\text{O}$	8.08
Sepiolite [$\text{Mg}_4\text{Si}_6\text{O}_{15}(\text{OH})_2 \cdot 6\text{H}_2\text{O}$]	$\text{sepiolite} + 8\text{H}^+ \leftrightarrow 4\text{Mg}^{2+} + 6\text{SiO}_2(\text{aq}) + 11\text{H}_2\text{O}$	45.83
$\text{Zn}(\text{OH})_2\text{-}\gamma$	$\text{Zn}(\text{OH})_2\text{-}\gamma + 2\text{H}^+ \leftrightarrow \text{Zn}^{2+} + 2\text{H}_2\text{O}$	11.88

3.0 Modeling Results and Discussion

Saturation indices were calculated for 43 1:1 water extract samples. The discussion in this section is focused primarily on phases that are part of the secondary phase reaction network established for LAWA44 glass (Pierce et al. 2004). This secondary phase reaction network is based on modeling of LAWA44 PCT results and was later found to be largely consistent with modeling of PCT results conducted on a large number of other ILAW glass samples (Pierce et al. 2013). Other plausible secondary phases that warrant consideration for possible inclusion in or replacement of other phases within the secondary phase reaction network are also included in the discussion. Phases with saturation indices that are near equilibrium but are likely to be present naturally in the background sediments (e.g., dolomite and coesite) are not discussed.

3.1 Saturation Indices of 1:1 Water Extracts

Saturation indices calculated for the most relevant phases in 1:1 water extracts of selected samples are shown in Table 2, Table 3, and Table 4. Saturation index results for $\text{TiO}_2(\text{am})$, $\text{ZrO}_2(\text{am})$ [(am) indicates an amorphous phase], and sepiolite (Table 1) were not included in the tables because Ti and Zr were not detected above the estimated quantification limit (EQL) in any of the samples and sepiolite was always highly undersaturated. Also included in the tables are the measured pH values of the water extracts. Elevated pH relative to background is a good indicator of an influence from glass dissolution on the sediments. Results for background samples and outer top samples from lysimeter D-14 are shown in Table 2. The outer top samples from lysimeter D-14 are included in Table 2 because these samples do not appear to have been significantly impacted by the glass corrosion and are therefore considered to be representative of background samples. Results for the center samples from lysimeters D-10 and D-11 (HAN28F glass) are shown in Table 3 and center samples from lysimeter D-14 (LAWA44 glass) are shown in Table 4. Besides the background samples, the discussion is focused on the center samples because these samples were located in closest proximity to the glass samples and have the highest potential for impacts from glass dissolution.

Review of the data in Table 2 indicates that for all the background samples, calcite (CaCO_3) and chalcedony (SiO_2) are near-equilibrium in all samples. With the exception of sample D10BG, the aluminum concentrations in all samples were below the EQL. For D10BG, gibbsite was highly oversaturated, but dawsonite appears to be essentially at equilibrium. Iron was below the EQL in all the background samples, so SI values could not be calculated for $\text{Fe}(\text{OH})_3(\text{am})$ [Table 2]. In the absence of sepiolite, several alternative phases were considered for controlling magnesium concentrations. These are magnesite (MgCO_3), chlinochlore-7A [$\text{Mg}_5\text{Al}_2\text{Si}_3\text{O}_{10}(\text{OH})_8$], and saponite-Mg [$\text{Mg}_{3.165}\text{Al}_{0.33}\text{Si}_{3.67}\text{O}_{10}(\text{OH})_2$]. Magnesite was consistently well below equilibrium in all the background samples. SI values for chlinochlore-7A and saponite-Mg could be calculated only for sample D10BG because aluminum was below the EQL for all other samples. For sample D10BG, chlinochlore-7A was highly undersaturated and saponite-Mg was oversaturated. The three zinc-containing phases [$\text{Zn}(\text{OH})_2\text{-}\gamma$, zincite (ZnO), and smithsonite (ZnCO_3)] were all unsaturated in the background samples. The pH of the background sample extracts ranged from 7.88 to 8.11, with an average of 8.04.

Table 2. Saturation Indices Calculated for Noteworthy Phases in 1:1 Water Extracts of Background Samples and Outer Top Samples from Lysimeter D-14; Also Included are pH Values of the Water Extracts (blank cells indicate that a phase component was below the EQL, precluding calculation of SI values)

Phase	Sample ID						
	D10BG	D11BG	D14BG	D14SWTOP	D14NWTOP	D14NETOP	D14SETOP
Analcime	-1.74	-	-	-	-	-	-
Calcite	-0.55	-0.37	-0.36	-0.25	-0.33	-0.32	-0.30
Chalcedony	0.18	0.20	0.27	0.35	0.33	0.32	0.32
Fe(OH) ₃ (am)	-	-	-	-	-	-	-
Gibbsite	2.40	-	-	-	-	-	-
Dawsonite	-0.27	-	-	-	-	-	-
Magnesite	-1.62	-1.37	-1.26	-1.26	-1.27	-1.26	-1.19
Clinochlore-7A	-3.86	-	-	-	-	-	-
Saponite-Mg	0.85	-	-	-	-	-	-
Zn(OH) ₂ -γ	-1.70	-1.45	-	-1.37	-	-	-1.34
Zincite	-1.30	-1.04	-	-0.96	-	-	-0.93
Smithsonite	-1.12	-1.02	-	-0.92	-	-	-0.93
pH	7.88	8.04	8.02	8.09	8.08	8.07	8.11

The center samples collected from the D-10 and D-11 lysimeters are expected to have the highest influence from the glass samples. This is because they are located within the center of the three glass samples (Figure 7 and Figure 8) and these two lysimeters contained HAN28F glass. This glass corrodes relatively quickly (Meyer et al. 2001) and will likely impact adjacent sediments to a greater extent than the LAWA44 glass in the D-14 lysimeter. This is apparent from the pH measurements (Table 3), which range from 8.18 to 9.97 with an average of 9.02. These values clearly indicate that corrosion of the HAN28F glass has measurably impacted the sediments located near the center.

The SI values shown in Table 3 indicate that analcime is essentially at equilibrium in the majority of the samples (5 out of 7). With the exception of sample D1019MMB_ts, gibbsite is significantly oversaturated in all samples. Dawsonite is essentially at saturation for four of the seven samples (D1019MMTOP, D1019MMB_ts, D1019MMB_bs, and D1119MMT_bs) and somewhat oversaturated in three of the samples (D1119MMT_ts, D1119MMB_ts, and D1119MMB_bs). These results indicate that dawsonite may be a more appropriate phase in the secondary phase reaction network than gibbsite under field conditions. This could be due to the presence of a significant pool of calcite in the sediments that provides a continuous source of carbonate, and is in contrast to the PCT tests where carbonate concentrations are limited. At this time the presence of dawsonite at the surface of corroding glass has not been confirmed.

Table 3. Saturation Indices Calculated for Noteworthy Phases in 1:1 Water Extracts of Center Samples from Lysimeters D-10 and D-11 (HAN28F glass); Also Included are pH Values of the Extracts (blank cells indicate that a phase component was below the EQL, precluding calculation of SI values)

Phase	Sample ID						
	D1019 MMTOP	D1019 MMB_ts	D1019 MMB_bs	D1119 MMT_ts	D1119 MMT_bs	D1119 MMB_ts	D1119 MMB_bs
Analcime	-1.52	-0.22	-1.22	0.05	-0.08	-0.29	-0.22
Calcite	-0.45	1.44	0.98	1.09	1.16	0.11	0.18
Chalcedony	0.06	0.11	-0.18	0.34	0.26	0.35	0.36
Fe(OH) ₃ (am)	-2.54	-2.07	-	-2.04	-2.10	-2.02	-2.00
Gibbsite	2.25	1.09	0.15	1.92	1.49	2.61	2.54
Dawsonite	-0.03	0.04	-0.25	0.71	0.37	0.70	0.63
Magnesite	-1.88	0.11	0.10	-0.52	-0.24	-1.31	-1.25
Clinocllore-7A	-4.62	9.10	5.64	3.89	6.09	-0.44	0.35
Saponite-Mg	0.30	10.15	8.33	6.48	8.13	3.11	3.70
Zn(OH) ₂ -γ	-1.06	2.14	2.21	-	-	-0.90	-0.67
Zincite	-0.66	2.54	2.62	-	-	-0.49	-0.27
Smithsonite	-0.72	1.29	1.50	-	-	-0.51	-0.39
pH	8.18	9.84	9.97	9.01	9.38	8.33	8.42

Chalcedony is virtually at equilibrium for all samples in Table 3. In contrast, calcite is near equilibrium for only three (D1019MMTOP, D1119MMB_ts, and D1119MMB_bs) of the seven samples. Four of the samples (D1019MMB_ts, D1019MMB_bs, D1119MMT_ts, and D1119MMT_bs) are significantly oversaturated with respect to calcite. This oversaturation with respect to calcite is correlated with pH; all of the extracts with oversaturated SI values have pH values of 9 or above. As ILAW glasses corrode, NaOH is released to solution, increasing the pH and sodium concentration. As the sodium concentration increases, it can exchange for calcium on ion-exchange sites of clay minerals, increasing the calcium concentration in solution. As the pH in solution increases, bicarbonate is increasingly deprotonated to carbonate. Both of these processes result in an increase in the SI for calcite. The water extractions were shaken for only one hour. Apparently this was insufficient time for calcite to precipitate and reestablish equilibrium. It is possible that under field conditions, equilibrium would occur because contact times are much greater than that of the extraction tests.

For samples that had quantifiable concentrations of iron, the SI values for Fe(OH)₃(am) all fell within a relatively narrow range (-2.13 ± 0.20). This suggests that these samples are at equilibrium with an Fe(OH)₃(s) phase that has a lower solubility than that assumed for the secondary phase reaction network. This would be consistent with an Fe(OH)₃(s) phase that is more crystalline than the Fe(OH)₃(am) phase assumed for the secondary phase reaction network, and could have been promoted by repeated wet-dry cycles that would have occurred in the lysimeter tests. This would not occur in the PCT experiments because the glass samples are maintained continuously in water.

In four of the seven samples (D1019MMB_ts, D1019MMB_bs, D1119MMT_ts, and D1119MMT_bs) magnesite is essentially at equilibrium. These samples are the samples that have pH values of 9 or above. In the other three samples (with pH values of 8.42 or less) magnesite is significantly undersaturated. In the case of sample D1019MMTOP, saponite-Mg is near saturation and

chlinochlore-7A is highly undersaturated. For samples D1119MMB_ts and D1119MMB_bs, chlinochlore-7A appears to be near saturation and saponite-Mg is highly oversaturated. It is expected that precipitation of secondary phases will be greatest at the glass-water interface, where pH and concentrations of soluble constituents from the glass will be highest. Because of this, it is hypothesized that magnesite is the most probable secondary phase for controlling the concentrations of Mg that leach from glass. At this time the presence of magnesite at the surface of corroding glass has not been confirmed.

Saturation index values calculated for the zinc minerals shown in Table 3 suggest that when there are measurable values of zinc; zincite (ZnO) is closer to being in equilibrium than $Zn(OH)_2-\gamma$ for samples D1010MMTOP, D1119MMB_ts, and D1119MMB_bs. For samples D1019MMB_ts and D1019MMB_bs, all the zinc phases are highly oversaturated, with smithsonite ($ZnCO_3$) being the least oversaturated.

Saturation indices calculated for phases of interest in the 1:1 water extracts of center samples from lysimeter D-14 (LAWA44 glass) and pH values of the extracts are shown in Table 4. Based on the pH values measured for these samples, it is apparent that corrosion of the LAWA44 had a minimal effect on the sediments from the D-14 lysimeter. Both calcite and chalcedony are effectively at equilibrium for all four samples, similar to the background samples. Many of the samples had components that were below their EQLs, precluding the calculation of SI values for a number of phases. With the exception of gibbsite, dawsonite and saponite-Mg for sample D1419MMT_bs, nearly all the SI values that were calculated indicated that the remaining phases were undersaturated. The most significant impacts due to glass corrosion were observed in sample D1419MMT_bs, which had an extract pH of 8.33. In this sample both gibbsite and saponite-Mg were significantly oversaturated. Analcime was undersaturated, but not to a great extent, and dawsonite appeared to be essentially at saturation. All these results are consistent with the observation that the impact on lysimeter D-14 sediments due to corrosion of LAWA44 glass was minimal.

Table 4. Saturation Indices Calculated for Noteworthy Phases in 1:1 Water Extracts of Center Samples from Lysimeter D-14 (LAWA44 glass); Also Included are pH Values of the Extracts (blank cells indicate that a phase component was below the EQL, precluding calculation of SI values)

Phase	Sample ID			
	D1419 MMT_ts	D1419 MMT_bs	D1419 MMB_ts	D1419 MMB_bs
Analcime	-	-0.88	-	-
Calcite	-0.33	0.25	-0.26	-0.18
Chalcedony	0.26	0.33	0.31	0.27
Fe(OH) ₃ (am)	-	-2.64	-	-
Gibbsite	-	2.01	-	-
Dawsonite	-	0.18	-	-
Magnesite	-1.22	-1.18	-1.23	-1.12
Clinochlore-7A	-	-1.30	-	-
Saponite-Mg	-	3.09	-	-
Zn(OH) ₂ -γ	-1.94	-	-	-1.55
Zincite	-1.54	-	-	-1.15
Smithsonite	-1.25	-	-	-0.97
pH	7.83	8.33	7.97	8.02

4.0 Conclusions

The results of the geochemical modeling of the 1:1 water extracts suggest that the secondary phase reaction network determined for ILAW glass that were derived from PCT results may be different when glass is buried in Hanford sediment. Several factors may be responsible for this effect. The most important geochemical factor is the availability of carbonate minerals (e.g., calcite) that typically occurs in Hanford sediment. The presence of carbonate-containing minerals in the sediments results in pore waters that are typically in equilibrium with calcite. It is believed that this results in dawsonite $[\text{NaAl CO}_3(\text{OH})_2]$ replacing gibbsite within the secondary phase reaction network when glass is corroded in Hanford sediment. It was also found that sepiolite was not likely to form as a secondary phase when glass corrodes in Hanford sediment. Potential alternative phases include magnesite (MgCO_3) and clinocllore $[\text{Mg}_5\text{Al}_2\text{Si}_3\text{O}_{10}(\text{OH})_8]$. The repeated wetting and drying cycles that occurred in the lysimeter experiments may have also had an impact on the nature of the secondary phase reaction network. For example, the solubility of several sparingly soluble metal oxides [e.g., $\text{Fe}(\text{OH})_3$, $\text{TiO}_2(\text{am})$, and $\text{ZrO}_2(\text{am})$] was much lower in the 1:1 extracts of the lysimeter samples than was found for the PCT experiments.

In order to validate that the alternative secondary phases predicted by the geochemical modeling, it is important to conduct solid-phase characterization to demonstrate their occurrence at or near the surface of the glass. Solid-phase characterization work was done as part of the lysimeter sample characterization completed in FY 2013 (Pierce et al. 2013); however, the results were inconclusive with regards to validating the alternative secondary phases identified by the geochemical modeling of the 1:1 water extracts of the lysimeter samples. To overcome this impediment, a complimentary approach is recommended to optimize our ability to identify the secondary phases that form during glass corrosion in contact with Hanford sediments. This will involve a flow-through column experiment designed to optimize secondary phase formation on glass samples that have been fabricated specifically to optimize sample preparation and characterization methods. Advanced microscopy techniques including SEM-EDS (scanning electron microscopy-energy dispersive spectroscopy), FIB (focused ion beam), and TEM-SAED (transmission electron microscopy-selected area electron diffraction) will be used to characterize the secondary solid phases that form. SEM-EDS can be used to identify likely secondary phases based upon morphology and elemental composition. Once likely secondary phases have been identified by SEM-EDS, phase confirmation can be made using TEM-SAED. The FIB can be used to isolate submicron-size subsamples found using SEM-EDS for TEM analysis (TEM requires very thin samples, typically ~100 nanometers). Once the sample prepared with the FIB has been transferred to the TEM, SAED analysis can be used to identify the specific phase under interrogation.

5.0 References

- Bacon DH and BP McGrail. 2001. *Waste Form Release Calculations for the 2001 Immobilized Low-Activity Waste Performance Assessment*. PNNL-13369, Pacific Northwest National Laboratory, Richland, Washington.
- Bethke C. and S Yeakel. 2010. *The Geochemist's Workbench, Release 8.0, Reference Manual*. Urbana, Illinois: Hydrogeology Program.
- Fayer MJ, EM Murphy, JL Downs, FO Khan, CW Lindenmeier, and BN Bjornstad. 1999. *Recharge Data Package for the Immobilized Low-Activity Waste 2001 Performance Assessment*. PNNL-13033, Pacific Northwest National Laboratory, Richland, Washington.
- McGrail B, D Bacon, R Serne, and E Pierce. 2003. *A Strategy to Assess Performance of Selected Low-Activity Waste Forms in an Integrated Disposal Facility*. PNNL-14362, Pacific Northwest National Laboratory, Richland, Washington.
- Meyer PD, BP McGrail, and DH Bacon. 2001. *Test Plan for Field Experiments to Support the Immobilized Low-Activity Waste Disposal Performance Assessment at the Hanford Site*. PNNL-13670, Pacific Northwest National Laboratory, Richland, Washington.
- Pierce EM, BP McGrail, EA Rodriguez, HT Schaefer, KP Saripalli, RJ Serne, KM Krupka, PF Martin, SR Baum, KN Geiszler, LR Reed, and WJ Shaw. 2004. *Waste Form Release Data Package for the 2005 Integrated Disposal Facility Performance Assessment*. PNNL-14805, Pacific Northwest National Laboratory, Richland, Washington.
- Pierce EM, SN Kerisit, EJ Krogstad, SD Burton, BN Bjornstad, VL Freedman, KJ Cantrell, MM Valenta, JV Crum, and JH Westsik, Jr. 2013. *Integrated Disposal Facility FY 2012 Glass Testing Summary Report*. PNNL-21812 Rev. 1, Pacific Northwest National Laboratory, Richland, Washington.

Appendix A

Geochemist's Workbench Output

Appendix A

Geochemist's Workbench Output

Sample D10BG

```

Step #      0                Xi = 0.0000
Temperature = 20.0 C        Pressure = 1.013 bars
pH = 7.880                log fO2 = -0.756
Eh = 0.7610 volts         pe = 13.0836
Ionic strength = 0.001889
Charge imbalance = -0.000281 eq/kg (-19.12% error)
Activity of water = 1.000000
Solvent mass = 1.000000 kg
Solution mass = 1.000166 kg
Solution density = 1.016 g/cm3
Chlorinity = 0.000009 molal
Dissolved solids = 166 mg/kg sol'n
Elect. conductivity = 136.12 uS/cm (or umho/cm)
Hardness = 36.12 mg/kg sol'n as CaCO3
  carbonate = 36.12 mg/kg sol'n as CaCO3
  non-carbonate = 0.00 mg/kg sol'n as CaCO3
Rock mass = 0.000000 kg
Carbonate alkalinity= 71.70 mg/kg sol'n as CaCO3
Water type = Ca-HCO3
  
```

No minerals in system.

Aqueous species	molality	mg/kg sol'n	act. coef.	log act.
HCO3-	0.001415	86.33	0.9534	-2.8700
Na+	0.0005382	12.37	0.9534	-3.2898
SiO2(aq)	0.0004206	25.27	1.0000	-3.3761
Ca++	0.0002778	11.13	0.8299	-3.6373
O2(aq)	0.0002460	7.871	1.0000	-3.6090
K+	7.548e-005	2.951	0.9527	-4.1432
Mg++	7.418e-005	1.803	0.8338	-4.2086
SO4--	5.910e-005	5.676	0.8257	-4.3116
CO2(aq)	4.338e-005	1.909	1.0000	-4.3627
F-	3.012e-005	0.5721	0.9531	-4.5420
NO3-	1.276e-005	0.7911	0.9527	-4.9152
Cl-	8.520e-006	0.3020	0.9527	-5.0906
AlO2-	8.497e-006	0.5011	0.9534	-5.0915
CO3--	5.114e-006	0.3068	0.8268	-5.3739
CaHCO3+	3.704e-006	0.3744	0.9534	-5.4521
HSiO3-	3.279e-006	0.2528	0.9534	-5.5050
Zn++	3.167e-006	0.2070	0.8299	-5.5804
ReO4-	2.405e-006	0.6015	0.9534	-5.6397
CaCO3(aq)	1.881e-006	0.1883	1.0000	-5.7256
CaSO4(aq)	1.422e-006	0.1935	1.0000	-5.8471
NaHCO3(aq)	1.092e-006	0.09170	1.0000	-5.9619
MgHCO3+	9.704e-007	0.08278	0.9534	-6.0338
MgSO4(aq)	6.871e-007	0.08269	1.0000	-6.1630
OH-	5.332e-007	0.009067	0.9531	-6.2940
HALO2(aq)	3.959e-007	0.02375	1.0000	-6.4024
MgCO3(aq)	2.385e-007	0.02010	1.0000	-6.6225
NaHSiO3(aq)	8.011e-008	0.008016	1.0000	-7.0963
Ba++	7.370e-008	0.01012	0.8278	-7.2146
MoO4--	5.949e-008	0.009513	0.8268	-7.3082

MgF+	4.257e-008	0.001843	0.9534	-7.3916
CaF+	3.286e-008	0.001941	0.9534	-7.5040
KSO4-	2.797e-008	0.003780	0.9534	-7.5740
ZnSO4(aq)	2.373e-008	0.003831	1.0000	-7.6246
H+	1.379e-008	1.389e-005	0.9563	-7.8800

(only species > 1e-8 molal listed)

Mineral saturation states

	log Q/K		log Q/K
Stilbite	11.6999s/sat	Wairakite	0.8802s/sat
Muscovite	10.7807s/sat	Saponite-Mg	0.8508s/sat
Beidellite-Ca	8.0299s/sat	Witherite	0.8463s/sat
Beidellite-Mg	7.9642s/sat	Quartz	0.7557s/sat
Illite	7.9517s/sat	Albite_high	0.7510s/sat
Mesolite	7.6646s/sat	Tridymite	0.5581s/sat
Paragonite	7.5991s/sat	Sillimanite	0.5564s/sat
Beidellite-K	7.5808s/sat	Saponite-K	0.4667s/sat
Beidellite-Na	7.5084s/sat	Phlogopite	0.4448s/sat
Montmor-Mg	7.1219s/sat	Saponite-Na	0.3945s/sat
Montmor-Ca	7.1161s/sat	Cristobalite(alp)	0.1937s/sat
Beidellite-H	7.0109s/sat	Chalcedony	0.1798s/sat
Kaolinite	6.9725s/sat	Coesite	-0.0675
Pyrophyllite	6.8076s/sat	Saponite-H	-0.1032
Herschelite	6.7708s/sat	Ice	-0.1194
Montmor-K	6.7388s/sat	Cristobalite(bet)	-0.2644
Montmor-Na	6.6626s/sat	Dawsonite	-0.2692
Scolecite	6.5220s/sat	Jadeite	-0.2763
Laumontite	5.4507s/sat	Talc	-0.3094
Celadonite	4.6950s/sat	Kalsilite	-0.3682
Margarite	4.6471s/sat	Clinocllore-14A	-0.4410
Maximum_Microcli	4.3754s/sat	Dolomite	-0.5113
K-Feldspar	4.3742s/sat	Dolomite-ord	-0.5113
Amesite-14A	3.5031s/sat	Calcite	-0.5495
Lawsonite	3.4096s/sat	Analcime-K	-0.5566
Mordenite	3.3308s/sat	SiO2(am)	-0.5724
Sanidine_high	3.1423s/sat	Aragonite	-0.6941
Diaspore	2.9707s/sat	Smithsonite	-1.1212
Zn2SiO4	2.7680s/sat	Anorthite	-1.1314
Boehmite	2.5582s/sat	Zincite	-1.2989
Gibbsite	2.3987s/sat	Monohydrocalcite	-1.3703
Albite_low	2.1033s/sat	Barite	-1.4597
Albite	2.1032s/sat	Magnesite	-1.6218
Corundum	1.8424s/sat	Zn(OH)2(gamma)	-1.7036
Prehnite	1.2676s/sat	Zn(OH)2(epsilon)	-1.7289
Kyanite	1.2133s/sat	Analcime	-1.7374
Natrolite	0.9913s/sat	Zn(OH)2(beta)	-2.0048
Clinzoisite	0.9642s/sat	Dolomite-dis	-2.0931
Andalusite	0.9298s/sat	Nepheline	-2.4982
Zoisite	0.9183s/sat	Fluorite	-2.6344
Saponite-Ca	0.9158s/sat		

(only minerals with log Q/K > -3 listed)

Gases

	fugacity	log fug.
O2(g)	0.1755	-0.756
H2O(g)	0.01903	-1.721
CO2(g)	0.001085	-2.965
HF(g)	1.913e-014	-13.718
HCl(g)	3.176e-020	-19.498
NO2(g)	3.235e-021	-20.490
N2(g)	4.094e-022	-21.388
NO(g)	3.235e-027	-26.490

Cl2(g)	1.243e-031	-30.906
SiF4(g)	1.137e-038	-37.944
H2(g)	8.946e-043	-42.048
CO(g)	3.100e-049	-48.509
SO2(g)	1.104e-057	-56.957
NH3(g)	1.802e-071	-70.744
Zn(g)	7.616e-076	-75.118
Na(g)	1.466e-077	-76.834
K(g)	4.125e-079	-78.385
F2(g)	2.904e-084	-83.537
Mg(g)	2.696e-132	-131.569
H2S(g)	1.565e-146	-145.806
CH4(g)	3.292e-148	-147.483
Ca(g)	7.074e-155	-154.150
Al(g)	4.844e-192	-191.315
C(g)	5.847e-193	-192.233
Si(g)	2.248e-224	-223.648
S2(g)	2.072e-234	-233.684
C2H4(g)	6.465e-242	-241.189

Original basis	total moles	In fluid		Sorbed		Kd L/kg
		moles	mg/kg	moles	mg/kg	
Al+++	8.90e-006	8.90e-006	0.240			
Ba++	7.38e-008	7.38e-008	0.0101			
Ca++	0.000285	0.000285	11.4			
Cl-	8.52e-006	8.52e-006	0.302			
F-	3.02e-005	3.02e-005	0.574			
H+	-1.57e-005	-1.57e-005	-0.0158			
H2O	55.5	55.5	1.00e+006			
HCO3-	0.00147	0.00147	89.8			
K+	7.55e-005	7.55e-005	2.95			
Mg++	7.61e-005	7.61e-005	1.85			
MoO4--	5.95e-008	5.95e-008	0.00951			
NH3(aq)	1.28e-005	1.28e-005	0.217			
Na+	0.000539	0.000539	12.4			
O2(aq)	0.000272	0.000272	8.69			
ReO4-	2.40e-006	2.40e-006	0.602			
SO4--	6.13e-005	6.13e-005	5.88			
SiO2(aq)	0.000424	0.000424	25.5			
Zn++	3.19e-006	3.19e-006	0.209			

Elemental composition	total moles	In fluid		Sorbed	
		moles	mg/kg	moles	mg/kg
Aluminum	8.899e-006	8.899e-006	0.2401		
Barium	7.381e-008	7.381e-008	0.01013		
Calcium	0.0002848	0.0002848	11.41		
Carbon	0.001471	0.001471	17.67		
Chlorine	8.521e-006	8.521e-006	0.3021		
Fluorine	3.020e-005	3.020e-005	0.5736		
Hydrogen	111.0	111.0	1.119e+005		
Magnesium	7.612e-005	7.612e-005	1.850		
Molybdenum	5.949e-008	5.949e-008	0.005707		
Nitrogen	1.276e-005	1.276e-005	0.1787		
Oxygen	55.51	55.51	8.881e+005		
Potassium	7.551e-005	7.551e-005	2.952		
Rhenium	2.405e-006	2.405e-006	0.4477		
Silicon	0.0004240	0.0004240	11.91		
Sodium	0.0005393	0.0005393	12.40		
Sulfur	6.126e-005	6.126e-005	1.964		
Zinc	3.190e-006	3.190e-006	0.2086		

Sample D10NTOP

```

Step #      0                Xi = 0.0000
Temperature = 20.0 C        Pressure = 1.013 bars
pH = 7.800                 log fO2 = -0.756
Eh = 0.7656 volts         pe = 13.1636
Ionic strength = 0.002025
Charge imbalance = -0.000370 eq/kg (-22.83% error)
Activity of water = 0.999999
Solvent mass = 1.000000 kg
Solution mass = 1.000180 kg
Solution density = 1.016 g/cm3
Chlorinity = 0.000028 molal
Dissolved solids = 180 mg/kg sol'n
Elect. conductivity = 150.44 uS/cm (or umho/cm)
Hardness = 32.15 mg/kg sol'n as CaCO3
  carbonate = 32.15 mg/kg sol'n as CaCO3
  non-carbonate = 0.00 mg/kg sol'n as CaCO3
Rock mass = 0.000000 kg
Carbonate alkalinity = 78.20 mg/kg sol'n as CaCO3
Water type = Na-HCO3
  
```

No minerals in system.

Aqueous species	molality	mg/kg sol'n	act. coef.	log act.
HCO3-	0.001546	94.32	0.9519	-2.8322
Na+	0.0007217	16.59	0.9519	-3.1631
SiO2(aq)	0.0004211	25.30	1.0000	-3.3756
O2(aq)	0.0002460	7.871	1.0000	-3.6090
Ca++	0.0002389	9.572	0.8249	-3.7055
SO4--	8.412e-005	8.080	0.8204	-4.1610
K+	7.924e-005	3.098	0.9512	-4.1228
Mg++	7.345e-005	1.785	0.8291	-4.2154
CO2(aq)	5.689e-005	2.503	1.0000	-4.2450
F-	3.622e-005	0.6881	0.9515	-4.4626
Cl-	2.772e-005	0.9827	0.9512	-4.5789
NO3-	1.255e-005	0.7783	0.9512	-4.9230
CO3--	4.669e-006	0.2801	0.8216	-5.4161
CaHCO3+	3.459e-006	0.3496	0.9519	-5.4825
Zn++	2.755e-006	0.1801	0.8249	-5.6435
HSiO3-	2.735e-006	0.2108	0.9519	-5.5844
ReO4-	2.405e-006	0.6015	0.9519	-5.6404
CaSO4(aq)	1.719e-006	0.2340	1.0000	-5.7647
NaHCO3(aq)	1.594e-006	0.1339	1.0000	-5.7974
CaCO3(aq)	1.459e-006	0.1460	1.0000	-5.8360
MgHCO3+	1.044e-006	0.08904	0.9519	-6.0028
MgSO4(aq)	9.568e-007	0.1151	1.0000	-6.0192
OH-	4.442e-007	0.007554	0.9515	-6.3740
MgCO3(aq)	2.130e-007	0.01796	1.0000	-6.6716
NaHSiO3(aq)	8.933e-008	0.008939	1.0000	-7.0490
Ba++	7.157e-008	0.009826	0.8227	-7.2301
MoO4--	5.949e-008	0.009513	0.8216	-7.3109
MgF+	5.040e-008	0.002182	0.9519	-7.3190
KSO4-	4.153e-008	0.005613	0.9519	-7.4030
CaF+	3.378e-008	0.001995	0.9519	-7.4928
ZnSO4(aq)	2.903e-008	0.004686	1.0000	-7.5372
H+	1.660e-008	1.672e-005	0.9549	-7.8000
NaCO3-	1.045e-008	0.0008673	0.9519	-8.0023
(only species > 1e-8 molal listed)				

Mineral saturation states

	log Q/K		log Q/K
Zn2SiO4	2.3224s/sat	Aragonite	-0.8045
Witherite	0.7886s/sat	Talc	-0.8076
Quartz	0.7562s/sat	Smithsonite	-1.2265
Tridymite	0.5586s/sat	Barite	-1.3247
Cristobalite(alp)	0.1942s/sat	Monohydrocalcite	-1.4807
Chalcedony	0.1803s/sat	Zincite	-1.5220
Coesite	-0.0670	Magnesite	-1.6709
Ice	-0.1194	Zn(OH)2(gamma)	-1.9267
Cristobalite(bet)	-0.2638	Zn(OH)2(epsilon)	-1.9520
SiO2(am)	-0.5719	Zn(OH)2(beta)	-2.2279
Calcite	-0.6599	Dolomite-dis	-2.2526
Dolomite	-0.6708	Fluorite	-2.5437
Dolomite-ord	-0.6708		

(only minerals with log Q/K > -3 listed)

Gases	fugacity	log fug.
O2(g)	0.1755	-0.756
H2O(g)	0.01903	-1.721
CO2(g)	0.001423	-2.847
HF(g)	2.762e-014	-13.559
HCl(g)	1.241e-019	-18.906
NO2(g)	3.821e-021	-20.418
N2(g)	5.709e-022	-21.243
NO(g)	3.820e-027	-26.418
Cl2(g)	1.896e-030	-29.722
SiF4(g)	4.942e-038	-37.306
H2(g)	8.946e-043	-42.048
CO(g)	4.066e-049	-48.391
SO2(g)	2.257e-057	-56.647
NH3(g)	2.128e-071	-70.672
Zn(g)	4.556e-076	-75.341
Na(g)	1.633e-077	-76.787
K(g)	3.596e-079	-78.444
F2(g)	6.051e-084	-83.218
Mg(g)	1.836e-132	-131.736
H2S(g)	3.199e-146	-145.495
CH4(g)	4.317e-148	-147.365
Ca(g)	4.183e-155	-154.379
C(g)	7.668e-193	-192.115
Si(g)	2.251e-224	-223.648
S2(g)	8.659e-234	-233.063
C2H4(g)	1.112e-241	-240.954

Original basis	total moles	In fluid		Sorbed		Kd L/kg
		moles	mg/kg	moles	mg/kg	
Ba++	7.17e-008	7.17e-008	0.00984			
Ca++	0.000246	0.000246	9.84			
Cl-	2.77e-005	2.77e-005	0.983			
F-	3.63e-005	3.63e-005	0.690			
H+	3.47e-005	3.47e-005	0.0350			
H2O	55.5	55.5	1.00e+006			
HCO3-	0.00162	0.00162	98.5			
K+	7.93e-005	7.93e-005	3.10			
Mg++	7.57e-005	7.57e-005	1.84			
MoO4--	5.95e-008	5.95e-008	0.00951			
NH3(aq)	1.26e-005	1.26e-005	0.214			
Na+	0.000723	0.000723	16.6			
O2(aq)	0.000271	0.000271	8.67			

ReO4-	2.40e-006	2.40e-006	0.602
SO4--	8.69e-005	8.69e-005	8.34
SiO2(aq)	0.000424	0.000424	25.5
Zn++	2.78e-006	2.78e-006	0.182

Elemental composition	In fluid			Sorbed	
	total moles	moles	mg/kg	moles	mg/kg
Barium	7.166e-008	7.166e-008	0.009839		
Calcium	0.0002455	0.0002455	9.839		
Carbon	0.001615	0.001615	19.40		
Chlorine	2.773e-005	2.773e-005	0.9829		
Fluorine	3.631e-005	3.631e-005	0.6897		
Hydrogen	111.0	111.0	1.119e+005		
Magnesium	7.571e-005	7.571e-005	1.840		
Molybdenum	5.949e-008	5.949e-008	0.005707		
Nitrogen	1.255e-005	1.255e-005	0.1758		
Oxygen	55.52	55.52	8.881e+005		
Potassium	7.928e-005	7.928e-005	3.099		
Rhenium	2.405e-006	2.405e-006	0.4477		
Silicon	0.0004240	0.0004240	11.91		
Sodium	0.0007234	0.0007234	16.63		
Sulfur	8.687e-005	8.687e-005	2.785		
Zinc	2.784e-006	2.784e-006	0.1820		

Sample D10NETOP

```

Step #      0          Xi = 0.0000
Temperature = 20.0 C   Pressure = 1.013 bars
pH = 7.890           log fO2 = -0.756
Eh = 0.7604 volts    pe = 13.0736
Ionic strength      = 0.002073
Charge imbalance    = -0.000241 eq/kg (-14.5% error)
Activity of water   = 0.999998
Solvent mass        = 1.000000 kg
Solution mass       = 1.000182 kg
Solution density    = 1.016 g/cm3
Chlorinity          = 0.000052 molal
Dissolved solids    = 182 mg/kg sol'n
Elect. conductivity = 156.71 uS/cm (or umho/cm)
Hardness            = 30.18 mg/kg sol'n as CaCO3
  carbonate         = 30.18 mg/kg sol'n as CaCO3
  non-carbonate     = 0.00 mg/kg sol'n as CaCO3
Rock mass           = 0.000000 kg
Carbonate alkalinity = 72.30 mg/kg sol'n as CaCO3
Water type          = Na-HCO3
  
```

No minerals in system.

Aqueous species	molality	mg/kg sol'n	act. coef.	log act.
HCO3-	0.001427	87.06	0.9513	-2.8672
Na+	0.0008798	20.22	0.9513	-3.0773
SiO2(aq)	0.0004830	29.02	1.0000	-3.3160
O2(aq)	0.0002460	7.871	1.0000	-3.6090
Ca++	0.0002284	9.150	0.8231	-3.7259
SO4--	0.0001134	10.89	0.8186	-4.0323
K+	7.244e-005	2.832	0.9507	-4.1620
Mg++	6.417e-005	1.559	0.8274	-4.2749
Cl-	5.217e-005	1.849	0.9507	-4.3045
F-	4.584e-005	0.8708	0.9510	-4.3605
CO2(aq)	4.266e-005	1.877	1.0000	-4.3700
NO3-	1.298e-005	0.8048	0.9507	-4.9086
CO3--	5.311e-006	0.3186	0.8198	-5.3611
HSiO3-	3.862e-006	0.2977	0.9513	-5.4349
CaHCO3+	3.046e-006	0.3078	0.9513	-5.5380
ReO4-	2.405e-006	0.6015	0.9513	-5.6406
CaSO4(aq)	2.206e-006	0.3002	1.0000	-5.6565
NaHCO3(aq)	1.792e-006	0.1505	1.0000	-5.7466
CaCO3(aq)	1.580e-006	0.1581	1.0000	-5.8015
MgSO4(aq)	1.122e-006	0.1350	1.0000	-5.9500
MgHCO3+	8.401e-007	0.07166	0.9513	-6.0973
OH-	5.468e-007	0.009298	0.9510	-6.2840
MgCO3(aq)	2.108e-007	0.01777	1.0000	-6.6761
NaHSiO3(aq)	1.536e-007	0.01537	1.0000	-6.8137
Ba++	6.941e-008	0.009530	0.8209	-7.2443
MoO4--	5.949e-008	0.009513	0.8198	-7.3119
MgF+	5.562e-008	0.002408	0.9513	-7.2764
KSO4-	5.107e-008	0.006901	0.9513	-7.3135
CaF+	4.078e-008	0.002409	0.9513	-7.4112
NaCO3-	1.446e-008	0.001200	0.9513	-7.8615
H+	1.350e-008	1.360e-005	0.9545	-7.8900

(only species > 1e-8 molal listed)

Mineral saturation states

	log Q/K		log Q/K
Witherite	0.8293s/sat	Calcite	-0.6254
Quartz	0.8158s/sat	Dolomite	-0.6408
Tridymite	0.6182s/sat	Dolomite-ord	-0.6408
Cristobalite(alp)	0.2538s/sat	Aragonite	-0.7700
Chalcedony	0.2399s/sat	Barite	-1.2102
Coesite	-0.0075	Monohydrocalcite	-1.4462
Ice	-0.1194	Magnesite	-1.6754
Cristobalite(bet)	-0.2043	Dolomite-dis	-2.2226
Talc	-0.2080	Fluorite	-2.3601
SiO2(am)	-0.5123		

(only minerals with log Q/K > -3 listed)

Gases fugacity log fug.

O2(g)	0.1755	-0.756
H2O(g)	0.01903	-1.721
CO2(g)	0.001067	-2.972
HF(g)	2.839e-014	-13.547
HCl(g)	1.897e-019	-18.722
NO2(g)	3.210e-021	-20.494
N2(g)	4.029e-022	-21.395
NO(g)	3.209e-027	-26.494
Cl2(g)	4.430e-030	-29.354
SiF4(g)	6.334e-038	-37.198
H2(g)	8.946e-043	-42.048
CO(g)	3.049e-049	-48.516
SO2(g)	2.005e-057	-56.698
NH3(g)	1.788e-071	-70.748
Na(g)	2.448e-077	-76.611
K(g)	4.042e-079	-78.393
F2(g)	6.397e-084	-83.194
Mg(g)	2.423e-132	-131.616
H2S(g)	2.842e-146	-145.546
CH4(g)	3.237e-148	-147.490
Ca(g)	6.040e-155	-154.219
C(g)	5.750e-193	-192.240
Si(g)	2.582e-224	-223.588
S2(g)	6.838e-234	-233.165
C2H4(g)	6.252e-242	-241.204

Original basis	total moles	In fluid		Sorbed		Kd L/kg
		moles	mg/kg	moles	mg/kg	
Ba++	6.95e-008	6.95e-008	0.00954			
Ca++	0.000235	0.000235	9.43			
Cl-	5.22e-005	5.22e-005	1.85			
F-	4.59e-005	4.59e-005	0.873			
H+	1.80e-005	1.80e-005	0.0182			
H2O	55.5	55.5	1.00e+006			
HCO3-	0.00148	0.00148	90.4			
K+	7.25e-005	7.25e-005	2.83			
Mg++	6.64e-005	6.64e-005	1.61			
MoO4--	5.95e-008	5.95e-008	0.00951			
NH3(aq)	1.30e-005	1.30e-005	0.221			
Na+	0.000882	0.000882	20.3			
O2(aq)	0.000272	0.000272	8.70			
ReO4-	2.40e-006	2.40e-006	0.602			
SO4--	0.000117	0.000117	11.2			
SiO2(aq)	0.000487	0.000487	29.3			

Elemental composition	In fluid			Sorbed	
	total moles	moles	mg/kg	moles	mg/kg
Barium	6.951e-008	6.951e-008	0.009544		
Calcium	0.0002352	0.0002352	9.426		
Carbon	0.001483	0.001483	17.80		
Chlorine	5.218e-005	5.218e-005	1.850		
Fluorine	4.594e-005	4.594e-005	0.8727		
Hydrogen	111.0	111.0	1.119e+005		
Magnesium	6.640e-005	6.640e-005	1.614		
Molybdenum	5.949e-008	5.949e-008	0.005707		
Nitrogen	1.298e-005	1.298e-005	0.1818		
Oxygen	55.52	55.52	8.880e+005		
Potassium	7.249e-005	7.249e-005	2.834		
Rhenium	2.405e-006	2.405e-006	0.4477		
Silicon	0.0004870	0.0004870	13.68		
Sodium	0.0008818	0.0008818	20.27		
Sulfur	0.0001168	0.0001168	3.744		

Sample D10STOP

```

Step #      0          Xi = 0.0000
Temperature = 20.0 C   Pressure = 1.013 bars
pH = 8.010          log fO2 = -0.757
Eh = 0.7534 volts    pe = 12.9532
Ionic strength      = 0.001954
Charge imbalance    = -0.000334 eq/kg (-20.82% error)
Activity of water   = 0.999999
Solvent mass        = 1.000000 kg
Solution mass       = 1.000179 kg
Solution density    = 1.016 g/cm3
Chlorinity          = 0.000033 molal
Dissolved solids    = 179 mg/kg sol'n
Elect. conductivity = 148.84 uS/cm (or umho/cm)
Hardness            = 26.33 mg/kg sol'n as CaCO3
  carbonate         = 26.33 mg/kg sol'n as CaCO3
  non-carbonate     = 0.00 mg/kg sol'n as CaCO3
Rock mass           = 0.000000 kg
Carbonate alkalinity = 74.90 mg/kg sol'n as CaCO3
Water type          = Na-HCO3
  
```

No minerals in system.

Aqueous species	molality	mg/kg sol'n	act. coef.	log act.
HCO3-	0.001475	89.99	0.9526	-2.8522
Na+	0.0008541	19.63	0.9526	-3.0896
SiO2(aq)	0.0004610	27.69	1.0000	-3.3363
O2(aq)	0.0002451	7.841	1.0000	-3.6107
Ca++	0.0002022	8.101	0.8274	-3.7765
SO4--	8.826e-005	8.477	0.8232	-4.1388
K+	6.817e-005	2.665	0.9520	-4.1878
Mg++	5.293e-005	1.286	0.8315	-4.3565
F-	4.617e-005	0.8770	0.9523	-4.3569
CO2(aq)	3.350e-005	1.474	1.0000	-4.4750
Cl-	3.330e-005	1.180	0.9520	-4.4989
NO3-	9.665e-006	0.5992	0.9520	-5.0361
CO3--	7.208e-006	0.4324	0.8242	-5.2262
AlO2-	6.519e-006	0.3844	0.9526	-5.2069
HSiO3-	4.852e-006	0.3740	0.9526	-5.3352
Fe(OH)3(aq)	3.806e-006	0.4067	1.0000	-5.4195
CaHCO3+	2.802e-006	0.2832	0.9526	-5.5736
ReO4-	2.405e-006	0.6015	0.9526	-5.6400
CaCO3(aq)	1.918e-006	0.1920	1.0000	-5.7171
NaHCO3(aq)	1.803e-006	0.1515	1.0000	-5.7439
CaSO4(aq)	1.536e-006	0.2091	1.0000	-5.8136
MgSO4(aq)	7.279e-007	0.08760	1.0000	-6.1380
OH-	7.199e-007	0.01224	0.9523	-6.1640
MgHCO3+	7.198e-007	0.06140	0.9526	-6.1639
MgCO3(aq)	2.384e-007	0.02010	1.0000	-6.6226
HALO2(aq)	2.250e-007	0.01350	1.0000	-6.6478
NaHSiO3(aq)	1.878e-007	0.01879	1.0000	-6.7262
Ba++	7.080e-008	0.009721	0.8253	-7.2333
MoO4--	5.949e-008	0.009513	0.8242	-7.3095
MgF+	4.643e-008	0.002010	0.9526	-7.3543
KSO4-	3.761e-008	0.005083	0.9526	-7.4458
CaF+	3.655e-008	0.002159	0.9526	-7.4581
NaCO3-	1.915e-008	0.001590	0.9526	-7.7388
H+	1.023e-008	1.031e-005	0.9556	-8.0100

(only species > 1e-8 molal listed)

Mineral saturation states

	log Q/K		log Q/K
Nontronite-Ca	17.9043s/sat	Gibbsite	2.1533s/sat
Nontronite-Mg	17.8373s/sat	Smectite-low-Fe-	1.8282s/sat
Nontronite-Na	17.4720s/sat	Corundum	1.3515s/sat
Nontronite-K	17.4634s/sat	Saponite-Ca	1.3374s/sat
Nontronite-H	16.8653s/sat	Natrolite	1.2804s/sat
Clinoptilolite-h	15.3853s/sat	Saponite-Mg	1.2710s/sat
Clinoptilolite-C	15.3563s/sat	Prehnite	1.1377s/sat
Hematite	12.6694s/sat	Witherite	0.9753s/sat
Clinoptilolite-K	11.7580s/sat	Albite_high	0.9553s/sat
Clinoptilolite-h	11.6482s/sat	Saponite-Na	0.9051s/sat
Stilbite	11.6048s/sat	Saponite-K	0.8965s/sat
Clinoptilolite-h	11.5536s/sat	Quartz	0.7955s/sat
Clinoptilolite-N	11.5528s/sat	Kyanite	0.7623s/sat
Muscovite	10.2493s/sat	Magnetite	0.7441s/sat
Beidellite-Ca	7.6240s/sat	Phlogopite	0.7408s/sat
Illite	7.6058s/sat	Wairakite	0.6694s/sat
Mesolite	7.5986s/sat	Tridymite	0.5979s/sat
Beidellite-Mg	7.5570s/sat	Clinozoisite	0.5889s/sat
Epidote-ord	7.4976s/sat	Zoisite	0.5430s/sat
Epidote	7.4972s/sat	Andalusite	0.4788s/sat
Paragonite	7.3126s/sat	Saponite-H	0.2985s/sat
Beidellite-Na	7.1917s/sat	Cristobalite(alp	0.2335s/sat
Beidellite-K	7.1832s/sat	Chalcedony	0.2196s/sat
Herschelite	6.9531s/sat	Talc	0.1863s/sat
Montmor-Mg	6.9268s/sat	Sillimanite	0.1053s/sat
Montmor-Ca	6.9224s/sat	Coesite	-0.0277
Beidellite-H	6.5851s/sat	Jadeite	-0.1118
Kaolinite	6.5613s/sat	Ice	-0.1194
Montmor-Na	6.5579s/sat	Cristobalite(bet	-0.2246
Montmor-K	6.5534s/sat	Clinochlore-14A	-0.2515
Pyrophyllite	6.4760s/sat	Dawsonite	-0.2966
Scolecite	6.2713s/sat	Kalsilite	-0.4884
Goethite	5.8602s/sat	Dolomite	-0.5029
Andradite	5.7370s/sat	Dolomite-ord	-0.5029
Laumontite	5.2398s/sat	SiO2(am)	-0.5326
Celadonite	4.8064s/sat	Calcite	-0.5410
Maximum_Microcli	4.3348s/sat	Analcime-K	-0.6290
K-Feldspar	4.3337s/sat	Aragonite	-0.6856
Margarite	3.8658s/sat	Smectite-high-Fe	-1.1703
Mordenite	3.4557s/sat	Barite	-1.3057
Lawsonite	3.1192s/sat	Monohydrocalcite	-1.3618
Sanidine_high	3.1017s/sat	Anorthite	-1.4219
Ferrite-Ca	3.0874s/sat	Analcime	-1.5747
Amesite-14A	3.0498s/sat	Magnesite	-1.6219
Ferrite-Mg	2.9298s/sat	Dolomite-dis	-2.0847
Diaspore	2.7252s/sat	Nepheline	-2.3735
Boehmite	2.3128s/sat	Fluorite	-2.4033
Albite_low	2.3076s/sat	Fe(OH)3	-2.8277
Albite	2.3075s/sat		

(only minerals with log Q/K > -3 listed)

Gases	fugacity	log fug.
O2(g)	0.1748	-0.757
H2O(g)	0.01903	-1.721
CO2(g)	0.0008377	-3.077
HF(g)	2.172e-014	-13.663
HCl(g)	9.196e-020	-19.036
NO2(g)	1.817e-021	-20.741
N2(g)	1.301e-022	-21.886

NO(g)	1.820e-027	-26.740
Cl2(g)	1.040e-030	-29.983
SiF4(g)	2.070e-038	-37.684
H2(g)	8.963e-043	-42.048
CO(g)	2.399e-049	-48.620
SO2(g)	9.048e-058	-57.043
NH3(g)	1.019e-071	-70.992
Na(g)	3.140e-077	-76.503
K(g)	5.026e-079	-78.299
F2(g)	3.736e-084	-83.428
Mg(g)	3.497e-132	-131.456
H2S(g)	1.290e-146	-145.889
CH4(g)	2.562e-148	-147.591
Ca(g)	9.359e-155	-154.029
Al(g)	2.761e-192	-191.559
C(g)	4.533e-193	-192.344
Si(g)	2.474e-224	-223.607
S2(g)	1.403e-234	-233.853
C2H4(g)	3.900e-242	-241.409

Original basis	total moles	In fluid		Sorbed		Kd L/kg
		moles	mg/kg	moles	mg/kg	
Al+++	6.75e-006	6.75e-006	0.182			
Ba++	7.09e-008	7.09e-008	0.00974			
Ca++	0.000208	0.000208	8.35			
Cl-	3.33e-005	3.33e-005	1.18			
F-	4.63e-005	4.63e-005	0.879			
Fe++	3.81e-006	3.81e-006	0.213			
H+	-2.57e-005	-2.57e-005	-0.0259			
H2O	55.5	55.5	1.00e+006			
HCO3-	0.00152	0.00152	92.9			
K+	6.82e-005	6.82e-005	2.67			
Mg++	5.47e-005	5.47e-005	1.33			
MoO4--	5.95e-008	5.95e-008	0.00951			
NH3(aq)	9.67e-006	9.67e-006	0.165			
Na+	0.000856	0.000856	19.7			
O2(aq)	0.000265	0.000265	8.49			
ReO4-	2.40e-006	2.40e-006	0.602			
SO4--	9.06e-005	9.06e-005	8.70			
SiO2(aq)	0.000466	0.000466	28.0			

Elemental composition	total moles	In fluid		Sorbed	
		moles	mg/kg	moles	mg/kg
Aluminum	6.747e-006	6.747e-006	0.1820		
Barium	7.094e-008	7.094e-008	0.009741		
Calcium	0.0002085	0.0002085	8.353		
Carbon	0.001523	0.001523	18.29		
Chlorine	3.331e-005	3.331e-005	1.181		
Fluorine	4.626e-005	4.626e-005	0.8786		
Hydrogen	111.0	111.0	1.119e+005		
Iron	3.806e-006	3.806e-006	0.2125		
Magnesium	5.466e-005	5.466e-005	1.328		
Molybdenum	5.949e-008	5.949e-008	0.005707		
Nitrogen	9.665e-006	9.665e-006	0.1354		
Oxygen	55.52	55.52	8.880e+005		
Potassium	6.821e-005	6.821e-005	2.666		
Rhenium	2.405e-006	2.405e-006	0.4477		
Silicon	0.0004660	0.0004660	13.09		
Sodium	0.0008561	0.0008561	19.68		
Sulfur	9.056e-005	9.056e-005	2.903		

Sample D10WTOP

```

Step #      0          Xi = 0.0000
Temperature = 20.0 C   Pressure = 1.013 bars
pH = 8.060          log fO2 = -0.756
Eh = 0.7505 volts    pe = 12.9036
Ionic strength      = 0.002131
Charge imbalance    = -0.000347 eq/kg (-20.35% error)
Activity of water   = 0.999999
Solvent mass        = 1.000000 kg
Solution mass       = 1.000185 kg
Solution density    = 1.016 g/cm3
Chlorinity          = 0.000040 molal
Dissolved solids    = 185 mg/kg sol'n
Elect. conductivity = 160.82 uS/cm (or umho/cm)
Hardness            = 29.44 mg/kg sol'n as CaCO3
  carbonate         = 29.44 mg/kg sol'n as CaCO3
  non-carbonate     = 0.00 mg/kg sol'n as CaCO3
Rock mass           = 0.000000 kg
Carbonate alkalinity = 75.80 mg/kg sol'n as CaCO3
Water type          = Na-HCO3
  
```

No minerals in system.

Aqueous species	molality	mg/kg sol'n	act. coef.	log act.
HCO3-	0.001490	90.91	0.9507	-2.8487
Na+	0.0008797	20.22	0.9507	-3.0776
SiO2(aq)	0.0004465	26.82	1.0000	-3.3502
O2(aq)	0.0002460	7.871	1.0000	-3.6090
Ca++	0.0002140	8.574	0.8211	-3.7552
SO4--	0.0001354	13.00	0.8165	-3.9566
K+	7.922e-005	3.097	0.9500	-4.1234
Mg++	6.967e-005	1.693	0.8255	-4.2402
F-	3.990e-005	0.7579	0.9504	-4.4211
Cl-	3.968e-005	1.407	0.9500	-4.4236
CO2(aq)	3.010e-005	1.324	1.0000	-4.5215
NO3-	1.147e-005	0.7114	0.9500	-4.9625
CO3--	8.219e-006	0.4931	0.8177	-5.1726
HSiO3-	5.284e-006	0.4073	0.9507	-5.2990
CaHCO3+	2.973e-006	0.3005	0.9507	-5.5488
CaSO4(aq)	2.454e-006	0.3341	1.0000	-5.6101
ReO4-	2.405e-006	0.6015	0.9507	-5.6409
CaCO3(aq)	2.279e-006	0.2281	1.0000	-5.6422
NaHCO3(aq)	1.869e-006	0.1570	1.0000	-5.7284
MgSO4(aq)	1.447e-006	0.1741	1.0000	-5.8395
MgHCO3+	9.502e-007	0.08106	0.9507	-6.0441
OH-	8.094e-007	0.01376	0.9504	-6.1140
MgCO3(aq)	3.525e-007	0.02971	1.0000	-6.4529
NaHSiO3(aq)	2.098e-007	0.02100	1.0000	-6.6781
Ba++	7.222e-008	0.009915	0.8188	-7.2282
KSO4-	6.648e-008	0.008984	0.9507	-7.1993
MoO4--	5.949e-008	0.009513	0.8177	-7.3130
MgF+	5.243e-008	0.002270	0.9507	-7.3023
CaF+	3.318e-008	0.001960	0.9507	-7.5011
NaCO3-	2.232e-008	0.001852	0.9507	-7.6733
(only species > 1e-8 molal listed)				

Mineral saturation states

	log Q/K		log Q/K
Witherite	1.0340s/sat	Dolomite-ord	-0.2584
Quartz	0.7816s/sat	Calcite	-0.4662

Talc	0.7796s/sat	SiO2(am)	-0.5465
Tridymite	0.5840s/sat	Aragonite	-0.6108
Cristobalite(alp)	0.2196s/sat	Barite	-1.1183
Chalcedony	0.2057s/sat	Monohydrocalcite	-1.2869
Coesite	-0.0416	Magnesite	-1.4522
Ice	-0.1194	Dolomite-dis	-1.8402
Cristobalite(bet)	-0.2384	Fluorite	-2.5106
Dolomite	-0.2584	Chrysotile	-2.7843

(only minerals with log Q/K > -3 listed)

Gases	fugacity	log fug.
O2(g)	0.1755	-0.756
H2O(g)	0.01903	-1.721
CO2(g)	0.0007527	-3.123
HF(g)	1.670e-014	-13.777
HCl(g)	9.747e-020	-19.011
NO2(g)	1.917e-021	-20.717
N2(g)	1.437e-022	-21.843
NO(g)	1.916e-027	-26.717
Cl2(g)	1.170e-030	-29.932
SiF4(g)	7.000e-039	-38.155
H2(g)	8.946e-043	-42.048
CO(g)	2.151e-049	-48.667
SO2(g)	1.091e-057	-56.962
NH3(g)	1.068e-071	-70.972
Na(g)	3.618e-077	-76.442
K(g)	6.533e-079	-78.185
F2(g)	2.212e-084	-83.655
Mg(g)	5.743e-132	-131.241
H2S(g)	1.547e-146	-145.811
CH4(g)	2.284e-148	-147.641
Ca(g)	1.235e-154	-153.908
C(g)	4.057e-193	-192.392
Si(g)	2.387e-224	-223.622
S2(g)	2.025e-234	-233.694
C2H4(g)	3.112e-242	-241.507

Original basis	total moles	In fluid moles	mg/kg	Sorbed moles	mg/kg	Kd L/kg
Ba++	7.24e-008	7.24e-008	0.00994			
Ca++	0.000222	0.000222	8.88			
Cl-	3.97e-005	3.97e-005	1.41			
F-	4.00e-005	4.00e-005	0.760			
H+	1.46e-006	1.46e-006	0.00147			
H2O	55.5	55.5	1.00e+006			
HCO3-	0.00154	0.00154	93.8			
K+	7.93e-005	7.93e-005	3.10			
Mg++	7.25e-005	7.25e-005	1.76			
MoO4--	5.95e-008	5.95e-008	0.00951			
NH3(aq)	1.15e-005	1.15e-005	0.195			
Na+	0.000882	0.000882	20.3			
O2(aq)	0.000269	0.000269	8.61			
ReO4-	2.40e-006	2.40e-006	0.602			
SO4--	0.000139	0.000139	13.4			
SiO2(aq)	0.000452	0.000452	27.2			

Elemental composition	total moles	In fluid moles	mg/kg	Sorbed moles	mg/kg
Barium	7.238e-008	7.238e-008	0.009937		
Calcium	0.0002217	0.0002217	8.885		

Carbon	0.001537	0.001537	18.46
Chlorine	3.969e-005	3.969e-005	1.407
Fluorine	3.999e-005	3.999e-005	0.7596
Hydrogen	111.0	111.0	1.119e+005
Magnesium	7.247e-005	7.247e-005	1.761
Molybdenum	5.949e-008	5.949e-008	0.005707
Nitrogen	1.147e-005	1.147e-005	0.1607
Oxygen	55.52	55.52	8.880e+005
Potassium	7.928e-005	7.928e-005	3.099
Rhenium	2.405e-006	2.405e-006	0.4477
Silicon	0.0004520	0.0004520	12.69
Sodium	0.0008818	0.0008818	20.27
Sulfur	0.0001393	0.0001393	4.467

Sample D1019MMTOP

```

Step #      0          Xi = 0.0000
Temperature = 20.0 C   Pressure = 1.013 bars
pH = 8.180           log fO2 = -0.759
Eh = 0.7435 volts    pe = 12.7828
Ionic strength      = 0.001939
Charge imbalance    = -0.000325 eq/kg (-19.13% error)
Activity of water   = 0.999999
Solvent mass        = 1.000000 kg
Solution mass       = 1.000181 kg
Solution density    = 1.016 g/cm3
Chlorinity          = 0.000025 molal
Dissolved solids    = 181 mg/kg sol'n
Elect. conductivity = 153.44 uS/cm (or umho/cm)
Hardness            = 17.50 mg/kg sol'n as CaCO3
  carbonate         = 17.50 mg/kg sol'n as CaCO3
  non-carbonate     = 0.00 mg/kg sol'n as CaCO3
Rock mass           = 0.000000 kg
Carbonate alkalinity = 83.60 mg/kg sol'n as CaCO3
Water type          = Na-HCO3
  
```

No minerals in system.

Aqueous species	molality	mg/kg sol'n	act. coef.	log act.
HCO3-	0.001639	100.0	0.9528	-2.8063
Na+	0.001127	25.91	0.9528	-2.9690
SiO2(aq)	0.0003216	19.32	1.0000	-3.4926
O2(aq)	0.0002442	7.812	1.0000	-3.6123
Ca++	0.0001512	6.060	0.8280	-3.9023
K+	6.366e-005	2.488	0.9522	-4.2174
SO4--	5.381e-005	5.168	0.8237	-4.3534
F-	3.358e-005	0.6379	0.9525	-4.4950
CO2(aq)	2.517e-005	1.108	1.0000	-4.5991
Cl-	2.512e-005	0.8902	0.9522	-4.6213
Mg++	1.766e-005	0.4292	0.8320	-4.8328
NO3-	1.335e-005	0.8275	0.9522	-4.8959
AlO2-	1.215e-005	0.7165	0.9528	-4.9364
CO3--	1.184e-005	0.7105	0.8248	-5.0102
Fe(OH)3(aq)	7.383e-006	0.7889	1.0000	-5.1318
HSiO3-	5.007e-006	0.3859	0.9528	-5.3214
Zn++	3.483e-006	0.2277	0.8280	-5.5401
NaHCO3(aq)	2.646e-006	0.2222	1.0000	-5.5774
ReO4-	2.405e-006	0.6015	0.9528	-5.6400
CaCO3(aq)	2.361e-006	0.2363	1.0000	-5.6269
CaHCO3+	2.331e-006	0.2356	0.9528	-5.6535
OH-	1.065e-006	0.01810	0.9525	-5.9940
CaSO4(aq)	7.016e-007	0.09550	1.0000	-6.1539
HALO2(aq)	2.835e-007	0.01701	1.0000	-6.5474
MgHCO3+	2.671e-007	0.02279	0.9528	-6.5943
NaHSiO3(aq)	2.559e-007	0.02560	1.0000	-6.5920
MgSO4(aq)	1.483e-007	0.01785	1.0000	-6.8289
MgCO3(aq)	1.309e-007	0.01103	1.0000	-6.8831
MoO4--	1.036e-007	0.01657	0.8248	-7.0683
Ba++	7.286e-008	0.01000	0.8259	-7.2206
NaCO3-	4.156e-008	0.003449	0.9528	-7.4023
ZnSO4(aq)	2.366e-008	0.003819	1.0000	-7.6261
KSO4-	2.143e-008	0.002896	0.9528	-7.6900
CaF+	1.990e-008	0.001176	0.9528	-7.7221
MgF+	1.128e-008	0.0004882	0.9528	-7.9688

(only species > 1e-8 molal listed)

Mineral saturation states

	log Q/K		log Q/K
Nontronite-Ca	17.9747s/sat	Magnetite	1.6077s/sat
Nontronite-Mg	17.8499s/sat	Natrolite	1.5934s/sat
Nontronite-Na	17.6029s/sat	Corundum	1.5524s/sat
Nontronite-K	17.5448s/sat	Smectite-low-Fe-	1.4504s/sat
Nontronite-H	16.9004s/sat	Prehnite	1.2981s/sat
Clinoptilolite-h	13.8366s/sat	Witherite	1.2039s/sat
Clinoptilolite-C	13.8076s/sat	Albite_high	0.8773s/sat
Hematite	13.2450s/sat	Clinozoisite	0.8498s/sat
Ferrite-Zn	12.1440s/sat	Kyanite	0.8069s/sat
Stilbite	11.0165s/sat	Zoisite	0.8038s/sat
Clinoptilolite-h	10.6409s/sat	Quartz	0.6392s/sat
Clinoptilolite-N	10.6401s/sat	Andalusite	0.5233s/sat
Clinoptilolite-K	10.3244s/sat	Wairakite	0.4593s/sat
Muscovite	10.2220s/sat	Tridymite	0.4416s/sat
Clinoptilolite-h	10.2146s/sat	Saponite-Ca	0.4232s/sat
Epidote-ord	7.9458s/sat	Saponite-Mg	0.2989s/sat
Epidote	7.9454s/sat	Sillimanite	0.1499s/sat
Mesolite	7.6652s/sat	Phlogopite	0.1036s/sat
Paragonite	7.4355s/sat	Cristobalite(alp)	0.0772s/sat
Illite	7.3399s/sat	Chalcedony	0.0633s/sat
Beidellite-Ca	7.3198s/sat	Saponite-Na	0.0514s/sat
Beidellite-Mg	7.1949s/sat	Saponite-K	-0.0067
Herschelite	7.0957s/sat	Dawsonite	-0.0297
Beidellite-Na	6.9480s/sat	Jadeite	-0.0335
Beidellite-K	6.8899s/sat	Ice	-0.1194
Andradite	6.4863s/sat	Coesite	-0.1840
Montmor-Ca	6.4553s/sat	Cristobalite(bet)	-0.3808
Kaolinite	6.4495s/sat	Kalsilite	-0.4039
Montmor-Mg	6.4019s/sat	Calcite	-0.4509
Beidellite-H	6.2456s/sat	Aragonite	-0.5954
Scolecite	6.2175s/sat	Saponite-H	-0.6511
Montmor-Na	6.1514s/sat	Zincite	-0.6585
Goethite	6.1479s/sat	Dolomite	-0.6732
Montmor-K	6.0973s/sat	Dolomite-ord	-0.6732
Pyrophyllite	6.0517s/sat	SiO2(am)	-0.6889
Laumontite	5.0298s/sat	Analcime-K	-0.7167
Celadonite	4.2856s/sat	Smithsonite	-0.7172
Margarite	4.1692s/sat	Talc	-0.8480
Maximum_Microcli	4.1067s/sat	Zn(OH)2(gamma)	-1.0633
K-Feldspar	4.1055s/sat	Zn(OH)2(epsilon)	-1.0886
Zn2SiO4	3.9322s/sat	Clinochlore-14A	-1.2014
Ferrite-Ca	3.8771s/sat	Monohydrocalcite	-1.2716
Ferrite-Mg	3.3689s/sat	Anorthite	-1.3194
Lawsonite	3.2217s/sat	Zn(OH)2(beta)	-1.3645
Mordenite	2.9262s/sat	Smectite-high-Fe	-1.4845
Sanidine_high	2.8736s/sat	Barite	-1.5075
Diaspore	2.8257s/sat	Analcime	-1.5183
Amesite-14A	2.5935s/sat	Magnesite	-1.8823
Boehmite	2.4132s/sat	Nepheline	-2.1389
Gibbsite	2.2537s/sat	Dolomite-dis	-2.2550
Albite_low	2.2297s/sat	Fe(OH)3	-2.5399
Albite	2.2296s/sat	Fluorite	-2.8054

(only minerals with log Q/K > -3 listed)

Gases	fugacity	log fug.
O2(g)	0.1742	-0.759
H2O(g)	0.01903	-1.721
CO2(g)	0.0006295	-3.201
HF(g)	1.068e-014	-13.971

HCl(g)	4.690e-020	-19.329
NO2(g)	1.698e-021	-20.770
N2(g)	1.145e-022	-21.941
NO(g)	1.705e-027	-26.768
Cl2(g)	2.699e-031	-30.569
SiF4(g)	8.455e-040	-39.073
H2(g)	8.979e-043	-42.047
CO(g)	1.806e-049	-48.743
SO2(g)	2.528e-058	-57.597
NH3(g)	9.586e-072	-71.018
Zn(g)	3.339e-075	-74.476
Na(g)	6.136e-077	-76.212
K(g)	6.950e-079	-78.158
F2(g)	9.022e-085	-84.045
Mg(g)	2.560e-132	-131.592
H2S(g)	3.624e-147	-146.441
CH4(g)	1.939e-148	-147.712
Ca(g)	1.536e-154	-153.814
Al(g)	3.489e-192	-191.457
C(g)	3.419e-193	-192.466
Si(g)	1.732e-224	-223.761
S2(g)	1.103e-235	-234.957
C2H4(g)	2.227e-242	-241.652

Original basis	total moles	In fluid		Sorbed		Kd L/kg
		moles	mg/kg	moles	mg/kg	
Al+++	1.24e-005	1.24e-005	0.336			
Ba++	7.31e-008	7.31e-008	0.0100			
Ca++	0.000157	0.000157	6.28			
Cl-	2.51e-005	2.51e-005	0.890			
F-	3.36e-005	3.36e-005	0.639			
Fe++	7.38e-006	7.38e-006	0.412			
H+	-7.31e-005	-7.31e-005	-0.0737			
H2O	55.5	55.5	1.00e+006			
HCO3-	0.00168	0.00168	103.			
K+	6.37e-005	6.37e-005	2.49			
Mg++	1.82e-005	1.82e-005	0.443			
MoO4--	1.04e-007	1.04e-007	0.0166			
NH3(aq)	1.33e-005	1.33e-005	0.227			
Na+	0.00113	0.00113	26.0			
O2(aq)	0.000273	0.000273	8.73			
ReO4-	2.40e-006	2.40e-006	0.602			
SO4--	5.47e-005	5.47e-005	5.25			
SiO2(aq)	0.000327	0.000327	19.6			
Zn++	3.51e-006	3.51e-006	0.229			

Elemental composition	total moles	In fluid		Sorbed	
		moles	mg/kg	moles	mg/kg
Aluminum	1.244e-005	1.244e-005	0.3355		
Barium	7.309e-008	7.309e-008	0.01004		
Calcium	0.0001567	0.0001567	6.277		
Carbon	0.001684	0.001684	20.23		
Chlorine	2.512e-005	2.512e-005	0.8904		
Fluorine	3.362e-005	3.362e-005	0.6386		
Hydrogen	111.0	111.0	1.119e+005		
Iron	7.383e-006	7.383e-006	0.4123		
Magnesium	1.822e-005	1.822e-005	0.4428		
Molybdenum	1.036e-007	1.036e-007	0.009937		
Nitrogen	1.335e-005	1.335e-005	0.1869		
Oxygen	55.52	55.52	8.880e+005		
Potassium	6.368e-005	6.368e-005	2.489		

Rhenium	2.405e-006	2.405e-006	0.4477
Silicon	0.0003269	0.0003269	9.180
Sodium	0.001130	0.001130	25.97
Sulfur	5.470e-005	5.470e-005	1.754
Zinc	3.507e-006	3.507e-006	0.2292

Sample D10NBTW

```

Step #      0          Xi = 0.0000
Temperature = 20.0 C   Pressure = 1.013 bars
pH = 8.050          log fO2 = -0.756
Eh = 0.7511 volts    pe = 12.9136
Ionic strength      = 0.002010
Charge imbalance    = -0.000350 eq/kg (-21.43% error)
Activity of water   = 0.999999
Solvent mass       = 1.000000 kg
Solution mass      = 1.000179 kg
Solution density    = 1.016 g/cm3
Chlorinity         = 0.000041 molal
Dissolved solids   = 178 mg/kg sol'n
Elect. conductivity = 151.53 uS/cm (or umho/cm)
Hardness           = 27.70 mg/kg sol'n as CaCO3
  carbonate        = 27.70 mg/kg sol'n as CaCO3
  non-carbonate    = 0.00 mg/kg sol'n as CaCO3
Rock mass          = 0.000000 kg
Carbonate alkalinity = 75.70 mg/kg sol'n as CaCO3
Water type         = Na-HCO3
  
```

No minerals in system.

Aqueous species	molality	mg/kg sol'n	act. coef.	log act.
HCO3-	0.001489	90.84	0.9520	-2.8484
Na+	0.0008327	19.14	0.9520	-3.1009
SiO2(aq)	0.0004224	25.38	1.0000	-3.3743
O2(aq)	0.0002460	7.871	1.0000	-3.6090
Ca++	0.0002056	8.238	0.8254	-3.7704
SO4--	9.964e-005	9.570	0.8210	-4.0872
K+	7.923e-005	3.097	0.9514	-4.1227
Mg++	6.221e-005	1.512	0.8296	-4.2873
Cl-	4.135e-005	1.466	0.9514	-4.4052
F-	3.810e-005	0.7236	0.9517	-4.4406
CO2(aq)	3.082e-005	1.356	1.0000	-4.5112
AlO2-	1.481e-005	0.8733	0.9520	-4.8508
CO3--	7.993e-006	0.4796	0.8221	-5.1824
HSiO3-	4.878e-006	0.3760	0.9520	-5.3331
CaHCO3+	2.869e-006	0.2900	0.9520	-5.5636
Zn++	2.809e-006	0.1837	0.8254	-5.6348
ReO4-	2.405e-006	0.6015	0.9520	-5.6403
CaCO3(aq)	2.152e-006	0.2154	1.0000	-5.6671
NaHCO3(aq)	1.773e-006	0.1489	1.0000	-5.7514
CaSO4(aq)	1.755e-006	0.2388	1.0000	-5.7558
MgSO4(aq)	9.610e-007	0.1157	1.0000	-6.0173
MgHCO3+	8.520e-007	0.07268	0.9520	-6.0909
OH-	7.898e-007	0.01343	0.9517	-6.1240
HALO2(aq)	4.659e-007	0.02794	1.0000	-6.3317
MgCO3(aq)	3.093e-007	0.02607	1.0000	-6.5097
NaHSiO3(aq)	1.839e-007	0.01840	1.0000	-6.7355
Ba++	6.721e-008	0.009228	0.8232	-7.2570
MoO4--	5.949e-008	0.009513	0.8221	-7.3106
KSO4-	4.922e-008	0.006652	0.9520	-7.3292
MgF+	4.492e-008	0.001945	0.9520	-7.3689
ZnSO4(aq)	3.510e-008	0.005667	1.0000	-7.4546
CaF+	3.060e-008	0.001807	0.9520	-7.5357
NaCO3-	2.066e-008	0.001714	0.9520	-7.7063

(only species > 1e-8 molal listed)

Mineral saturation states

	log Q/K		log Q/K
Stilbite	12.1274s/sat	Saponite-K	1.3437s/sat
Muscovite	11.1887s/sat	Saponite-Na	1.3271s/sat
Illite	8.3003s/sat	Wairakite	1.2359s/sat
Beidellite-Ca	8.2355s/sat	Albite_high	1.1862s/sat
Mesolite	8.1894s/sat	Andalusite	1.0730s/sat
Beidellite-Mg	8.1788s/sat	Clinochlore-14A	1.0125s/sat
Paragonite	8.1756s/sat	Witherite	0.9954s/sat
Beidellite-K	7.8151s/sat	Quartz	0.7576s/sat
Beidellite-Na	7.7983s/sat	Saponite-H	0.7110s/sat
Herschelite	7.6147s/sat	Sillimanite	0.6995s/sat
Montmor-Mg	7.3767s/sat	Tridymite	0.5599s/sat
Montmor-Ca	7.3619s/sat	Talc	0.4820s/sat
Beidellite-H	7.1823s/sat	Cristobalite(alp	0.1955s/sat
Kaolinite	7.1175s/sat	Chalcedony	0.1816s/sat
Montmor-K	7.0134s/sat	Jadeite	0.1570s/sat
Montmor-Na	6.9927s/sat	Dawsonite	0.0120s/sat
Pyrophyllite	6.9564s/sat	Coesite	-0.0657
Scolecite	6.8758s/sat	Kalsilite	-0.1053
Laumontite	5.8064s/sat	Ice	-0.1194
Celadonite	5.2249s/sat	Cristobalite(bet	-0.2625
Margarite	5.1404s/sat	Analcime-K	-0.3022
Amesite-14A	4.8348s/sat	Dolomite	-0.3400
Maximum_Microcli	4.6421s/sat	Dolomite-ord	-0.3400
K-Feldspar	4.6409s/sat	Calcite	-0.4911
Lawsonite	3.7616s/sat	SiO2(am)	-0.5706
Mordenite	3.5961s/sat	Aragonite	-0.6356
Sanidine_high	3.4090s/sat	Anorthite	-0.7794
Zn2SiO4	3.3411s/sat	Smithsonite	-0.9840
Diaspore	3.0413s/sat	Zincite	-1.0133
Boehmite	2.6289s/sat	Barite	-1.2778
Albite_low	2.5385s/sat	Monohydrocalcite	-1.3118
Albite	2.5384s/sat	Analcime	-1.3212
Gibbsite	2.4693s/sat	Zn(OH)2(gamma)	-1.4180
Corundum	1.9837s/sat	Zn(OH)2(epsilon)	-1.4433
Natrolite	1.8561s/sat	Magnesite	-1.5090
Prehnite	1.8284s/sat	Zn(OH)2(beta)	-1.7192
Saponite-Ca	1.7641s/sat	Dolomite-dis	-1.9218
Saponite-Mg	1.7081s/sat	Nepheline	-2.0667
Clinzoisite	1.5956s/sat	Clinochlore-7A	-2.4024
Zoisite	1.5497s/sat	Fluorite	-2.5647
Phlogopite	1.4955s/sat	Cordierite_hydr	-2.6095
Kyanite	1.3565s/sat		

(only minerals with log Q/K > -3 listed)

Gases	fugacity	log fug.
O2(g)	0.1755	-0.756
H2O(g)	0.01903	-1.721
CO2(g)	0.0007707	-3.113
HF(g)	1.634e-014	-13.787
HCl(g)	1.041e-019	-18.983
Cl2(g)	1.334e-030	-29.875
SiF4(g)	6.069e-039	-38.217
H2(g)	8.946e-043	-42.048
CO(g)	2.203e-049	-48.657
SO2(g)	8.458e-058	-57.073
Zn(g)	1.470e-075	-74.833
Na(g)	3.351e-077	-76.475
K(g)	6.395e-079	-78.194
F2(g)	2.117e-084	-83.674

Mg(g)	4.921e-132	-131.308
H2S(g)	1.199e-146	-145.921
CH4(g)	2.339e-148	-147.631
Ca(g)	1.139e-154	-153.943
Al(g)	5.700e-192	-191.244
C(g)	4.154e-193	-192.382
Si(g)	2.258e-224	-223.646
S2(g)	1.216e-234	-233.915
C2H4(g)	3.263e-242	-241.486

Original basis	total moles	In fluid		Sorbed		Kd L/kg
		moles	mg/kg	moles	mg/kg	
Al+++	1.53e-005	1.53e-005	0.412			
Ba++	6.74e-008	6.74e-008	0.00925			
Ca++	0.000212	0.000212	8.51			
Cl-	4.14e-005	4.14e-005	1.47			
F-	3.82e-005	3.82e-005	0.725			
H+	-4.62e-005	-4.62e-005	-0.0465			
H2O	55.5	55.5	1.00e+006			
HCO3-	0.00154	0.00154	93.7			
K+	7.93e-005	7.93e-005	3.10			
Mg++	6.44e-005	6.44e-005	1.56			
MoO4--	5.95e-008	5.95e-008	0.00951			
Na+	0.000835	0.000835	19.2			
O2(aq)	0.000246	0.000246	7.87			
ReO4-	2.40e-006	2.40e-006	0.602			
SO4--	0.000102	0.000102	9.84			
SiO2(aq)	0.000427	0.000427	25.7			
Zn++	2.84e-006	2.84e-006	0.186			

Elemental composition	total moles	In fluid		Sorbed	
		moles	mg/kg	moles	mg/kg
Aluminum	1.528e-005	1.528e-005	0.4123		
Barium	6.736e-008	6.736e-008	0.009249		
Calcium	0.0002124	0.0002124	8.511		
Carbon	0.001536	0.001536	18.44		
Chlorine	4.136e-005	4.136e-005	1.466		
Fluorine	3.818e-005	3.818e-005	0.7251		
Hydrogen	111.0	111.0	1.119e+005		
Magnesium	6.438e-005	6.438e-005	1.564		
Molybdenum	5.949e-008	5.949e-008	0.005707		
Oxygen	55.52	55.52	8.880e+005		
Potassium	7.928e-005	7.928e-005	3.099		
Rhenium	2.405e-006	2.405e-006	0.4477		
Silicon	0.0004275	0.0004275	12.00		
Sodium	0.0008347	0.0008347	19.19		
Sulfur	0.0001024	0.0001024	3.284		
Zinc	2.844e-006	2.844e-006	0.1860		

Sample D10NBOT

```

Step #      0          Xi = 0.0000
Temperature = 20.0 C   Pressure = 1.013 bars
pH = 8.130           log fO2 = -0.756
Eh = 0.7464 volts    pe = 12.8336
Ionic strength = 0.001950
Charge imbalance = -0.000304 eq/kg (-19.44% error)
Activity of water = 1.000000
Solvent mass = 1.000000 kg
Solution mass = 1.000174 kg
Solution density = 1.016 g/cm3
Chlorinity = 0.000010 molal
Dissolved solids = 174 mg/kg sol'n
Elect. conductivity = 145.00 uS/cm (or umho/cm)
Hardness = 30.99 mg/kg sol'n as CaCO3
  carbonate = 30.99 mg/kg sol'n as CaCO3
  non-carbonate = 0.00 mg/kg sol'n as CaCO3
Rock mass = 0.000000 kg
Carbonate alkalinity = 75.80 mg/kg sol'n as CaCO3
Water type = Na-HCO3
  
```

No minerals in system.

Aqueous species	molality	mg/kg sol'n	act. coef.	log act.
HCO3-	0.001487	90.70	0.9527	-2.8488
Na+	0.0007216	16.59	0.9527	-3.1627
SiO2(aq)	0.0004318	25.94	1.0000	-3.3647
O2(aq)	0.0002460	7.871	1.0000	-3.6090
Ca++	0.0002332	9.345	0.8276	-3.7145
K+	8.252e-005	3.226	0.9520	-4.1048
SO4--	7.181e-005	6.898	0.8233	-4.2282
Mg++	6.672e-005	1.621	0.8317	-4.2558
F-	3.540e-005	0.6725	0.9524	-4.4722
CO2(aq)	2.561e-005	1.127	1.0000	-4.5916
NO3-	1.300e-005	0.8058	0.9520	-4.9075
Cl-	1.041e-005	0.3689	0.9520	-5.0040
CO3--	9.575e-006	0.5745	0.8244	-5.1027
HSiO3-	5.991e-006	0.4618	0.9527	-5.2435
CaHCO3+	3.258e-006	0.3293	0.9527	-5.5081
CaCO3(aq)	2.941e-006	0.2943	1.0000	-5.5316
Zn++	2.595e-006	0.1697	0.8276	-5.6680
ReO4-	2.405e-006	0.6015	0.9527	-5.6400
NaHCO3(aq)	1.536e-006	0.1290	1.0000	-5.8136
CaSO4(aq)	1.442e-006	0.1963	1.0000	-5.8409
OH-	9.489e-007	0.01614	0.9524	-6.0440
MgHCO3+	9.147e-007	0.07803	0.9527	-6.0598
MgSO4(aq)	7.469e-007	0.08989	1.0000	-6.1267
MgCO3(aq)	3.995e-007	0.03368	1.0000	-6.3985
NaHSiO3(aq)	1.960e-007	0.01961	1.0000	-6.7078
MoO4--	1.005e-007	0.01607	0.8244	-7.0816
Ba++	7.290e-008	0.01001	0.8255	-7.2206
MgF+	4.489e-008	0.001944	0.9527	-7.3689
KSO4-	3.705e-008	0.005007	0.9527	-7.4522
CaF+	3.234e-008	0.001910	0.9527	-7.5113
ZnSO4(aq)	2.350e-008	0.003794	1.0000	-7.6289
NaCO3-	2.150e-008	0.001785	0.9527	-7.6885
(only species > 1e-8 molal listed)				

Mineral saturation states

	log Q/K		log Q/K
Zn2SiO4	3.6041s/sat	SiO2(am)	-0.5610
Witherite	1.1115s/sat	Zincite	-0.8865
Talc	1.0948s/sat	Smithsonite	-0.9377
Quartz	0.7671s/sat	Monohydrocalcite	-1.1763
Tridymite	0.5695s/sat	Zn(OH)2(gamma)	-1.2912
Cristobalite(alp)	0.2051s/sat	Zn(OH)2(epsilon)	-1.3166
Chalcedony	0.1912s/sat	Barite	-1.3823
Coesite	-0.0561	Magnesite	-1.3978
Dolomite	-0.0933	Zn(OH)2(beta)	-1.5925
Dolomite-ord	-0.0933	Dolomite-dis	-1.6751
Ice	-0.1194	Chrysotile	-2.4399
Cristobalite(bet)	-0.2530	Fluorite	-2.5719
Calcite	-0.3555	Enstatite	-2.9062
Aragonite	-0.5001		

(only minerals with log Q/K > -3 listed)

Gases	fugacity	log fug.
O2(g)	0.1755	-0.756
H2O(g)	0.01903	-1.721
CO2(g)	0.0006405	-3.193
HF(g)	1.264e-014	-13.898
HCl(g)	2.180e-020	-19.662
NO2(g)	1.852e-021	-20.732
N2(g)	1.341e-022	-21.872
NO(g)	1.852e-027	-26.732
Cl2(g)	5.854e-032	-31.233
SiF4(g)	2.221e-039	-38.654
H2(g)	8.946e-043	-42.048
CO(g)	1.831e-049	-48.737
SO2(g)	4.229e-058	-57.374
NH3(g)	1.032e-071	-70.986
Zn(g)	1.968e-075	-74.706
Na(g)	3.494e-077	-76.457
K(g)	8.013e-079	-78.096
F2(g)	1.267e-084	-83.897
Mg(g)	7.649e-132	-131.116
H2S(g)	5.995e-147	-146.222
CH4(g)	1.944e-148	-147.711
Ca(g)	1.873e-154	-153.728
C(g)	3.452e-193	-192.462
Si(g)	2.308e-224	-223.637
S2(g)	3.042e-235	-234.517
C2H4(g)	2.254e-242	-241.647

Original basis	total moles	In fluid		Sorbed		Kd L/kg
		moles	mg/kg	moles	mg/kg	
Ba++	7.31e-008	7.31e-008	0.0100			
Ca++	0.000241	0.000241	9.65			
Cl-	1.04e-005	1.04e-005	0.369			
F-	3.55e-005	3.55e-005	0.674			
H+	-7.45e-006	-7.45e-006	-0.00751			
H2O	55.5	55.5	1.00e+006			
HCO3-	0.00153	0.00153	93.4			
K+	8.26e-005	8.26e-005	3.23			
Mg++	6.88e-005	6.88e-005	1.67			
MoO4--	1.01e-007	1.01e-007	0.0161			
NH3(aq)	1.30e-005	1.30e-005	0.221			
Na+	0.000723	0.000723	16.6			

O2(aq)	0.000272	0.000272	8.70
ReO4-	2.40e-006	2.40e-006	0.602
SO4--	7.41e-005	7.41e-005	7.11
SiO2(aq)	0.000438	0.000438	26.3
Zn++	2.62e-006	2.62e-006	0.171

Elemental composition	In fluid			Sorbed	
	total moles	moles	mg/kg	moles	mg/kg
Barium	7.309e-008	7.309e-008	0.01004		
Calcium	0.0002409	0.0002409	9.652		
Carbon	0.001531	0.001531	18.39		
Chlorine	1.041e-005	1.041e-005	0.3690		
Fluorine	3.548e-005	3.548e-005	0.6740		
Hydrogen	111.0	111.0	1.119e+005		
Magnesium	6.883e-005	6.883e-005	1.673		
Molybdenum	1.005e-007	1.005e-007	0.009642		
Nitrogen	1.300e-005	1.300e-005	0.1820		
Oxygen	55.51	55.51	8.881e+005		
Potassium	8.256e-005	8.256e-005	3.227		
Rhenium	2.405e-006	2.405e-006	0.4477		
Silicon	0.0004380	0.0004380	12.30		
Sodium	0.0007234	0.0007234	16.63		
Sulfur	7.406e-005	7.406e-005	2.375		
Zinc	2.619e-006	2.619e-006	0.1712		

Sample D10EBOT

```

Step #      0          Xi = 0.0000
Temperature = 20.0 C   Pressure = 1.013 bars
pH = 8.850           log fO2 = -0.761
Eh = 0.7045 volts    pe = 12.1124
Ionic strength      = 0.003023
Charge imbalance    = -0.000565 eq/kg (-21.31% error)
Activity of water   = 0.999999
Solvent mass        = 1.000000 kg
Solution mass       = 1.000268 kg
Solution density    = 1.016 g/cm3
Chlorinity          = 0.000020 molal
Dissolved solids    = 268 mg/kg sol'n
Elect. conductivity = 235.10 uS/cm (or umho/cm)
Hardness            = 21.26 mg/kg sol'n as CaCO3
  carbonate         = 21.26 mg/kg sol'n as CaCO3
  non-carbonate     = 0.00 mg/kg sol'n as CaCO3
Rock mass           = 0.000000 kg
Carbonate alkalinity = 130.00 mg/kg sol'n as CaCO3
Water type          = Na-HCO3
  
```

No minerals in system.

Aqueous species	molality	mg/kg sol'n	act. coef.	log act.
HCO3-	0.002401	146.4	0.9422	-2.6455
Na+	0.001929	44.34	0.9422	-2.7404
SiO2(aq)	0.0004543	27.29	1.0000	-3.3427
O2(aq)	0.0002433	7.783	1.0000	-3.6139
Ca++	0.0001690	6.770	0.7937	-3.8725
SO4--	9.312e-005	8.943	0.7876	-4.1347
CO3--	8.384e-005	5.030	0.7891	-4.1794
F-	7.916e-005	1.504	0.9418	-4.1275
K+	6.038e-005	2.360	0.9413	-4.2454
HSiO3-	3.344e-005	2.578	0.9422	-4.5015
Cl-	2.017e-005	0.7150	0.9413	-4.7215
Mg++	1.979e-005	0.4809	0.7995	-4.8007
AlO2-	1.909e-005	1.125	0.9422	-4.7451
CaCO3(aq)	1.713e-005	1.714	1.0000	-4.7663
NO3-	1.528e-005	0.9475	0.9413	-4.8420
Fe(OH)3(aq)	1.098e-005	1.173	1.0000	-4.9595
CO2(aq)	7.794e-006	0.3429	1.0000	-5.1083
NaHCO3(aq)	6.486e-006	0.5447	1.0000	-5.1880
OH-	5.036e-006	0.08563	0.9418	-5.3240
ReO4-	4.788e-006	1.198	0.9422	-5.3457
CaHCO3+	3.655e-006	0.3695	0.9422	-5.4629
NaHSiO3(aq)	2.861e-006	0.2863	1.0000	-5.5435
MoO4--	2.544e-006	0.4068	0.7891	-5.6973
CaSO4(aq)	1.243e-006	0.1692	1.0000	-5.9055
MgCO3(aq)	9.547e-007	0.08047	1.0000	-6.0201
NaCO3-	4.818e-007	0.03998	0.9422	-6.3429
MgHCO3+	4.212e-007	0.03593	0.9422	-6.4014
MgSO4(aq)	2.642e-007	0.03179	1.0000	-6.5781
Ba++	9.898e-008	0.01359	0.7907	-7.1065
HALO2(aq)	9.417e-008	0.005648	1.0000	-7.0261
CaF+	5.024e-008	0.002967	0.9422	-7.3248
KSO4-	3.361e-008	0.004542	0.9422	-7.4993
MgF+	2.862e-008	0.001239	0.9422	-7.5692
NaF(aq)	1.313e-008	0.0005512	1.0000	-7.8817

(only species > 1e-8 molal listed)

Mineral saturation states			
	log Q/K		log Q/K
Antigorite	19.1995s/sat	Saponite-H	3.8575s/sat
Nontronite-Ca	18.9376s/sat	Prehnite	3.5301s/sat
Nontronite-Mg	18.8131s/sat	Sanidine_high	3.4867s/sat
Nontronite-Na	18.6363s/sat	Tremolite	3.1981s/sat
Nontronite-K	18.4935s/sat	Albite_low	3.0993s/sat
Nontronite-H	17.6372s/sat	Albite	3.0992s/sat
Clinoptilolite-h	16.7414s/sat	Smectite-low-Fe-	3.0174s/sat
Clinoptilolite-C	16.7123s/sat	Natrolite	2.8830s/sat
Clinoptilolite-h	14.2866s/sat	Clinozoisite	2.6030s/sat
Clinoptilolite-N	14.2858s/sat	Zoisite	2.5571s/sat
Hematite	13.5895s/sat	Diaspore	2.3470s/sat
Clinoptilolite-K	13.0806s/sat	Witherite	2.1489s/sat
Clinoptilolite-h	12.9708s/sat	Magnetite	2.1250s/sat
Stilbite	12.5173s/sat	Boehmite	1.9345s/sat
Andradite	11.3900s/sat	Gibbsite	1.7750s/sat
Epidote-ord	10.3501s/sat	Albite_high	1.7470s/sat
Epidote	10.3496s/sat	Clinochlore-7A	1.7366s/sat
Muscovite	9.8777s/sat	Wairakite	1.4713s/sat
Mesolite	8.6712s/sat	Dolomite	1.0503s/sat
Herschelite	8.3903s/sat	Dolomite-ord	1.0503s/sat
Illite	7.4919s/sat	Quartz	0.7891s/sat
Paragonite	7.3478s/sat	Jadeite	0.6863s/sat
Scolecite	7.0796s/sat	Corundum	0.5950s/sat
Beidellite-Ca	6.9807s/sat	Tridymite	0.5915s/sat
Montmor-Ca	6.9344s/sat	Calcite	0.4097s/sat
Montmor-Mg	6.8813s/sat	Smectite-high-Fe	0.3931s/sat
Beidellite-Mg	6.8561s/sat	Chrysotile	0.2893s/sat
Montmor-Na	6.7010s/sat	Aragonite	0.2651s/sat
Beidellite-Na	6.6793s/sat	Cristobalite(alp)	0.2271s/sat
Montmor-K	6.5622s/sat	Chalcedony	0.2132s/sat
Beidellite-K	6.5366s/sat	Kyanite	-0.0006
Amesite-14A	6.4670s/sat	Coesite	-0.0341
Celadonite	6.4208s/sat	Kalsilite	-0.0907
Goethite	6.3202s/sat	Dawsonite	-0.1190
Laumontite	6.0418s/sat	Ice	-0.1194
Kaolinite	5.7920s/sat	Cristobalite(bet)	-0.2309
Pyrophyllite	5.6940s/sat	Analcime-K	-0.2541
Beidellite-H	5.6804s/sat	Andalusite	-0.2841
Ferrite-Ca	5.5915s/sat	Monohydrocalcite	-0.4110
Saponite-Ca	5.1578s/sat	Dolomite-dis	-0.5315
Clinochlore-14A	5.1516s/sat	SiO2(am)	-0.5390
Ferrite-Mg	5.0856s/sat	Anorthite	-0.6071
Saponite-Mg	5.0339s/sat	Sillimanite	-0.6576
Saponite-Na	4.8566s/sat	Analcime	-0.8093
Phlogopite	4.8330s/sat	Magnesite	-1.0194
Maximum_Microcli	4.7198s/sat	Barite	-1.1747
K-Feldspar	4.7186s/sat	Diopside	-1.2652
Saponite-K	4.7138s/sat	Nepheline	-1.5690
Mordenite	3.9558s/sat	Enstatite	-1.9891
Lawsonite	3.9339s/sat	Grossular	-2.0004
Margarite	3.9240s/sat	Fluorite	-2.0407
Talc	3.8681s/sat	Fe(OH)3	-2.3676

(only minerals with log Q/K > -3 listed)

Gases	fugacity	log fug.
O2(g)	0.1736	-0.761
H2O(g)	0.01903	-1.721
CO2(g)	0.0001949	-3.710
HF(g)	5.324e-015	-14.274
HCl(g)	7.962e-021	-20.099
NO2(g)	4.114e-022	-21.386
N2(g)	6.769e-024	-23.169
NO(g)	4.137e-028	-27.383
Cl2(g)	7.764e-033	-32.110
SiF4(g)	7.363e-041	-40.133
H2(g)	8.996e-043	-42.046
CO(g)	5.602e-050	-49.252
SO2(g)	1.915e-059	-58.718
NH3(g)	2.337e-072	-71.631
Na(g)	4.863e-076	-75.313
K(g)	3.051e-078	-77.516
F2(g)	2.236e-085	-84.650
Mg(g)	6.041e-131	-130.219
H2S(g)	2.761e-148	-147.559
CH4(g)	6.048e-149	-148.218
Ca(g)	3.604e-153	-152.443
Al(g)	1.162e-192	-191.935
C(g)	1.062e-193	-192.974
Si(g)	2.455e-224	-223.610
S2(g)	6.379e-238	-237.195
C2H4(g)	2.158e-243	-242.666

Original basis	total moles	In fluid		Sorbed		Kd L/kg
		moles	mg/kg	moles	mg/kg	
Al+++	1.92e-005	1.92e-005	0.518			
Ba++	1.01e-007	1.01e-007	0.0139			
Ca++	0.000191	0.000191	7.65			
Cl-	2.02e-005	2.02e-005	0.715			
F-	7.93e-005	7.93e-005	1.51			
Fe++	1.10e-005	1.10e-005	0.613			
H+	-0.000250	-0.000250	-0.252			
H2O	55.5	55.5	1.00e+006			
HCO3-	0.00252	0.00252	154.			
K+	6.04e-005	6.04e-005	2.36			
Mg++	2.15e-005	2.15e-005	0.521			
MoO4--	2.54e-006	2.54e-006	0.407			
NH3(aq)	1.53e-005	1.53e-005	0.260			
Na+	0.00194	0.00194	44.6			
O2(aq)	0.000277	0.000277	8.85			
ReO4-	4.79e-006	4.79e-006	1.20			
SO4--	9.47e-005	9.47e-005	9.09			
SiO2(aq)	0.000491	0.000491	29.5			

Elemental composition	total moles	In fluid		Sorbed	
		moles	mg/kg	moles	mg/kg
Aluminum	1.919e-005	1.919e-005	0.5175		
Barium	1.010e-007	1.010e-007	0.01387		
Calcium	0.0001910	0.0001910	7.654		
Carbon	0.002521	0.002521	30.28		
Chlorine	2.018e-005	2.018e-005	0.7153		
Fluorine	7.925e-005	7.925e-005	1.505		
Hydrogen	111.0	111.0	1.119e+005		
Iron	1.098e-005	1.098e-005	0.6129		
Magnesium	2.146e-005	2.146e-005	0.5214		

Molybdenum	2.544e-006	2.544e-006	0.2440
Nitrogen	1.528e-005	1.528e-005	0.2140
Oxygen	55.52	55.52	8.880e+005
Potassium	6.041e-005	6.041e-005	2.361
Rhenium	4.788e-006	4.788e-006	0.8914
Silicon	0.0004906	0.0004906	13.77
Sodium	0.001939	0.001939	44.57
Sulfur	9.466e-005	9.466e-005	3.035

Sample D1019MMB_ts

```

Step #      0          Xi = 0.0000
Temperature = 20.0 C   Pressure = 1.013 bars
pH = 9.840           log fO2 = -0.766
Eh = 0.6468 volts    pe = 11.1209
Ionic strength      = 0.011060
Charge imbalance    = -0.003078 eq/kg (-34.93% error)
Activity of water   = 0.999998
Solvent mass        = 1.000000 kg
Solution mass       = 1.000735 kg
Solution density    = 1.017 g/cm3
Chlorinity          = 0.000048 molal
Dissolved solids    = 735 mg/kg sol'n
Elect. conductivity = 750.91 uS/cm (or umho/cm)
Hardness            = 32.41 mg/kg sol'n as CaCO3
  carbonate         = 32.41 mg/kg sol'n as CaCO3
  non-carbonate     = 0.00 mg/kg sol'n as CaCO3
Rock mass           = 0.000000 kg
Carbonate alkalinity = 475.00 mg/kg sol'n as CaCO3
Water type          = Na-HCO3
  
```

No minerals in system.

Aqueous species	molality	mg/kg sol'n	act. coef.	log act.
Na+	0.006952	159.7	0.8988	-2.2042
HCO3-	0.005121	312.3	0.8988	-2.3369
CO3--	0.002009	120.5	0.6548	-2.8809
SiO2(aq)	0.0003566	21.41	1.0000	-3.4478
BO2-	0.0002876	12.30	0.8988	-3.5876
HSiO3-	0.0002690	20.72	0.8988	-3.6167
O2(aq)	0.0002400	7.675	1.0000	-3.6197
F-	0.0002117	4.019	0.8973	-3.7214
CaCO3(aq)	0.0001823	18.23	1.0000	-3.7392
Ca++	0.0001077	4.312	0.6668	-4.1439
SO4--	8.884e-005	8.528	0.6506	-4.2381
NaHSiO3(aq)	7.544e-005	7.545	1.0000	-4.1224
B(OH)3(aq)	7.481e-005	4.622	1.0000	-4.1260
K+	6.845e-005	2.674	0.8958	-4.2124
NO3-	5.350e-005	3.315	0.8958	-4.3194
OH-	5.165e-005	0.8778	0.8973	-4.3340
Cl-	4.771e-005	1.690	0.8958	-4.3692
NaHCO3(aq)	4.537e-005	3.808	1.0000	-4.3433
AlO2-	4.044e-005	2.383	0.8988	-4.4395
NaCO3-	3.453e-005	2.864	0.8988	-4.5081
Fe(OH)3(aq)	2.203e-005	2.353	1.0000	-4.6569
Mg++	1.569e-005	0.3811	0.6816	-4.9708
MgCO3(aq)	1.283e-005	1.081	1.0000	-4.8917
ReO4-	1.269e-005	3.172	0.8988	-4.9430
HPO4--	8.226e-006	0.7889	0.6506	-5.2715
MoO4--	7.028e-006	1.123	0.6548	-5.3370
CaHCO3+	4.174e-006	0.4217	0.8988	-5.4257
Zn++	3.273e-006	0.2139	0.6668	-5.6610
CO2(aq)	1.623e-006	0.07137	1.0000	-5.7897
SeO4--	1.111e-006	0.1587	0.6506	-6.1411
MgHCO3+	6.073e-007	0.05178	0.8988	-6.2629
CaSO4(aq)	5.245e-007	0.07135	1.0000	-6.2803
MgSO4(aq)	1.407e-007	0.01693	1.0000	-6.8516
Ba++	1.337e-007	0.01835	0.6589	-7.0551
NaF(aq)	1.150e-007	0.004825	1.0000	-6.9393
CaF+	7.183e-008	0.004240	0.8988	-7.1900
MgF+	5.166e-008	0.002236	0.8988	-7.3331

NaOH(aq)	4.779e-008	0.001910	1.0000	-7.3207
BaCO3(aq)	4.622e-008	0.009113	1.0000	-7.3352
NaCl(aq)	4.354e-008	0.002543	1.0000	-7.3611
PO4---	4.114e-008	0.003904	0.3797	-7.8063
NaAlO2(aq)	3.914e-008	0.003206	1.0000	-7.4073
KSO4-	2.997e-008	0.004047	0.8988	-7.5697
ZnSO4(aq)	2.335e-008	0.003767	1.0000	-7.6317
HALO2(aq)	1.948e-008	0.001168	1.0000	-7.7105
H2PO4-	1.450e-008	0.001406	0.8988	-7.8848

(only species > 1e-8 molal listed)

Mineral saturation states

	log Q/K		log Q/K
Antigorite	102.4991s/sat	Clinozoisite	3.6515s/sat
Nontronite-Ca	19.2128s/sat	Albite_low	3.6257s/sat
Nontronite-Na	19.1333s/sat	Albite	3.6256s/sat
Nontronite-Mg	19.1051s/sat	Zoisite	3.6056s/sat
Nontronite-K	18.8245s/sat	Sanidine_high	3.5099s/sat
Nontronite-H	17.6306s/sat	Witherite	3.4988s/sat
Andradite	16.8055s/sat	Dolomite	3.2059s/sat
Ferrite-Zn	16.2927s/sat	Dolomite-ord	3.2059s/sat
Clinoptilolite-h	15.8192s/sat	Magnetite	3.0341s/sat
Clinoptilolite-C	15.7902s/sat	Margarite	2.6847s/sat
Clinoptilolite-h	15.6940s/sat	Zincite	2.5405s/sat
Clinoptilolite-N	15.6932s/sat	Albite_high	2.2734s/sat
Tremolite	14.8236s/sat	Zn(OH)2(gamma)	2.1358s/sat
Hematite	14.1946s/sat	Zn(OH)2(epsilon)	2.1105s/sat
Fluorapatite	14.0303s/sat	Diopside	2.0430s/sat
Clinoptilolite-K	12.7433s/sat	Smectite-high-Fe	1.8634s/sat
Clinoptilolite-h	12.6335s/sat	Zn(OH)2(beta)	1.8346s/sat
Clinochlore-14A	12.5168s/sat	Diaspore	1.6626s/sat
Epidote-ord	12.3855s/sat	Dolomite-dis	1.6241s/sat
Epidote	12.3851s/sat	Grossular	1.4411s/sat
Stilbite	12.2630s/sat	Calcite	1.4368s/sat
Amesite-14A	10.7586s/sat	Wairakite	1.3906s/sat
Zn2SiO4	10.3751s/sat	Jadeite	1.3178s/sat
Phlogopite	10.2858s/sat	Aragonite	1.2923s/sat
Saponite-Ca	10.2577s/sat	Smithsonite	1.2912s/sat
Saponite-Na	10.1781s/sat	Boehmite	1.2501s/sat
Saponite-Mg	10.1505s/sat	Gibbsite	1.0906s/sat
Saponite-K	9.8693s/sat	Quartz	0.6840s/sat
Herschelite	9.4070s/sat	Monohydrocalcite	0.6161s/sat
Mesolite	9.1470s/sat	Whitlockite	0.6030s/sat
Clinochlore-7A	9.1018s/sat	Tridymite	0.4864s/sat
Talc	8.8772s/sat	Huntite	0.1560s/sat
Saponite-H	8.6755s/sat	Kalsilite	0.1428s/sat
Muscovite	8.5321s/sat	Cristobalite(alp)	0.1220s/sat
Celadonite	8.1487s/sat	Magnesite	0.1090s/sat
Ferrite-Ca	7.9051s/sat	Chalcedony	0.1081s/sat
Ferrite-Mg	7.5006s/sat	Dawsonite	0.0414s/sat
Anthophyllite	7.3778s/sat	Ice	-0.1194
Scolecite	7.1040s/sat	Coesite	-0.1393
Goethite	6.6228s/sat	Pargasite	-0.1427
Illite	6.6160s/sat	Analcime-K	-0.1435
Paragonite	6.5054s/sat	Analcime	-0.2156
Montmor-Ca	6.2500s/sat	Enstatite	-0.2843
Montmor-Na	6.2384s/sat	Cristobalite(bet)	-0.3361
Montmor-Mg	6.2137s/sat	Anorthite	-0.4776
Laumontite	5.9611s/sat	SiO2(am)	-0.6441
Montmor-K	5.9335s/sat	Corundum	-0.7738
Chrysotile	5.5087s/sat	Nepheline	-0.8324
Hydroxylapatite	5.3567s/sat	Barite	-1.2267

Beidellite-Ca	5.2821s/sat	Kyanite	-1.4746
Prehnite	5.2630s/sat	Fluorite	-1.4997
Beidellite-Na	5.2025s/sat	Okenite	-1.7416
Beidellite-Mg	5.1743s/sat	Andalusite	-1.7581
Beidellite-K	4.8937s/sat	Wollastonite	-1.8735
Maximum_Microcli	4.7430s/sat	Brucite	-1.9277
K-Feldspar	4.7418s/sat	Fe(OH)3	-2.0651
Natrolite	4.2512s/sat	Pseudowollastoni	-2.1216
Kaolinite	4.2129s/sat	Sillimanite	-2.1315
Lawsonite	4.0634s/sat	Gyrolite	-2.3409
Smectite-low-Fe-	4.0008s/sat	Forsterite	-2.4839
Pyrophyllite	3.9046s/sat	Cordierite_hydr	-2.6993
Mordenite	3.8260s/sat	Artinite	-2.8073
Beidellite-H	3.6999s/sat	Nesquehonite	-2.9096
(only minerals with log Q/K > -3 listed)			

Gases	fugacity	log fug.
O2(g)	0.1712	-0.766
H2O(g)	0.01903	-1.721
CO2(g)	4.059e-005	-4.392
HF(g)	1.388e-015	-14.858
HCl(g)	1.834e-021	-20.737
NO2(g)	1.407e-022	-21.852
N2(g)	8.135e-025	-24.090
NO(g)	1.424e-028	-27.846
Cl2(g)	4.091e-034	-33.388
H2(g)	9.056e-043	-42.043
BF3(g)	8.031e-043	-42.095
SiF4(g)	2.670e-043	-42.573
CO(g)	1.174e-050	-49.930
SO2(g)	1.591e-061	-60.798
Zn(g)	5.327e-072	-71.274
NH3(g)	8.184e-073	-72.087
Na(g)	1.639e-074	-73.785
K(g)	3.227e-077	-76.491
F2(g)	1.510e-086	-85.821
Mg(g)	3.925e-129	-128.406
CH4(g)	1.294e-149	-148.888
H2S(g)	2.341e-150	-149.631
Ca(g)	1.855e-151	-150.732
Al(g)	2.428e-193	-192.615
C(g)	2.242e-194	-193.649
B(g)	1.396e-206	-205.855
Si(g)	1.954e-224	-223.709
S2(g)	4.524e-242	-241.344
C2H4(g)	9.743e-245	-244.011

Original basis	total moles	In fluid		Sorbed		Kd L/kg
		moles	mg/kg	moles	mg/kg	
Al+++	4.05e-005	4.05e-005	1.09			
B(OH)3(aq)	0.000362	0.000362	22.4			
Ba++	1.80e-007	1.80e-007	0.0247			
Ca++	0.000295	0.000295	11.8			
Cl-	4.78e-005	4.78e-005	1.69			
F-	0.000212	0.000212	4.02			
Fe++	2.20e-005	2.20e-005	1.23			
H+	-0.00318	-0.00318	-3.20			
H2O	55.5	55.5	9.99e+005			
HCO3-	0.00741	0.00741	452.			
HPO4--	8.28e-006	8.28e-006	0.794			
K+	6.85e-005	6.85e-005	2.68			

Mg ⁺⁺	2.93e-005	2.93e-005	0.712
MoO ₄ ⁻⁻	7.03e-006	7.03e-006	1.12
NH ₃ (aq)	5.35e-005	5.35e-005	0.910
Na ⁺	0.00711	0.00711	163.
O ₂ (aq)	0.000353	0.000353	11.3
ReO ₄ ⁻	1.27e-005	1.27e-005	3.17
SO ₄ ⁻⁻	8.96e-005	8.96e-005	8.60
SeO ₃ ⁻⁻	1.11e-006	1.11e-006	0.141
SiO ₂ (aq)	0.000701	0.000701	42.1
Zn ⁺⁺	3.30e-006	3.30e-006	0.215

Elemental composition	In fluid			Sorbed	
	total moles	moles	mg/kg	moles	mg/kg
Aluminum	4.050e-005	4.050e-005	1.092		
Barium	1.799e-007	1.799e-007	0.02469		
Boron	0.0003624	0.0003624	3.915		
Calcium	0.0002947	0.0002947	11.80		
Carbon	0.007412	0.007412	88.96		
Chlorine	4.776e-005	4.776e-005	1.692		
Fluorine	0.0002119	0.0002119	4.023		
Hydrogen	111.0	111.0	1.118e+005		
Iron	2.203e-005	2.203e-005	1.230		
Magnesium	2.932e-005	2.932e-005	0.7122		
Molybdenum	7.028e-006	7.028e-006	0.6738		
Nitrogen	5.350e-005	5.350e-005	0.7488		
Oxygen	55.53	55.53	8.879e+005		
Phosphorus	8.282e-006	8.282e-006	0.2563		
Potassium	6.848e-005	6.848e-005	2.676		
Rhenium	1.269e-005	1.269e-005	2.361		
Selenium	1.111e-006	1.111e-006	0.08764		
Silicon	0.0007010	0.0007010	19.67		
Sodium	0.007108	0.007108	163.3		
Sulfur	8.956e-005	8.956e-005	2.870		
Zinc	3.297e-006	3.297e-006	0.2154		

Sample D1019MMB_bs

```

Step #      0          Xi = 0.0000
Temperature = 20.0 C   Pressure = 1.013 bars
pH = 9.970           log fO2 = -0.757
Eh = 0.6394 volts    pe = 10.9934
Ionic strength = 0.027044
Charge imbalance = -0.006343 eq/kg (-30.45% error)
Activity of water = 1.000000
Solvent mass = 1.000000 kg
Solution mass = 1.001546 kg
Solution density = 1.017 g/cm3
Chlorinity = 0.000000 molal
Dissolved solids = 1544 mg/kg sol'n
Elect. conductivity = 1654.46 uS/cm (or umho/cm)
Hardness = 10.36 mg/kg sol'n as CaCO3
  carbonate = 10.36 mg/kg sol'n as CaCO3
  non-carbonate = 0.00 mg/kg sol'n as CaCO3
Rock mass = 0.000000 kg
Carbonate alkalinity = 1130.00 mg/kg sol'n as CaCO3
Water type = Na-CO3
  
```

No minerals in system.

Aqueous species	molality	mg/kg sol'n	act. coef.	log act.
Na+	0.01749	401.5	0.8563	-1.8245
HCO3-	0.009877	601.8	0.8563	-2.0727
CO3--	0.006029	361.2	0.5409	-2.4867
BO2-	0.0009465	40.46	0.8563	-3.0912
F-	0.0003737	7.090	0.8532	-3.4964
O2(aq)	0.0002455	7.844	1.0000	-3.6099
NaCO3-	0.0002153	17.85	0.8563	-3.7342
NaHCO3(aq)	0.0001998	16.76	1.0000	-3.6993
HSiO3-	0.0001959	15.08	0.8563	-3.7753
SiO2(aq)	0.0001835	11.01	1.0000	-3.7364
B(OH)3(aq)	0.0001739	10.74	1.0000	-3.7597
K+	0.0001387	5.416	0.8500	-3.9284
NaHSiO3(aq)	0.0001255	12.54	1.0000	-3.9013
SO4--	9.762e-005	9.363	0.5336	-4.2833
OH-	7.328e-005	1.244	0.8532	-4.2040
CaCO3(aq)	6.398e-005	6.394	1.0000	-4.1940
NO3-	3.891e-005	2.409	0.8500	-4.4805
Ca++	1.810e-005	0.7241	0.5617	-4.9929
ReO4-	1.386e-005	3.462	0.8563	-4.9257
HPO4--	1.263e-005	1.210	0.5336	-5.1714
MgCO3(aq)	1.258e-005	1.059	1.0000	-4.9003
MoO4--	9.865e-006	1.575	0.5409	-5.2728
Mg++	7.210e-006	0.1750	0.5868	-5.3736
AlO2-	6.590e-006	0.3881	0.8563	-5.2485
Zn++	2.547e-006	0.1663	0.5617	-5.8445
CO2(aq)	2.211e-006	0.09714	1.0000	-5.6555
SeO4--	1.409e-006	0.2012	0.5336	-6.1238
CaHCO3+	1.140e-006	0.1151	0.8563	-6.0105
MgHCO3+	4.633e-007	0.03947	0.8563	-6.4015
NaF(aq)	4.628e-007	0.01940	1.0000	-6.3346
NaOH(aq)	1.545e-007	0.006172	1.0000	-6.8110
PO4---	1.094e-007	0.01037	0.2426	-7.5762
CaSO4(aq)	6.692e-008	0.009096	1.0000	-7.1744
Ba++	6.322e-008	0.008668	0.5481	-7.4603
KSO4-	5.451e-008	0.007357	0.8563	-7.3309
MgSO4(aq)	5.016e-008	0.006029	1.0000	-7.2996
BaCO3(aq)	4.506e-008	0.008878	1.0000	-7.3462

MgF+	3.601e-008	0.001557	0.8563	-7.5109
CaF+	1.792e-008	0.001057	0.8563	-7.8140
NaAlO2(aq)	1.457e-008	0.001192	1.0000	-7.8366
H2PO4-	1.421e-008	0.001376	0.8563	-7.9147
ZnSO4(aq)	1.379e-008	0.002223	1.0000	-7.8604

(only species > 1e-8 molal listed)

Mineral saturation states

	log Q/K		log Q/K
Antigorite	85.8330s/sat	Kaolinite	1.7577s/sat
Fluorapatite	10.7008s/sat	Smithsonite	1.5019s/sat
Tremolite	10.6229s/sat	Mordenite	1.4966s/sat
Zn2SiO4	10.2395s/sat	Prehnite	1.3413s/sat
Clinochlore-14A	9.0591s/sat	Dolomite-dis	1.1607s/sat
Saponite-Na	8.5490s/sat	Lawsonite	1.0193s/sat
Phlogopite	8.4667s/sat	Calcite	0.9821s/sat
Saponite-Ca	8.3631s/sat	Albite_high	0.9783s/sat
Saponite-Mg	8.3295s/sat	Pyrophyllite	0.8723s/sat
Saponite-K	8.2085s/sat	Aragonite	0.8375s/sat
Stilbite	7.7194s/sat	Diopside	0.7340s/sat
Talc	7.2944s/sat	Diaspore	0.7236s/sat
Herschelite	7.1633s/sat	Beidellite-H	0.4529s/sat
Saponite-H	6.8781s/sat	Quartz	0.3954s/sat
Mesolite	6.3674s/sat	Jadeite	0.3113s/sat
Celadonite	6.3266s/sat	Boehmite	0.3112s/sat
Amesite-14A	5.8544s/sat	Tridymite	0.1978s/sat
Clinochlore-7A	5.6441s/sat	Monohydrocalcite	0.1613s/sat
Muscovite	5.2634s/sat	Gibbsite	0.1516s/sat
Chrysotile	4.5031s/sat	Magnesite	0.1004s/sat
Anthophyllite	4.0695s/sat	Ice	-0.1194
Scolecite	3.7713s/sat	Cristobalite(alp)	-0.1666
Illite	3.6590s/sat	Chalcedony	-0.1805
Montmor-Na	3.6370s/sat	Dawsonite	-0.2537
Witherite	3.4878s/sat	Huntite	-0.3245
Montmor-Mg	3.4205s/sat	Coesite	-0.4278
Montmor-Ca	3.3833s/sat	Cristobalite(bet)	-0.6247
Maximum_Microcli	3.3522s/sat	Kalsilite	-0.6708
K-Feldspar	3.3511s/sat	Enstatite	-0.7157
Paragonite	3.3323s/sat	SiO2(am)	-0.9327
Montmor-K	3.3006s/sat	Clinozoisite	-1.2091
Dolomite	2.7425s/sat	Analcime	-1.2165
Dolomite-ord	2.7425s/sat	Analcime-K	-1.2362
Zincite	2.6170s/sat	Zoisite	-1.2550
Natrolite	2.5269s/sat	Whitlockite	-1.4836
Laumontite	2.3397s/sat	Nepheline	-1.5502
Albite_low	2.3307s/sat	Barite	-1.6772
Albite	2.3306s/sat	Fluorite	-1.8987
Zn(OH)2(gamma)	2.2123s/sat	Brucite	-2.0705
Zn(OH)2(epsilon)	2.1869s/sat	Wairakite	-2.2307
Beidellite-Na	2.1237s/sat	Margarite	-2.2374
Sanidine_high	2.1192s/sat	Corundum	-2.6518
Beidellite-Ca	1.9379s/sat	Wollastonite	-2.7511
Hydroxylapatite	1.9322s/sat	Okenite	-2.9078
Zn(OH)2(beta)	1.9110s/sat	Nesquehonite	-2.9182
Beidellite-Mg	1.9037s/sat	Artinite	-2.9587
Beidellite-K	1.7834s/sat	Pseudowollastoni	-2.9992

(only minerals with log Q/K > -3 listed)

Gases

	fugacity	log fug.
O2(g)	0.1751	-0.757
H2O(g)	0.01903	-1.721

CO2(g)	5.528e-005	-4.257
HF(g)	1.727e-015	-14.763
NO2(g)	7.159e-023	-22.145
N2(g)	2.013e-025	-24.696
NO(g)	7.166e-029	-28.145
BF3(g)	3.599e-042	-41.444
H2(g)	8.955e-043	-42.048
SiF4(g)	3.296e-043	-42.482
CO(g)	1.582e-050	-49.801
SO2(g)	7.792e-062	-61.108
Zn(g)	6.281e-072	-71.202
NH3(g)	4.003e-073	-72.398
Na(g)	5.270e-074	-73.278
K(g)	8.326e-077	-76.080
F2(g)	2.365e-086	-85.626
Mg(g)	2.794e-129	-128.554
CH4(g)	1.685e-149	-148.774
H2S(g)	1.108e-150	-149.955
Ca(g)	4.726e-152	-151.326
C(g)	2.986e-194	-193.525
Al(g)	2.747e-194	-193.561
B(g)	3.191e-206	-205.496
Si(g)	9.828e-225	-224.008
S2(g)	1.037e-242	-241.984
C2H4(g)	1.690e-244	-243.772

Original basis	total moles	In fluid		Sorbed		Kd L/kg
		moles	mg/kg	moles	mg/kg	
Al+++	6.61e-006	6.61e-006	0.178			
B(OH)3(aq)	0.00112	0.00112	69.2			
Ba++	1.08e-007	1.08e-007	0.0148			
Ca++	8.33e-005	8.33e-005	3.33			
F-	0.000374	0.000374	7.10			
H+	-0.00773	-0.00773	-7.77			
H2O	55.5	55.5	9.98e+005			
HCO3-	0.0164	0.0164	999.			
HPO4--	1.28e-005	1.28e-005	1.22			
K+	0.000139	0.000139	5.42			
Mg++	2.03e-005	2.03e-005	0.494			
MoO4--	9.86e-006	9.86e-006	1.58			
NH3(aq)	3.89e-005	3.89e-005	0.662			
Na+	0.0180	0.0180	414.			
O2(aq)	0.000324	0.000324	10.4			
ReO4-	1.39e-005	1.39e-005	3.46			
SO4--	9.78e-005	9.78e-005	9.38			
SeO3--	1.41e-006	1.41e-006	0.179			
SiO2(aq)	0.000505	0.000505	30.3			
Zn++	2.56e-006	2.56e-006	0.167			

Elemental composition	total moles	In fluid		Sorbed	
		moles	mg/kg	moles	mg/kg
Aluminum	6.606e-006	6.606e-006	0.1780		
Barium	1.083e-007	1.083e-007	0.01485		
Boron	0.001120	0.001120	12.09		
Calcium	8.330e-005	8.330e-005	3.333		
Carbon	0.01640	0.01640	196.7		
Fluorine	0.0003743	0.0003743	7.099		
Hydrogen	111.0	111.0	1.117e+005		
Magnesium	2.034e-005	2.034e-005	0.4936		
Molybdenum	9.865e-006	9.865e-006	0.9449		
Nitrogen	3.891e-005	3.891e-005	0.5442		

Oxygen	55.56	55.56	8.876e+005
Phosphorus	1.275e-005	1.275e-005	0.3944
Potassium	0.0001388	0.0001388	5.418
Rhenium	1.386e-005	1.386e-005	2.576
Selenium	1.409e-006	1.409e-006	0.1111
Silicon	0.0005049	0.0005049	14.16
Sodium	0.01803	0.01803	414.0
Sulfur	9.780e-005	9.780e-005	3.131
Zinc	2.560e-006	2.560e-006	0.1672

Sample D10END

```

Step #      0          Xi = 0.0000
Temperature = 20.0 C   Pressure = 1.013 bars
pH = 7.890           log fO2 = -0.758
Eh = 0.7604 volts    pe = 13.0731
Ionic strength      = 0.002851
Charge imbalance    = -0.000719 eq/kg (-29.44% error)
Activity of water   = 0.999999
Solvent mass        = 1.000000 kg
Solution mass       = 1.000259 kg
Solution density    = 1.016 g/cm3
Chlorinity          = 0.000021 molal
Dissolved solids    = 259 mg/kg sol'n
Elect. conductivity = 216.20 uS/cm (or umho/cm)
Hardness            = 31.01 mg/kg sol'n as CaCO3
  carbonate         = 31.01 mg/kg sol'n as CaCO3
  non-carbonate     = 0.00 mg/kg sol'n as CaCO3
Rock mass           = 0.000000 kg
Carbonate alkalinity = 124.00 mg/kg sol'n as CaCO3
Water type          = Na-HCO3
  
```

No minerals in system.

Aqueous species	molality	mg/kg sol'n	act. coef.	log act.
HCO3-	0.002446	149.2	0.9437	-2.6368
Na+	0.001416	32.55	0.9437	-2.8741
SiO2(aq)	0.0004725	28.38	1.0000	-3.3256
Ca++	0.0002593	10.39	0.7985	-3.6839
O2(aq)	0.0002449	7.835	1.0000	-3.6110
SO4--	9.606e-005	9.226	0.7926	-4.1184
F-	8.118e-005	1.542	0.9433	-4.1159
CO2(aq)	7.252e-005	3.191	1.0000	-4.1395
K+	5.962e-005	2.330	0.9428	-4.2502
Mg++	3.813e-005	0.9266	0.8040	-4.5134
Cl-	2.142e-005	0.7593	0.9428	-4.6947
NO3-	1.455e-005	0.9022	0.9428	-4.8626
CO3--	9.320e-006	0.5591	0.7941	-5.1307
ReO4-	9.302e-006	2.327	0.9437	-5.0566
AlO2-	8.126e-006	0.4791	0.9437	-5.1153
CaHCO3+	5.750e-006	0.5811	0.9437	-5.2655
NaHCO3(aq)	4.865e-006	0.4086	1.0000	-5.3129
Fe(OH)3(aq)	4.494e-006	0.4801	1.0000	-5.3474
HSiO3-	3.808e-006	0.2935	0.9437	-5.4444
MoO4--	3.293e-006	0.5265	0.7941	-5.5826
CaCO3(aq)	2.958e-006	0.2960	1.0000	-5.5290
Zn++	2.723e-006	0.1780	0.7985	-5.6626
CaSO4(aq)	1.993e-006	0.2713	1.0000	-5.7005
MgHCO3+	8.314e-007	0.07091	0.9437	-6.1054
OH-	5.513e-007	0.009374	0.9433	-6.2840
MgSO4(aq)	5.315e-007	0.06396	1.0000	-6.2745
HALO2(aq)	3.662e-007	0.02196	1.0000	-6.4362
NaHSiO3(aq)	2.399e-007	0.02400	1.0000	-6.6200
MgCO3(aq)	2.070e-007	0.01745	1.0000	-6.6841
Ba++	8.793e-008	0.01207	0.7956	-7.1551
CaF+	7.955e-008	0.004698	0.9437	-7.1245
MgF+	5.687e-008	0.002462	0.9437	-7.2703
NaCO3-	3.956e-008	0.003283	0.9437	-7.4278
KSO4-	3.447e-008	0.004657	0.9437	-7.4878
ZnSO4(aq)	3.065e-008	0.004947	1.0000	-7.5136
H+	1.359e-008	1.369e-005	0.9479	-7.8900

(only species > 1e-8 molal listed)

Mineral saturation states

	log Q/K		log Q/K
Nontronite-Ca	18.1334s/sat	Natrolite	1.9267s/sat
Nontronite-Mg	18.0252s/sat	Smectite-low-Fe-	1.7830s/sat
Nontronite-Na	17.7569s/sat	Corundum	1.7747s/sat
Nontronite-K	17.6566s/sat	Prehnite	1.2983s/sat
Nontronite-H	17.1187s/sat	Albite_high	1.2945s/sat
Clinoptilolite-h	16.0169s/sat	Kyanite	1.1962s/sat
Clinoptilolite-C	15.9879s/sat	Witherite	1.1489s/sat
Hematite	12.8136s/sat	Wairakite	0.9881s/sat
Clinoptilolite-h	12.7718s/sat	Clinzoisite	0.9611s/sat
Clinoptilolite-N	12.7709s/sat	Magnetite	0.9605s/sat
Clinoptilolite-K	12.0126s/sat	Zoisite	0.9152s/sat
Stilbite	12.0010s/sat	Andalusite	0.9127s/sat
Clinoptilolite-h	11.9028s/sat	Quartz	0.8062s/sat
Ferrite-Zn	11.0101s/sat	Tridymite	0.6086s/sat
Muscovite	10.7338s/sat	Sillimanite	0.5392s/sat
Beidellite-Ca	8.1321s/sat	Dawsonite	0.3459s/sat
Paragonite	8.0750s/sat	Cristobalite(alp	0.2442s/sat
Beidellite-Mg	8.0238s/sat	Saponite-Ca	0.2314s/sat
Mesolite	8.0197s/sat	Chalcedony	0.2303s/sat
Illite	7.9213s/sat	Jadeite	0.2167s/sat
Beidellite-Na	7.7555s/sat	Saponite-Mg	0.1238s/sat
Epidote-ord	7.7304s/sat	Coesite	-0.0170
Epidote	7.7299s/sat	Ice	-0.1194
Beidellite-K	7.6554s/sat	Saponite-Na	-0.1451
Herschelite	7.5377s/sat	Cristobalite(bet	-0.2138
Montmor-Ca	7.1633s/sat	Saponite-K	-0.2453
Montmor-Mg	7.1266s/sat	Calcite	-0.3529
Beidellite-H	7.1175s/sat	Dolomite	-0.3763
Kaolinite	7.0059s/sat	Dolomite-ord	-0.3763
Pyrophyllite	6.9420s/sat	Phlogopite	-0.3888
Montmor-Na	6.8547s/sat	Kalsilite	-0.4485
Montmor-K	6.7585s/sat	Aragonite	-0.4975
Scolecite	6.5793s/sat	SiO2(am)	-0.5219
Goethite	5.9323s/sat	Analcime-K	-0.5791
Laumontite	5.5586s/sat	Saponite-H	-0.7832
Andradite	5.4714s/sat	Smithsonite	-0.9602
Margarite	4.5863s/sat	Talc	-0.9617
Celadonite	4.4815s/sat	Anorthite	-1.1246
Maximum_Microcli	4.3962s/sat	Monohydrocalcite	-1.1737
K-Feldspar	4.3950s/sat	Barite	-1.2071
Mordenite	3.7007s/sat	Analcime	-1.2581
Lawsonite	3.4164s/sat	Smectite-high-Fe	-1.3049
Sanidine_high	3.1631s/sat	Zincite	-1.3611
Ferrite-Ca	3.0842s/sat	Magnesite	-1.6834
Diaspore	2.9368s/sat	Zn(OH)2(gamma)	-1.7658
Zn2SiO4	2.6941s/sat	Clinochlore-14A	-1.7810
Ferrite-Mg	2.6770s/sat	Zn(OH)2(epsilon)	-1.7911
Albite_low	2.6468s/sat	Fluorite	-1.8288
Albite	2.6467s/sat	Dolomite-dis	-1.9581
Boehmite	2.5244s/sat	Nepheline	-2.0557
Gibbsite	2.3648s/sat	Zn(OH)2(beta)	-2.0670
Amesite-14A	2.3298s/sat	Fe(OH)3	-2.7556

(only minerals with log Q/K > -3 listed)

Gases	fugacity	log fug.
O2(g)	0.1747	-0.758
H2O(g)	0.01903	-1.721
CO2(g)	0.001814	-2.741

HF(g)	4.987e-014	-13.302
HCl(g)	7.724e-020	-19.112
NO2(g)	3.573e-021	-20.447
N2(g)	5.038e-022	-21.298
NO(g)	3.580e-027	-26.446
Cl2(g)	7.331e-031	-30.135
SiF4(g)	5.897e-037	-36.229
H2(g)	8.966e-043	-42.047
CO(g)	5.195e-049	-48.284
SO2(g)	1.649e-057	-56.783
NH3(g)	2.006e-071	-70.698
Zn(g)	6.614e-076	-75.180
Na(g)	3.913e-077	-76.407
K(g)	3.303e-079	-78.481
F2(g)	1.969e-083	-82.706
Mg(g)	1.403e-132	-131.853
H2S(g)	2.353e-146	-145.628
CH4(g)	5.553e-148	-147.255
Ca(g)	6.669e-155	-154.176
Al(g)	4.496e-192	-191.347
C(g)	9.820e-193	-192.008
Si(g)	2.537e-224	-223.596
S2(g)	4.663e-234	-233.331
C2H4(g)	1.832e-241	-240.737

Original basis	total moles	In fluid		Sorbed		Kd L/kg
		moles	mg/kg	moles	mg/kg	
Al+++	8.50e-006	8.50e-006	0.229			
Ba++	8.81e-008	8.81e-008	0.0121			
Ca++	0.000270	0.000270	10.8			
Cl-	2.14e-005	2.14e-005	0.760			
F-	8.13e-005	8.13e-005	1.54			
Fe++	4.49e-006	4.49e-006	0.251			
H+	-1.75e-006	-1.75e-006	-0.00176			
H2O	55.5	55.5	1.00e+006			
HCO3-	0.00254	0.00254	155.			
K+	5.97e-005	5.97e-005	2.33			
Mg++	3.98e-005	3.98e-005	0.966			
MoO4--	3.29e-006	3.29e-006	0.526			
NH3(aq)	1.46e-005	1.46e-005	0.248			
Na+	0.00142	0.00142	32.7			
O2(aq)	0.000275	0.000275	8.80			
ReO4-	9.30e-006	9.30e-006	2.33			
SO4--	9.87e-005	9.87e-005	9.47			
SiO2(aq)	0.000477	0.000477	28.6			
Zn++	2.75e-006	2.75e-006	0.180			

Elemental composition	total moles	In fluid		Sorbed	
		moles	mg/kg	moles	mg/kg
Aluminum	8.498e-006	8.498e-006	0.2292		
Barium	8.814e-008	8.814e-008	0.01210		
Calcium	0.0002701	0.0002701	10.82		
Carbon	0.002542	0.002542	30.52		
Chlorine	2.143e-005	2.143e-005	0.7595		
Fluorine	8.133e-005	8.133e-005	1.545		
Hydrogen	111.0	111.0	1.119e+005		
Iron	4.494e-006	4.494e-006	0.2509		
Magnesium	3.976e-005	3.976e-005	0.9662		
Molybdenum	3.293e-006	3.293e-006	0.3158		
Nitrogen	1.455e-005	1.455e-005	0.2038		
Oxygen	55.52	55.52	8.880e+005		

Potassium	5.965e-005	5.965e-005	2.332
Rhenium	9.302e-006	9.302e-006	1.732
Silicon	0.0004765	0.0004765	13.38
Sodium	0.001421	0.001421	32.66
Sulfur	9.865e-005	9.865e-005	3.163
Zinc	2.754e-006	2.754e-006	0.1800

Sample D10ETOP

```

Step #      0                Xi = 0.0000
Temperature = 20.0 C        Pressure = 1.013 bars
pH = 7.890                log fO2 = -0.758
Eh = 0.7604 volts         pe = 13.0731
Ionic strength = 0.002851
Charge imbalance = -0.000719 eq/kg (-29.44% error)
Activity of water = 0.999999
Solvent mass = 1.000000 kg
Solution mass = 1.000259 kg
Solution density = 1.016 g/cm3
Chlorinity = 0.000021 molal
Dissolved solids = 259 mg/kg sol'n
Elect. conductivity = 216.20 uS/cm (or umho/cm)
Hardness = 31.01 mg/kg sol'n as CaCO3
  carbonate = 31.01 mg/kg sol'n as CaCO3
  non-carbonate = 0.00 mg/kg sol'n as CaCO3
Rock mass = 0.000000 kg
Carbonate alkalinity= 124.00 mg/kg sol'n as CaCO3
Water type = Na-HCO3
  
```

No minerals in system.

Aqueous species	molality	mg/kg sol'n	act. coef.	log act.
HCO3-	0.002446	149.2	0.9437	-2.6368
Na+	0.001416	32.55	0.9437	-2.8741
SiO2(aq)	0.0004725	28.38	1.0000	-3.3256
Ca++	0.0002593	10.39	0.7985	-3.6839
O2(aq)	0.0002449	7.835	1.0000	-3.6110
SO4--	9.606e-005	9.226	0.7926	-4.1184
F-	8.118e-005	1.542	0.9433	-4.1159
CO2(aq)	7.252e-005	3.191	1.0000	-4.1395
K+	5.962e-005	2.330	0.9428	-4.2502
Mg++	3.813e-005	0.9266	0.8040	-4.5134
Cl-	2.142e-005	0.7593	0.9428	-4.6947
NO3-	1.455e-005	0.9022	0.9428	-4.8626
CO3--	9.320e-006	0.5591	0.7941	-5.1307
ReO4-	9.302e-006	2.327	0.9437	-5.0566
AlO2-	8.126e-006	0.4791	0.9437	-5.1153
CaHCO3+	5.750e-006	0.5811	0.9437	-5.2655
NaHCO3(aq)	4.865e-006	0.4086	1.0000	-5.3129
Fe(OH)3(aq)	4.494e-006	0.4801	1.0000	-5.3474
HSiO3-	3.808e-006	0.2935	0.9437	-5.4444
MoO4--	3.293e-006	0.5265	0.7941	-5.5826
CaCO3(aq)	2.958e-006	0.2960	1.0000	-5.5290
Zn++	2.723e-006	0.1780	0.7985	-5.6626
CaSO4(aq)	1.993e-006	0.2713	1.0000	-5.7005
MgHCO3+	8.314e-007	0.07091	0.9437	-6.1054
OH-	5.513e-007	0.009374	0.9433	-6.2840
MgSO4(aq)	5.315e-007	0.06396	1.0000	-6.2745
HAlO2(aq)	3.662e-007	0.02196	1.0000	-6.4362
NaHSiO3(aq)	2.399e-007	0.02400	1.0000	-6.6200
MgCO3(aq)	2.070e-007	0.01745	1.0000	-6.6841
Ba++	8.793e-008	0.01207	0.7956	-7.1551
CaF+	7.955e-008	0.004698	0.9437	-7.1245
MgF+	5.687e-008	0.002462	0.9437	-7.2703
NaCO3-	3.956e-008	0.003283	0.9437	-7.4278
KSO4-	3.447e-008	0.004657	0.9437	-7.4878
ZnSO4(aq)	3.065e-008	0.004947	1.0000	-7.5136
H+	1.359e-008	1.369e-005	0.9479	-7.8900

(only species > 1e-8 molal listed)

Mineral saturation states

	log Q/K		log Q/K
Nontronite-Ca	18.1334s/sat	Natrolite	1.9267s/sat
Nontronite-Mg	18.0252s/sat	Smectite-low-Fe-	1.7830s/sat
Nontronite-Na	17.7569s/sat	Corundum	1.7747s/sat
Nontronite-K	17.6566s/sat	Prehnite	1.2983s/sat
Nontronite-H	17.1187s/sat	Albite_high	1.2945s/sat
Clinoptilolite-h	16.0169s/sat	Kyanite	1.1962s/sat
Clinoptilolite-C	15.9879s/sat	Witherite	1.1489s/sat
Hematite	12.8136s/sat	Wairakite	0.9881s/sat
Clinoptilolite-h	12.7718s/sat	Clinzoisite	0.9611s/sat
Clinoptilolite-N	12.7709s/sat	Magnetite	0.9605s/sat
Clinoptilolite-K	12.0126s/sat	Zoisite	0.9152s/sat
Stilbite	12.0010s/sat	Andalusite	0.9127s/sat
Clinoptilolite-h	11.9028s/sat	Quartz	0.8062s/sat
Ferrite-Zn	11.0101s/sat	Tridymite	0.6086s/sat
Muscovite	10.7338s/sat	Sillimanite	0.5392s/sat
Beidellite-Ca	8.1321s/sat	Dawsonite	0.3459s/sat
Paragonite	8.0750s/sat	Cristobalite(alp	0.2442s/sat
Beidellite-Mg	8.0238s/sat	Saponite-Ca	0.2314s/sat
Mesolite	8.0197s/sat	Chalcedony	0.2303s/sat
Illite	7.9213s/sat	Jadeite	0.2167s/sat
Beidellite-Na	7.7555s/sat	Saponite-Mg	0.1238s/sat
Epidote-ord	7.7304s/sat	Coesite	-0.0170
Epidote	7.7299s/sat	Ice	-0.1194
Beidellite-K	7.6554s/sat	Saponite-Na	-0.1451
Herschelite	7.5377s/sat	Cristobalite(bet	-0.2138
Montmor-Ca	7.1633s/sat	Saponite-K	-0.2453
Montmor-Mg	7.1266s/sat	Calcite	-0.3529
Beidellite-H	7.1175s/sat	Dolomite	-0.3763
Kaolinite	7.0059s/sat	Dolomite-ord	-0.3763
Pyrophyllite	6.9420s/sat	Phlogopite	-0.3888
Montmor-Na	6.8547s/sat	Kalsilite	-0.4485
Montmor-K	6.7585s/sat	Aragonite	-0.4975
Scolecite	6.5793s/sat	SiO2(am)	-0.5219
Goethite	5.9323s/sat	Analcime-K	-0.5791
Laumontite	5.5586s/sat	Saponite-H	-0.7832
Andradite	5.4714s/sat	Smithsonite	-0.9602
Margarite	4.5863s/sat	Talc	-0.9617
Celadonite	4.4815s/sat	Anorthite	-1.1246
Maximum_Microcli	4.3962s/sat	Monohydrocalcite	-1.1737
K-Feldspar	4.3950s/sat	Barite	-1.2071
Mordenite	3.7007s/sat	Analcime	-1.2581
Lawsonite	3.4164s/sat	Smectite-high-Fe	-1.3049
Sanidine_high	3.1631s/sat	Zincite	-1.3611
Ferrite-Ca	3.0842s/sat	Magnesite	-1.6834
Diaspore	2.9368s/sat	Zn(OH)2(gamma)	-1.7658
Zn2SiO4	2.6941s/sat	Clinochlore-14A	-1.7810
Ferrite-Mg	2.6770s/sat	Zn(OH)2(epsilon)	-1.7911
Albite_low	2.6468s/sat	Fluorite	-1.8288
Albite	2.6467s/sat	Dolomite-dis	-1.9581
Boehmite	2.5244s/sat	Nepheline	-2.0557
Gibbsite	2.3648s/sat	Zn(OH)2(beta)	-2.0670
Amesite-14A	2.3298s/sat	Fe(OH)3	-2.7556

(only minerals with log Q/K > -3 listed)

Gases	fugacity	log fug.
O2(g)	0.1747	-0.758
H2O(g)	0.01903	-1.721
CO2(g)	0.001814	-2.741

HF(g)	4.987e-014	-13.302
HCl(g)	7.724e-020	-19.112
NO2(g)	3.573e-021	-20.447
N2(g)	5.038e-022	-21.298
NO(g)	3.580e-027	-26.446
Cl2(g)	7.331e-031	-30.135
SiF4(g)	5.897e-037	-36.229
H2(g)	8.966e-043	-42.047
CO(g)	5.195e-049	-48.284
SO2(g)	1.649e-057	-56.783
NH3(g)	2.006e-071	-70.698
Zn(g)	6.614e-076	-75.180
Na(g)	3.913e-077	-76.407
K(g)	3.303e-079	-78.481
F2(g)	1.969e-083	-82.706
Mg(g)	1.403e-132	-131.853
H2S(g)	2.353e-146	-145.628
CH4(g)	5.553e-148	-147.255
Ca(g)	6.669e-155	-154.176
Al(g)	4.496e-192	-191.347
C(g)	9.820e-193	-192.008
Si(g)	2.537e-224	-223.596
S2(g)	4.663e-234	-233.331
C2H4(g)	1.832e-241	-240.737

Original basis	total moles	In fluid		Sorbed		Kd L/kg
		moles	mg/kg	moles	mg/kg	
Al+++	8.50e-006	8.50e-006	0.229			
Ba++	8.81e-008	8.81e-008	0.0121			
Ca++	0.000270	0.000270	10.8			
Cl-	2.14e-005	2.14e-005	0.760			
F-	8.13e-005	8.13e-005	1.54			
Fe++	4.49e-006	4.49e-006	0.251			
H+	-1.75e-006	-1.75e-006	-0.00176			
H2O	55.5	55.5	1.00e+006			
HCO3-	0.00254	0.00254	155.			
K+	5.97e-005	5.97e-005	2.33			
Mg++	3.98e-005	3.98e-005	0.966			
MoO4--	3.29e-006	3.29e-006	0.526			
NH3(aq)	1.46e-005	1.46e-005	0.248			
Na+	0.00142	0.00142	32.7			
O2(aq)	0.000275	0.000275	8.80			
ReO4-	9.30e-006	9.30e-006	2.33			
SO4--	9.87e-005	9.87e-005	9.47			
SiO2(aq)	0.000477	0.000477	28.6			
Zn++	2.75e-006	2.75e-006	0.180			

Elemental composition	total moles	In fluid		Sorbed	
		moles	mg/kg	moles	mg/kg
Aluminum	8.498e-006	8.498e-006	0.2292		
Barium	8.814e-008	8.814e-008	0.01210		
Calcium	0.0002701	0.0002701	10.82		
Carbon	0.002542	0.002542	30.52		
Chlorine	2.143e-005	2.143e-005	0.7595		
Fluorine	8.133e-005	8.133e-005	1.545		
Hydrogen	111.0	111.0	1.119e+005		
Iron	4.494e-006	4.494e-006	0.2509		
Magnesium	3.976e-005	3.976e-005	0.9662		
Molybdenum	3.293e-006	3.293e-006	0.3158		
Nitrogen	1.455e-005	1.455e-005	0.2038		
Oxygen	55.52	55.52	8.880e+005		

Potassium	5.965e-005	5.965e-005	2.332
Rhenium	9.302e-006	9.302e-006	1.732
Silicon	0.0004765	0.0004765	13.38
Sodium	0.001421	0.001421	32.66
Sulfur	9.865e-005	9.865e-005	3.163
Zinc	2.754e-006	2.754e-006	0.1800

Sample D10NBOTg

```

Step #      0          Xi = 0.0000
Temperature = 20.0 C   Pressure = 1.013 bars
pH = 8.640           log fO2 = -1.407
Eh = 0.7073 volts    pe = 12.1607
Ionic strength      = 0.009809
Charge imbalance    = -0.000412 eq/kg (-5.05% error)
Activity of water   = 1.000000
Solvent mass        = 1.000000 kg
Solution mass       = 1.000862 kg
Solution density    = 1.017 g/cm3
Chlorinity          = 0.000000 molal
Dissolved solids    = 862 mg/kg sol'n
Elect. conductivity = 666.88 uS/cm (or umho/cm)
Hardness            = 108.19 mg/kg sol'n as CaCO3
  carbonate         = 108.19 mg/kg sol'n as CaCO3
  non-carbonate     = 0.00 mg/kg sol'n as CaCO3
Rock mass           = 0.000000 kg
Carbonate alkalinity = 339.00 mg/kg sol'n as CaCO3
Water type          = Na-HCO3
  
```

No minerals in system.

Aqueous species	molality	mg/kg sol'n	act. coef.	log act.
HCO3-	0.006265	381.9	0.9037	-2.2471
Na+	0.005973	137.2	0.9037	-2.2678
SiO2(aq)	0.001185	71.14	1.0000	-2.9262
Ca++	0.0007836	31.38	0.6801	-3.2733
Fe(OH)3(aq)	0.0007650	81.69	1.0000	-3.1163
SO4--	0.0005823	55.89	0.6651	-3.4119
AlO2-	0.0002988	17.61	0.9037	-3.5686
B(OH)3(aq)	0.0002260	13.96	1.0000	-3.6460
F-	0.0001578	2.996	0.9024	-3.8465
CO3--	0.0001526	9.150	0.6690	-3.9910
K+	0.0001278	4.992	0.9010	-3.9388
Mg++	0.0001095	2.659	0.6938	-4.1194
CaCO3(aq)	0.0001050	10.50	1.0000	-3.9787
HSiO3-	5.609e-005	4.320	0.9037	-4.2951
O2(aq)	5.486e-005	1.754	1.0000	-4.2607
BO2-	5.451e-005	2.331	0.9037	-4.3075
NaHCO3(aq)	4.820e-005	4.046	1.0000	-4.3169
CaHCO3+	3.791e-005	3.829	0.9037	-4.4652
CO2(aq)	3.164e-005	1.391	1.0000	-4.4998
CaSO4(aq)	2.609e-005	3.549	1.0000	-4.5835
ReO4-	2.236e-005	5.591	0.9037	-4.6944
MoO4--	1.570e-005	2.509	0.6690	-4.9787
NaHSiO3(aq)	1.367e-005	1.367	1.0000	-4.8644
Ti(OH)4(aq)	9.149e-006	1.060	1.0000	-5.0386
Zn++	8.283e-006	0.5412	0.6801	-5.2493
MgCO3(aq)	7.072e-006	0.5958	1.0000	-5.1504
MgSO4(aq)	6.698e-006	0.8055	1.0000	-5.1741
MgHCO3+	5.276e-006	0.4498	0.9037	-5.3217
OH-	3.241e-006	0.05507	0.9024	-5.5340
NaCO3-	2.302e-006	0.1909	0.9037	-5.6818
HALO2(aq)	2.294e-006	0.1375	1.0000	-5.6395
Ba++	1.067e-006	0.1465	0.6728	-6.1438
ZnSO4(aq)	4.038e-007	0.06514	1.0000	-6.3938
CaF+	3.976e-007	0.02347	0.9037	-6.4445
KSO4-	3.750e-007	0.05064	0.9037	-6.4699
MgF+	2.736e-007	0.01184	0.9037	-6.6069
NaAlO2(aq)	2.513e-007	0.02058	1.0000	-6.5999

NaF(aq)	7.448e-008	0.003125	1.0000	-7.1279
BaCO3(aq)	2.924e-008	0.005765	1.0000	-7.5340

(only species > 1e-8 molal listed)

Mineral saturation states

	log Q/K		log Q/K
Antigorite	45.8993s/sat	Sanidine_high	6.2192s/sat
Clinoptilolite-h	27.9193s/sat	Wairakite	6.0895s/sat
Clinoptilolite-C	27.8903s/sat	Albite_low	5.9979s/sat
Clinoptilolite-h	26.0645s/sat	Albite	5.9978s/sat
Clinoptilolite-N	26.0637s/sat	Smectite-high-Fe	5.3054s/sat
Nontronite-Ca	24.6393s/sat	Cordierite_hydr	5.0953s/sat
Nontronite-Mg	24.5285s/sat	Albite_high	4.6456s/sat
Nontronite-Na	24.3952s/sat	Diaspore	3.7336s/sat
Clinoptilolite-K	24.2828s/sat	Corundum	3.3682s/sat
Nontronite-K	24.1976s/sat	Boehmite	3.3211s/sat
Clinoptilolite-h	24.1730s/sat	Witherite	3.3000s/sat
Nontronite-H	23.3094s/sat	Kyanite	3.1890s/sat
Stilbite	18.5991s/sat	Anorthite	3.1781s/sat
Ferrite-Zn	17.3857s/sat	Jadeite	3.1684s/sat
Hematite	17.2758s/sat	Gibbsite	3.1616s/sat
Andradite	16.8633s/sat	Andalusite	2.9055s/sat
Epidote-ord	16.5741s/sat	Dolomite	2.7076s/sat
Epidote	16.5737s/sat	Dolomite-ord	2.7076s/sat
Muscovite	15.3834s/sat	Cordierite_anhyd	2.5628s/sat
Amesite-14A	13.8913s/sat	Grossular	2.5597s/sat
Herschelite	13.6636s/sat	Sillimanite	2.5320s/sat
Paragonite	13.0195s/sat	Dawsonite	2.1387s/sat
Mesolite	12.9793s/sat	Analcime-K	2.0193s/sat
Illite	12.2619s/sat	Chrysotile	1.9060s/sat
Beidellite-Ca	11.7693s/sat	Kalsilite	1.8089s/sat
Beidellite-Mg	11.6583s/sat	Analcime	1.6235s/sat
Beidellite-Na	11.5251s/sat	Anatase	1.5200s/sat
Beidellite-K	11.3276s/sat	Quartz	1.2056s/sat
Scolecite	11.2814s/sat	Calcite	1.1973s/sat
Montmor-Ca	11.0315s/sat	Dolomite-dis	1.1258s/sat
Montmor-Mg	10.9920s/sat	Aragonite	1.0528s/sat
Montmor-Na	10.8552s/sat	Tridymite	1.0079s/sat
Montmor-K	10.6617s/sat	Anthophyllite	0.7102s/sat
Laumontite	10.6600s/sat	Cristobalite(alp)	0.6436s/sat
Margarite	10.4824s/sat	Chalcedony	0.6297s/sat
Clinochlore-14A	10.4804s/sat	Smithsonite	0.5929s/sat
Beidellite-H	10.4395s/sat	Zincite	0.5523s/sat
Pyrophyllite	10.1329s/sat	Barite	0.5108s/sat
Celadonite	9.8310s/sat	Nepheline	0.4967s/sat
Ferrite-Ca	9.4570s/sat	Coesite	0.3823s/sat
Kaolinite	9.3980s/sat	Monohydrocalcite	0.3766s/sat
Ferrite-Mg	9.0332s/sat	Cronstedtite-7A	0.2178s/sat
Clinzoisite	8.3705s/sat	Cristobalite(bet)	0.1855s/sat
Phlogopite	8.3493s/sat	Zn(OH)2(gamma)	0.1475s/sat
Zoisite	8.3246s/sat	Zn(OH)2(epsilon)	0.1222s/sat
Tremolite	8.1944s/sat	Diopside	0.0081s/sat
Goethite	8.1634s/sat	Ice	-0.1194
Saponite-Ca	7.9571s/sat	SiO2(am)	-0.1225
Prehnite	7.9110s/sat	Magnesite	-0.1497
Saponite-Mg	7.8467s/sat	Zn(OH)2(beta)	-0.1537
Magnetite	7.8162s/sat	Fe(OH)3	-0.5245
Lawsonite	7.7191s/sat	Huntite	-0.8597
Saponite-Na	7.7130s/sat	Fluorite	-0.8793
Saponite-K	7.5154s/sat	Jarosite	-1.2232
Mordenite	7.5131s/sat	Enstatite	-1.3114
Smectite-low-Fe-	7.4860s/sat	Pargasite	-1.3171

Maximum_Microcli	7.4523s/sat	Analcime-dehy	-1.8634
K-Feldspar	7.4512s/sat	Gypsum	-2.1948
Natrolite	7.4308s/sat	Okenite	-2.2279
Clinochlore-7A	7.0654s/sat	Anhydrite	-2.4197
Zn2SiO4	6.9202s/sat	Sellaite	-2.4524
Saponite-H	6.6272s/sat	Wollastonite	-2.8813
Talc	6.3177s/sat		

(only minerals with log Q/K > -3 listed)

Gases	fugacity	log fug.
O2(g)	0.03913	-1.407
H2O(g)	0.01903	-1.721
CO2(g)	0.0007912	-3.102
HF(g)	1.649e-014	-13.783
SiF4(g)	1.769e-038	-37.752
BF3(g)	4.069e-039	-38.390
H2(g)	1.894e-042	-41.723
CO(g)	4.788e-049	-48.320
SO2(g)	5.603e-058	-57.252
Zn(g)	1.145e-073	-72.941
Na(g)	1.292e-075	-74.889
K(g)	5.530e-078	-77.257
F2(g)	1.019e-084	-83.992
Mg(g)	2.322e-130	-129.634
H2S(g)	7.542e-146	-145.122
CH4(g)	4.828e-147	-146.316
Ca(g)	1.147e-152	-151.941
Al(g)	8.648e-191	-190.063
C(g)	1.912e-192	-191.718
B(g)	1.276e-205	-204.894
Si(g)	2.841e-223	-222.547
S2(g)	1.074e-233	-232.969
C2H4(g)	3.101e-240	-239.508

Original basis	total moles	In fluid moles	mg/kg	Sorbed moles	mg/kg	Kd L/kg
Al+++	0.000301	0.000301	8.12			
B(OH)3(aq)	0.000280	0.000280	17.3			
Ba++	1.10e-006	1.10e-006	0.150			
Ca++	0.000953	0.000953	38.2			
F-	0.000159	0.000159	3.01			
Fe++	0.000765	0.000765	42.7			
H+	-0.00310	-0.00310	-3.12			
H2O	55.5	55.5	9.99e+005			
HCO3-	0.00665	0.00665	406.			
K+	0.000128	0.000128	5.01			
Mg++	0.000129	0.000129	3.13			
MoO4--	1.57e-005	1.57e-005	2.51			
Na+	0.00604	0.00604	139.			
O2(aq)	0.000246	0.000246	7.87			
ReO4-	2.24e-005	2.24e-005	5.59			
SO4--	0.000616	0.000616	59.1			
SiO2(aq)	0.00125	0.00125	75.3			
Ti(OH)4(aq)	9.15e-006	9.15e-006	1.06			
Zn++	8.69e-006	8.69e-006	0.568			

Elemental composition	total moles	In fluid moles	mg/kg	Sorbed moles	mg/kg
Aluminum	0.0003014	0.0003014	8.125		
Barium	1.097e-006	1.097e-006	0.1505		

Boron	0.0002805	0.0002805	3.029
Calcium	0.0009531	0.0009531	38.16
Carbon	0.006655	0.006655	79.86
Fluorine	0.0001586	0.0001586	3.010
Hydrogen	111.0	111.0	1.118e+005
Iron	0.0007650	0.0007650	42.69
Magnesium	0.0001288	0.0001288	3.128
Molybdenum	1.570e-005	1.570e-005	1.505
Oxygen	55.54	55.54	8.878e+005
Potassium	0.0001282	0.0001282	5.007
Rhenium	2.236e-005	2.236e-005	4.161
Silicon	0.001255	0.001255	35.21
Sodium	0.006038	0.006038	138.7
Sulfur	0.0006159	0.0006159	19.73
Titanium	9.149e-006	9.149e-006	0.4377
Zinc	8.687e-006	8.687e-006	0.5675

Sample D11BG

```

Step #      0          Xi = 0.0000
Temperature = 20.0 C   Pressure = 1.013 bars
pH = 8.040          log fO2 = -0.756
Eh = 0.7517 volts    pe = 12.9236
Ionic strength      = 0.002197
Charge imbalance    = -0.000465 eq/kg (-27.93% error)
Activity of water   = 0.999999
Solvent mass        = 1.000000 kg
Solution mass       = 1.000183 kg
Solution density    = 1.016 g/cm3
Chlorinity          = 0.000036 molal
Dissolved solids    = 183 mg/kg sol'n
Elect. conductivity = 159.86 uS/cm (or umho/cm)
Hardness            = 39.09 mg/kg sol'n as CaCO3
  carbonate         = 39.09 mg/kg sol'n as CaCO3
  non-carbonate     = 0.00 mg/kg sol'n as CaCO3
Rock mass           = 0.000000 kg
Carbonate alkalinity = 73.90 mg/kg sol'n as CaCO3
Water type          = Na-HCO3
  
```

No minerals in system.

Aqueous species	molality	mg/kg sol'n	act. coef.	log act.
HCO3-	0.001452	88.60	0.9500	-2.8602
Na+	0.0005808	13.35	0.9500	-3.2582
SiO2(aq)	0.0004434	26.63	1.0000	-3.3533
Ca++	0.0002869	11.49	0.8188	-3.6291
O2(aq)	0.0002460	7.871	1.0000	-3.6090
SO4--	0.0001450	13.92	0.8141	-3.9281
Mg++	8.987e-005	2.184	0.8233	-4.1308
K+	8.726e-005	3.411	0.9493	-4.0818
NO3-	6.301e-005	3.906	0.9493	-4.2232
Cl-	3.552e-005	1.259	0.9493	-4.4721
F-	3.316e-005	0.6299	0.9497	-4.5018
CO2(aq)	3.069e-005	1.350	1.0000	-4.5130
CO3--	7.666e-006	0.4599	0.8153	-5.2041
HSiO3-	5.014e-006	0.3865	0.9500	-5.3221
CaHCO3+	3.873e-006	0.3915	0.9500	-5.4342
CaSO4(aq)	3.504e-006	0.4769	1.0000	-5.4554
CaCO3(aq)	2.833e-006	0.2835	1.0000	-5.5477
Zn++	2.765e-006	0.1808	0.8188	-5.6452
ReO4-	2.235e-006	0.5592	0.9500	-5.6729
MgSO4(aq)	1.988e-006	0.2392	1.0000	-5.7016
NaHCO3(aq)	1.201e-006	0.1008	1.0000	-5.9206
MgHCO3+	1.191e-006	0.1016	0.9500	-5.9462
OH-	7.735e-007	0.01315	0.9497	-6.1340
MgCO3(aq)	4.217e-007	0.03555	1.0000	-6.3750
NaHSiO3(aq)	1.313e-007	0.01314	1.0000	-6.8818
Ba++	8.796e-008	0.01208	0.8165	-7.1438
KSO4-	7.820e-008	0.01057	0.9500	-7.1291
MgF+	5.606e-008	0.002427	0.9500	-7.2736
MoO4--	5.539e-008	0.008857	0.8153	-7.3453
ZnSO4(aq)	4.945e-008	0.007982	1.0000	-7.3058
CaF+	3.686e-008	0.002177	0.9500	-7.4557
NaCO3-	1.370e-008	0.001137	0.9500	-7.8855
(only species > 1e-8 molal listed)				

Mineral saturation states

	log Q/K		log Q/K
Zn2SiO4	3.3014s/sat	SiO2(am)	-0.5496
Witherite	1.0869s/sat	Barite	-1.0054
Talc	0.9755s/sat	Smithsonite	-1.0162
Quartz	0.7786s/sat	Zincite	-1.0436
Tridymite	0.5809s/sat	Monohydrocalcite	-1.1924
Cristobalite(alp)	0.2166s/sat	Magnesite	-1.3743
Chalcedony	0.2026s/sat	Zn(OH)2(gamma)	-1.4484
Coesite	-0.0447	Zn(OH)2(epsilon)	-1.4737
Dolomite	-0.0859	Dolomite-dis	-1.6677
Dolomite-ord	-0.0859	Zn(OH)2(beta)	-1.7496
Ice	-0.1194	Fluorite	-2.5458
Cristobalite(bet)	-0.2415	Chrysotile	-2.5822
Calcite	-0.3716	Enstatite	-2.9497
Aragonite	-0.5162		

(only minerals with log Q/K > -3 listed)

Gases	fugacity	log fug.
O2(g)	0.1755	-0.756
H2O(g)	0.01903	-1.721
CO2(g)	0.0007676	-3.115
HF(g)	1.452e-014	-13.838
HCl(g)	9.129e-020	-19.040
NO2(g)	1.101e-020	-19.958
N2(g)	4.743e-021	-20.324
NO(g)	1.101e-026	-25.958
Cl2(g)	1.026e-030	-29.989
SiF4(g)	3.975e-039	-38.401
H2(g)	8.946e-043	-42.048
CO(g)	2.194e-049	-48.659
SO2(g)	1.278e-057	-56.894
NH3(g)	6.135e-071	-70.212
Zn(g)	1.371e-075	-74.863
Na(g)	2.280e-077	-76.642
K(g)	6.868e-079	-78.163
F2(g)	1.673e-084	-83.777
Mg(g)	6.738e-132	-131.171
H2S(g)	1.811e-146	-145.742
CH4(g)	2.329e-148	-147.633
Ca(g)	1.506e-154	-153.822
C(g)	4.137e-193	-192.383
Si(g)	2.370e-224	-223.625
S2(g)	2.776e-234	-233.557
C2H4(g)	3.236e-242	-241.490

Original basis	total moles	In fluid		Sorbed		Kd L/kg
		moles	mg/kg	moles	mg/kg	
Ba++	8.81e-008	8.81e-008	0.0121			
Ca++	0.000297	0.000297	11.9			
Cl-	3.55e-005	3.55e-005	1.26			
F-	3.33e-005	3.33e-005	0.632			
H+	-4.92e-005	-4.92e-005	-0.0495			
H2O	55.5	55.5	1.00e+006			
HCO3-	0.00150	0.00150	91.5			
K+	8.73e-005	8.73e-005	3.41			
Mg++	9.35e-005	9.35e-005	2.27			
MoO4--	5.54e-008	5.54e-008	0.00886			
NH3(aq)	6.30e-005	6.30e-005	1.07			
Na+	0.000582	0.000582	13.4			

O2(aq)	0.000372	0.000372	11.9
ReO4-	2.24e-006	2.24e-006	0.559
SO4--	0.000151	0.000151	14.5
SiO2(aq)	0.000448	0.000448	26.9
Zn++	2.81e-006	2.81e-006	0.184

Elemental composition	In fluid			Sorbed	
	total moles	moles	mg/kg	moles	mg/kg
Barium	8.814e-008	8.814e-008	0.01210		
Calcium	0.0002971	0.0002971	11.91		
Carbon	0.001500	0.001500	18.01		
Chlorine	3.553e-005	3.553e-005	1.259		
Fluorine	3.325e-005	3.325e-005	0.6317		
Hydrogen	111.0	111.0	1.119e+005		
Magnesium	9.353e-005	9.353e-005	2.273		
Molybdenum	5.539e-008	5.539e-008	0.005313		
Nitrogen	6.301e-005	6.301e-005	0.8824		
Oxygen	55.52	55.52	8.880e+005		
Potassium	8.734e-005	8.734e-005	3.414		
Rhenium	2.235e-006	2.235e-006	0.4162		
Silicon	0.0004485	0.0004485	12.59		
Sodium	0.0005821	0.0005821	13.38		
Sulfur	0.0001506	0.0001506	4.828		
Zinc	2.814e-006	2.814e-006	0.1840		

Sample D11WTOP

```

Step #      0          Xi = 0.0000
Temperature = 20.0 C   Pressure = 1.013 bars
pH = 8.400          log fO2 = -0.758
Eh = 0.7307 volts    pe = 12.5631
Ionic strength      = 0.002741
Charge imbalance    = -0.000762 eq/kg (-31.11% error)
Activity of water   = 0.999999
Solvent mass        = 1.000000 kg
Solution mass       = 1.000256 kg
Solution density    = 1.016 g/cm3
Chlorinity          = 0.000035 molal
Dissolved solids    = 256 mg/kg sol'n
Elect. conductivity = 218.02 uS/cm (or umho/cm)
Hardness            = 19.83 mg/kg sol'n as CaCO3
  carbonate         = 19.83 mg/kg sol'n as CaCO3
  non-carbonate     = 0.00 mg/kg sol'n as CaCO3
Rock mass           = 0.000000 kg
Carbonate alkalinity = 124.00 mg/kg sol'n as CaCO3
Water type          = Na-HCO3
  
```

No minerals in system.

Aqueous species	molality	mg/kg sol'n	act. coef.	log act.
HCO3-	0.002403	146.6	0.9447	-2.6439
Na+	0.001624	37.34	0.9447	-2.8140
SiO2(aq)	0.0004397	26.41	1.0000	-3.3568
O2(aq)	0.0002449	7.833	1.0000	-3.6111
Ca++	0.0001644	6.589	0.8017	-3.8800
NO3-	8.682e-005	5.382	0.9439	-4.0865
SO4--	7.505e-005	7.208	0.7960	-4.2237
F-	7.140e-005	1.356	0.9443	-4.1712
K+	6.692e-005	2.616	0.9439	-4.1995
Cl-	3.469e-005	1.229	0.9439	-4.4849
CO3--	2.954e-005	1.773	0.7974	-4.6278
CO2(aq)	2.205e-005	0.9700	1.0000	-4.6567
Mg++	2.199e-005	0.5344	0.8071	-4.7508
HSiO3-	1.146e-005	0.8830	0.9447	-4.9656
AlO2-	8.163e-006	0.4813	0.9447	-5.1128
CaCO3(aq)	5.995e-006	0.5999	1.0000	-5.2222
NaHCO3(aq)	5.496e-006	0.4616	1.0000	-5.2600
Fe(OH)3(aq)	4.687e-006	0.5008	1.0000	-5.3291
CaHCO3+	3.597e-006	0.3636	0.9447	-5.4687
ReO4-	2.965e-006	0.7416	0.9447	-5.5527
OH-	1.782e-006	0.03030	0.9443	-5.7740
CaSO4(aq)	9.955e-007	0.1355	1.0000	-6.0019
NaHSiO3(aq)	8.296e-007	0.08300	1.0000	-6.0811
MgHCO3+	4.730e-007	0.04034	0.9447	-6.3499
MoO4--	4.083e-007	0.06528	0.7974	-6.4874
MgCO3(aq)	3.814e-007	0.03215	1.0000	-6.4186
MgSO4(aq)	2.414e-007	0.02905	1.0000	-6.6172
NaCO3-	1.445e-007	0.01199	0.9447	-6.8649
HALO2(aq)	1.138e-007	0.006826	1.0000	-6.9438
Ba++	6.828e-008	0.009374	0.7989	-7.2632
CaF+	4.454e-008	0.002631	0.9447	-7.3759
KSO4-	3.036e-008	0.004102	0.9447	-7.5425
MgF+	2.896e-008	0.001254	0.9447	-7.5629
NaF(aq)	1.003e-008	0.0004209	1.0000	-7.9989

(only species > 1e-8 molal listed)

Mineral saturation states

	log Q/K		log Q/K
Nontronite-Ca	18.0240s/sat	Boehmite	2.0169s/sat
Nontronite-Mg	17.9090s/sat	Saponite-K	2.0055s/sat
Nontronite-Na	17.6997s/sat	Smectite-low-Fe-	1.9582s/sat
Nontronite-K	17.5963s/sat	Natrolite	1.9582s/sat
Nontronite-H	16.8733s/sat	Phlogopite	1.9186s/sat
Clinoptilolite-h	15.2408s/sat	Gibbsite	1.8573s/sat
Clinoptilolite-C	15.2118s/sat	Prehnite	1.8374s/sat
Hematite	12.8503s/sat	Witherite	1.5437s/sat
Clinoptilolite-h	12.5440s/sat	Saponite-H	1.2826s/sat
Clinoptilolite-N	12.5431s/sat	Albite_high	1.2634s/sat
Clinoptilolite-K	11.7521s/sat	Talc	1.2614s/sat
Clinoptilolite-h	11.6423s/sat	Clinochlore-14A	1.0234s/sat
Stilbite	11.6021s/sat	Magnetite	1.0155s/sat
Muscovite	9.6782s/sat	Clinozoisite	0.9927s/sat
Epidote-ord	8.2878s/sat	Zoisite	0.9468s/sat
Epidote	8.2874s/sat	Quartz	0.7750s/sat
Andradite	7.8861s/sat	Corundum	0.7596s/sat
Mesolite	7.8424s/sat	Wairakite	0.6721s/sat
Herschelite	7.4697s/sat	Tridymite	0.5774s/sat
Illite	7.1768s/sat	Jadeite	0.2168s/sat
Paragonite	7.0288s/sat	Cristobalite(alp)	0.2130s/sat
Beidellite-Ca	6.9709s/sat	Chalcedony	0.1991s/sat
Beidellite-Mg	6.8559s/sat	Dolomite	0.1960s/sat
Beidellite-Na	6.6465s/sat	Dolomite-ord	0.1960s/sat
Montmor-Ca	6.5851s/sat	Kyanite	0.1499s/sat
Beidellite-K	6.5433s/sat	Calcite	-0.0461
Montmor-Mg	6.5415s/sat	Coesite	-0.0482
Montmor-Na	6.3286s/sat	Dawsonite	-0.1086
Scolecite	6.2945s/sat	Ice	-0.1194
Montmor-K	6.2293s/sat	Andalusite	-0.1336
Goethite	5.9506s/sat	Aragonite	-0.1907
Kaolinite	5.9284s/sat	Cristobalite(bet)	-0.2450
Beidellite-H	5.8204s/sat	Kalsilite	-0.4266
Pyrophyllite	5.8021s/sat	Sillimanite	-0.5071
Laumontite	5.2425s/sat	SiO2(am)	-0.5531
Celadonite	5.1924s/sat	Analcime-K	-0.5918
Maximum_Microcli	4.3556s/sat	Monohydrocalcite	-0.8669
K-Feldspar	4.3545s/sat	Smectite-high-Fe	-0.9460
Ferrite-Ca	3.9448s/sat	Analcime	-1.2617
Mordenite	3.5100s/sat	Anorthite	-1.3782
Ferrite-Mg	3.4963s/sat	Dolomite-dis	-1.3858
Amesite-14A	3.3677s/sat	Magnesite	-1.4179
Margarite	3.3176s/sat	Barite	-1.4205
Lawsonite	3.1628s/sat	Nepheline	-2.0244
Sanidine_high	3.1226s/sat	Fluorite	-2.1354
Albite_low	2.6157s/sat	Chrysotile	-2.2892
Albite	2.6156s/sat	Clinochlore-7A	-2.3915
Saponite-Ca	2.4332s/sat	Fe(OH)3	-2.7372
Diaspore	2.4293s/sat	Enstatite	-2.8533
Saponite-Mg	2.3187s/sat	Tremolite	-2.9802
Saponite-Na	2.1089s/sat		

(only minerals with log Q/K > -3 listed)

Gases	fugacity	log fug.
O2(g)	0.1747	-0.758
H2O(g)	0.01903	-1.721
CO2(g)	0.0005514	-3.259
HF(g)	1.357e-014	-13.867
HCl(g)	3.869e-020	-19.412

NO2(g)	6.593e-021	-20.181
N2(g)	1.716e-021	-20.765
NO(g)	6.608e-027	-26.180
Cl2(g)	1.839e-031	-30.735
SiF4(g)	3.008e-039	-38.522
H2(g)	8.967e-043	-42.047
CO(g)	1.579e-049	-48.801
SO2(g)	1.235e-058	-57.908
NH3(g)	3.704e-071	-70.431
Na(g)	1.454e-076	-75.837
K(g)	1.201e-078	-77.920
F2(g)	1.458e-084	-83.836
Mg(g)	8.504e-132	-131.070
H2S(g)	1.764e-147	-146.754
CH4(g)	1.689e-148	-147.772
Ca(g)	4.446e-154	-153.352
Al(g)	1.398e-192	-191.855
C(g)	2.986e-193	-192.525
Si(g)	2.362e-224	-223.627
S2(g)	2.620e-236	-235.582
C2H4(g)	1.694e-242	-241.771

Original basis	total moles	In fluid		Sorbed		Kd L/kg
		moles	mg/kg	moles	mg/kg	
Al+++	8.28e-006	8.28e-006	0.223			
Ba++	6.88e-008	6.88e-008	0.00945			
Ca++	0.000175	0.000175	7.01			
Cl-	3.47e-005	3.47e-005	1.23			
F-	7.15e-005	7.15e-005	1.36			
Fe++	4.69e-006	4.69e-006	0.262			
H+	-0.000157	-0.000157	-0.158			
H2O	55.5	55.5	1.00e+006			
HCO3-	0.00247	0.00247	151.			
K+	6.70e-005	6.70e-005	2.62			
Mg++	2.31e-005	2.31e-005	0.562			
MoO4--	4.08e-007	4.08e-007	0.0653			
NH3(aq)	8.68e-005	8.68e-005	1.48			
Na+	0.00163	0.00163	37.5			
O2(aq)	0.000420	0.000420	13.4			
ReO4-	2.96e-006	2.96e-006	0.742			
SO4--	7.63e-005	7.63e-005	7.33			
SiO2(aq)	0.000452	0.000452	27.2			

Elemental composition	In fluid		Sorbed		
	total moles	moles	mg/kg	moles	mg/kg
Aluminum	8.280e-006	8.280e-006	0.2233		
Barium	6.880e-008	6.880e-008	0.009445		
Calcium	0.0001751	0.0001751	7.015		
Carbon	0.002471	0.002471	29.67		
Chlorine	3.470e-005	3.470e-005	1.230		
Fluorine	7.148e-005	7.148e-005	1.358		
Hydrogen	111.0	111.0	1.119e+005		
Iron	4.687e-006	4.687e-006	0.2617		
Magnesium	2.312e-005	2.312e-005	0.5618		
Molybdenum	4.083e-007	4.083e-007	0.03916		
Nitrogen	8.682e-005	8.682e-005	1.216		
Oxygen	55.52	55.52	8.880e+005		
Potassium	6.695e-005	6.695e-005	2.617		
Rhenium	2.965e-006	2.965e-006	0.5519		
Silicon	0.0004520	0.0004520	12.69		
Sodium	0.001631	0.001631	37.49		
Sulfur	7.632e-005	7.632e-005	2.447		

Sample D11NETOP

```

Step #      0          Xi = 0.0000
Temperature = 20.0 C   Pressure = 1.013 bars
pH = 8.030          log fO2 = -0.756
Eh = 0.7523 volts    pe = 12.9336
Ionic strength      = 0.002172
Charge imbalance    = -0.000582 eq/kg (-32.45% error)
Activity of water   = 0.999999
Solvent mass        = 1.000000 kg
Solution mass       = 1.000201 kg
Solution density    = 1.016 g/cm3
Chlorinity          = 0.000029 molal
Dissolved solids    = 201 mg/kg sol'n
Elect. conductivity = 165.77 uS/cm (or umho/cm)
Hardness            = 30.13 mg/kg sol'n as CaCO3
  carbonate         = 30.13 mg/kg sol'n as CaCO3
  non-carbonate     = 0.00 mg/kg sol'n as CaCO3
Rock mass           = 0.000000 kg
Carbonate alkalinity = 88.80 mg/kg sol'n as CaCO3
Water type          = Na-HCO3
  
```

No minerals in system.

Aqueous species	molality	mg/kg sol'n	act. coef.	log act.
HCO3-	0.001747	106.6	0.9503	-2.7798
Na+	0.0008452	19.43	0.9503	-3.0952
SiO2(aq)	0.0004781	28.72	1.0000	-3.3205
O2(aq)	0.0002460	7.871	1.0000	-3.6090
Ca++	0.0002288	9.168	0.8197	-3.7269
NO3-	9.015e-005	5.589	0.9496	-4.0675
SO4--	7.683e-005	7.380	0.8150	-4.2033
K+	7.170e-005	2.803	0.9496	-4.1670
Mg++	6.226e-005	1.513	0.8241	-4.2898
F-	3.980e-005	0.7560	0.9499	-4.4224
CO2(aq)	3.779e-005	1.663	1.0000	-4.4226
Cl-	2.886e-005	1.023	0.9496	-4.5621
CO3--	9.005e-006	0.5403	0.8162	-5.1338
HSiO3-	5.282e-006	0.4071	0.9503	-5.2993
CaHCO3+	3.720e-006	0.3760	0.9503	-5.4516
CaCO3(aq)	2.660e-006	0.2662	1.0000	-5.5750
ReO4-	2.468e-006	0.6174	0.9503	-5.6298
NaHCO3(aq)	2.103e-006	0.1767	1.0000	-5.6771
CaSO4(aq)	1.484e-006	0.2021	1.0000	-5.8284
MgHCO3+	9.939e-007	0.08478	0.9503	-6.0248
OH-	7.557e-007	0.01285	0.9499	-6.1440
MgSO4(aq)	7.315e-007	0.08803	1.0000	-6.1358
MgCO3(aq)	3.439e-007	0.02899	1.0000	-6.4636
NaHSiO3(aq)	2.014e-007	0.02015	1.0000	-6.6960
MoO4--	1.775e-007	0.02838	0.8162	-6.8391
Ba++	6.791e-008	0.009324	0.8174	-7.2556
MgF+	4.666e-008	0.002020	0.9503	-7.3532
CaF+	3.533e-008	0.002087	0.9503	-7.4741
KSO4-	3.409e-008	0.004607	0.9503	-7.4895
NaCO3-	2.345e-008	0.001946	0.9503	-7.6520

(only species > 1e-8 molal listed)

Mineral saturation states

	log Q/K		log Q/K
Witherite	1.0454s/sat	Cristobalite(bet	-0.2087
Quartz	0.8113s/sat	Calcite	-0.3990

Tridymite	0.6137s/sat	SiO2(am)	-0.5168
Talc	0.5695s/sat	Aragonite	-0.5435
Cristobalite(alp)	0.2493s/sat	Monohydrocalcite	-1.2197
Chalcedony	0.2354s/sat	Barite	-1.3925
Coesite	-0.0119	Magnesite	-1.4629
Ice	-0.1194	Dolomite-dis	-1.7836
Dolomite	-0.2018	Fluorite	-2.4848
Dolomite-ord	-0.2018		

(only minerals with log Q/K > -3 listed)

Gases	fugacity	log fug.
O2(g)	0.1755	-0.756
H2O(g)	0.01903	-1.721
CO2(g)	0.0009452	-3.024
HF(g)	1.784e-014	-13.749
HCl(g)	7.592e-020	-19.120
NO2(g)	1.613e-020	-19.792
N2(g)	1.017e-020	-19.993
NO(g)	1.613e-026	-25.792
Cl2(g)	7.099e-031	-30.149
SiF4(g)	9.764e-039	-38.010
H2(g)	8.946e-043	-42.048
CO(g)	2.701e-049	-48.568
SO2(g)	7.099e-058	-57.149
NH3(g)	8.984e-071	-70.047
Na(g)	3.243e-077	-76.489
K(g)	5.516e-079	-78.258
F2(g)	2.524e-084	-83.598
Mg(g)	4.462e-132	-131.350
H2S(g)	1.006e-146	-145.997
CH4(g)	2.868e-148	-147.542
Ca(g)	1.148e-154	-153.940
C(g)	5.094e-193	-192.293
Si(g)	2.555e-224	-223.593
S2(g)	8.569e-235	-234.067
C2H4(g)	4.907e-242	-241.309

Original basis	total moles	In fluid moles	mg/kg	Sorbed moles	mg/kg	Kd L/kg
Ba++	6.81e-008	6.81e-008	0.00935			
Ca++	0.000237	0.000237	9.48			
Cl-	2.89e-005	2.89e-005	1.02			
F-	3.99e-005	3.99e-005	0.758			
H+	-7.06e-005	-7.06e-005	-0.0712			
H2O	55.5	55.5	1.00e+006			
HCO3-	0.00180	0.00180	110.			
K+	7.17e-005	7.17e-005	2.80			
Mg++	6.44e-005	6.44e-005	1.56			
MoO4--	1.77e-007	1.77e-007	0.0284			
NH3(aq)	9.01e-005	9.01e-005	1.53			
Na+	0.000848	0.000848	19.5			
O2(aq)	0.000426	0.000426	13.6			
ReO4-	2.47e-006	2.47e-006	0.617			
SO4--	7.91e-005	7.91e-005	7.60			
SiO2(aq)	0.000484	0.000484	29.0			

Elemental composition	total moles	In fluid moles	mg/kg	Sorbed moles	mg/kg
Barium	6.808e-008	6.808e-008	0.009347		
Calcium	0.0002367	0.0002367	9.485		

Carbon	0.001804	0.001804	21.66
Chlorine	2.887e-005	2.887e-005	1.023
Fluorine	3.988e-005	3.988e-005	0.7576
Hydrogen	111.0	111.0	1.119e+005
Magnesium	6.438e-005	6.438e-005	1.564
Molybdenum	1.775e-007	1.775e-007	0.01702
Nitrogen	9.015e-005	9.015e-005	1.262
Oxygen	55.52	55.52	8.880e+005
Potassium	7.173e-005	7.173e-005	2.804
Rhenium	2.468e-006	2.468e-006	0.4595
Silicon	0.0004835	0.0004835	13.58
Sodium	0.0008475	0.0008475	19.48
Sulfur	7.908e-005	7.908e-005	2.535

Sample D1119MMT_ts

```

Step #      0          Xi = 0.0000
Temperature = 20.0 C   Pressure = 1.013 bars
pH = 9.010           log fO2 = -0.766
Eh = 0.6951 volts    pe = 11.9509
Ionic strength      = 0.006464
Charge imbalance    = -0.002023 eq/kg (-35% error)
Activity of water   = 0.999998
Solvent mass        = 1.000000 kg
Solution mass       = 1.000565 kg
Solution density    = 1.017 g/cm3
Chlorinity          = 0.000047 molal
Dissolved solids    = 565 mg/kg sol'n
Elect. conductivity = 482.43 uS/cm (or umho/cm)
Hardness            = 38.34 mg/kg sol'n as CaCO3
  carbonate         = 38.34 mg/kg sol'n as CaCO3
  non-carbonate     = 0.00 mg/kg sol'n as CaCO3
Rock mass           = 0.000000 kg
Carbonate alkalinity = 321.00 mg/kg sol'n as CaCO3
Water type          = Na-HCO3
  
```

No minerals in system.

Aqueous species	molality	mg/kg sol'n	act. coef.	log act.
HCO3-	0.005664	345.4	0.9193	-2.2834
Na+	0.004137	95.05	0.9193	-2.4199
SiO2(aq)	0.0006058	36.38	1.0000	-3.2177
CO3--	0.0003076	18.45	0.7157	-3.6573
Ca++	0.0002636	10.56	0.7239	-3.7193
O2(aq)	0.0002400	7.676	1.0000	-3.6198
NO3-	9.572e-005	5.932	0.9174	-4.0564
SO4--	8.589e-005	8.247	0.7128	-4.2130
CaCO3(aq)	8.110e-005	8.112	1.0000	-4.0910
F-	8.069e-005	1.532	0.9183	-4.1302
HSiO3-	6.608e-005	5.091	0.9193	-4.2165
K+	5.435e-005	2.124	0.9174	-4.3022
Cl-	4.717e-005	1.671	0.9174	-4.3638
AlO2-	3.961e-005	2.335	0.9193	-4.4388
NaHCO3(aq)	3.123e-005	2.622	1.0000	-4.5054
Fe(OH)3(aq)	2.362e-005	2.523	1.0000	-4.6268
Mg++	2.047e-005	0.4971	0.7342	-4.8232
CO2(aq)	1.241e-005	0.5459	1.0000	-4.9062
CaHCO3+	1.227e-005	1.240	0.9193	-4.9475
NaHSiO3(aq)	1.154e-005	1.154	1.0000	-4.9379
OH-	7.465e-006	0.1269	0.9183	-5.1640
ReO4-	4.223e-006	1.056	0.9193	-5.4109
NaCO3-	3.438e-006	0.2852	0.9193	-5.5003
MgCO3(aq)	3.016e-006	0.2542	1.0000	-5.5205
CaSO4(aq)	1.477e-006	0.2010	1.0000	-5.8306
MgHCO3+	9.436e-007	0.08047	0.9193	-6.0618
MoO4--	6.125e-007	0.09790	0.7157	-6.3582
SeO4--	3.316e-007	0.04738	0.7128	-6.6264
MgSO4(aq)	2.094e-007	0.02520	1.0000	-6.6789
Ba++	1.847e-007	0.02535	0.7185	-6.8770
HALO2(aq)	1.319e-007	0.007909	1.0000	-6.8797
CaF+	7.284e-008	0.004301	0.9193	-7.1742
MgF+	2.769e-008	0.001198	0.9193	-7.5943
NaF(aq)	2.730e-008	0.001146	1.0000	-7.5638
NaCl(aq)	2.683e-008	0.001567	1.0000	-7.5715
KSO4-	2.524e-008	0.003409	0.9193	-7.6345
NaAlO2(aq)	2.386e-008	0.001955	1.0000	-7.6223

BaCO3(aq) 1.165e-008 0.002298 1.0000 -7.9336
 (only species > 1e-8 molal listed)

Mineral saturation states			
	log Q/K		log Q/K
Antigorite	37.7317s/sat	Natrolite	4.5118s/sat
Nontronite-Ca	20.1881s/sat	Clinozoisite	4.3636s/sat
Nontronite-Mg	20.0347s/sat	Zoisite	4.3177s/sat
Nontronite-Na	19.9673s/sat	Smectite-low-Fe-	4.1892s/sat
Clinoptilolite-h	19.8892s/sat	Sanidine_high	4.1113s/sat
Clinoptilolite-C	19.8601s/sat	Albite_low	4.1013s/sat
Nontronite-K	19.7000s/sat	Albite	4.1011s/sat
Nontronite-H	18.8097s/sat	Clinochlore-7A	3.8921s/sat
Clinoptilolite-h	18.2800s/sat	Magnetite	3.1246s/sat
Clinoptilolite-N	18.2792s/sat	Witherite	2.9004s/sat
Clinoptilolite-K	15.7657s/sat	Albite_high	2.7489s/sat
Clinoptilolite-h	15.6559s/sat	Wairakite	2.7374s/sat
Hematite	14.2549s/sat	Diaspore	2.4933s/sat
Stilbite	14.2371s/sat	Dolomite	2.2253s/sat
Andradite	13.8502s/sat	Dolomite-ord	2.2253s/sat
Epidote-ord	12.2970s/sat	Boehmite	2.0809s/sat
Epidote	12.2965s/sat	Gibbsite	1.9214s/sat
Muscovite	10.7950s/sat	Smectite-high-Fe	1.6699s/sat
Herschelite	10.0512s/sat	Jadeite	1.5632s/sat
Mesolite	9.9745s/sat	Chrysotile	1.4320s/sat
Paragonite	8.6424s/sat	Calcite	1.0850s/sat
Amesite-14A	8.4926s/sat	Aragonite	0.9405s/sat
Illite	8.4023s/sat	Quartz	0.9141s/sat
Scolecite	8.2207s/sat	Corundum	0.8877s/sat
Beidellite-Ca	7.8586s/sat	Tridymite	0.7165s/sat
Montmor-Ca	7.8551s/sat	Dawsonite	0.7100s/sat
Montmor-Mg	7.7731s/sat	Dolomite-dis	0.6435s/sat
Beidellite-Mg	7.7051s/sat	Kyanite	0.4171s/sat
Montmor-Na	7.7022s/sat	Anorthite	0.4089s/sat
Beidellite-Na	7.6377s/sat	Cristobalite(alp	0.3521s/sat
Celadonite	7.4679s/sat	Chalcedony	0.3382s/sat
Montmor-K	7.4389s/sat	Kalsilite	0.2839s/sat
Beidellite-K	7.3705s/sat	Monohydrocalcite	0.2643s/sat
Laumontite	7.3078s/sat	Analcime-K	0.2405s/sat
Clinochlore-14A	7.3070s/sat	Andalusite	0.1336s/sat
Ferrite-Ca	6.7301s/sat	Coesite	0.0909s/sat
Goethite	6.6529s/sat	Grossular	0.0871s/sat
Saponite-Ca	6.6356s/sat	Analcime	0.0475s/sat
Tremolite	6.6324s/sat	Cristobalite(bet	-0.1059
Pyrophyllite	6.4867s/sat	Ice	-0.1194
Saponite-Mg	6.4827s/sat	Sillimanite	-0.2398
Beidellite-H	6.4802s/sat	Diopside	-0.2444
Saponite-Na	6.4148s/sat	SiO2(am)	-0.4140
Phlogopite	6.3502s/sat	Magnesite	-0.5198
Kaolinite	6.3347s/sat	Nepheline	-0.8171
Saponite-K	6.1475s/sat	Barite	-1.0236
Ferrite-Mg	6.0485s/sat	Cordierite_hydr	-1.2502
Maximum_Microcli	5.3444s/sat	Anthophyllite	-1.3674
K-Feldspar	5.3432s/sat	Enstatite	-1.5665
Talc	5.2607s/sat	Fluorite	-1.8926
Saponite-H	5.2572s/sat	Fe(OH)3	-2.0350
Margarite	5.2327s/sat	Huntite	-2.0823
Prehnite	5.1443s/sat	Okenite	-2.5167
Mordenite	5.0364s/sat	Wollastonite	-2.8787
Lawsonite	4.9499s/sat		

(only minerals with log Q/K > -3 listed)

Gases	fugacity	log fug.
O2(g)	0.1712	-0.766
H2O(g)	0.01903	-1.721
CO2(g)	0.0003104	-3.508
HF(g)	3.661e-015	-14.436
HCl(g)	1.255e-020	-19.901
NO2(g)	1.743e-021	-20.759
N2(g)	1.249e-022	-21.904
NO(g)	1.765e-027	-26.753
Cl2(g)	1.917e-032	-31.717
SiF4(g)	2.196e-041	-40.658
H2(g)	9.057e-043	-42.043
CO(g)	8.981e-050	-49.047
SO2(g)	7.706e-060	-59.113
NH3(g)	1.014e-071	-70.994
Na(g)	1.475e-075	-74.831
K(g)	3.882e-078	-77.411
F2(g)	1.050e-085	-84.979
Mg(g)	1.207e-130	-129.918
H2S(g)	1.134e-148	-147.946
CH4(g)	9.897e-149	-148.005
Ca(g)	1.079e-152	-151.967
Al(g)	1.644e-192	-191.784
C(g)	1.715e-193	-192.766
Si(g)	3.319e-224	-223.479
S2(g)	1.061e-238	-237.974
C2H4(g)	5.701e-243	-242.244

Original basis	total moles	In fluid		Sorbed		Kd L/kg
		moles	mg/kg	moles	mg/kg	
Al+++	3.98e-005	3.98e-005	1.07			
Ba++	1.96e-007	1.96e-007	0.0270			
Ca++	0.000359	0.000359	14.4			
Cl-	4.72e-005	4.72e-005	1.67			
F-	8.08e-005	8.08e-005	1.53			
Fe++	2.36e-005	2.36e-005	1.32			
H+	-0.000770	-0.000770	-0.775			
H2O	55.5	55.5	9.99e+005			
HCO3-	0.00612	0.00612	373.			
K+	5.44e-005	5.44e-005	2.12			
Mg++	2.47e-005	2.47e-005	0.599			
MoO4--	6.12e-007	6.12e-007	0.0979			
NH3(aq)	9.57e-005	9.57e-005	1.63			
Na+	0.00418	0.00418	96.1			
O2(aq)	0.000438	0.000438	14.0			
ReO4-	4.22e-006	4.22e-006	1.06			
SO4--	8.76e-005	8.76e-005	8.41			
SeO3--	3.32e-007	3.32e-007	0.0421			
SiO2(aq)	0.000683	0.000683	41.0			

Elemental composition	total moles	In fluid		Sorbed	
		moles	mg/kg	moles	mg/kg
Aluminum	3.976e-005	3.976e-005	1.072		
Barium	1.964e-007	1.964e-007	0.02695		
Calcium	0.0003586	0.0003586	14.36		
Carbon	0.006116	0.006116	73.42		
Chlorine	4.720e-005	4.720e-005	1.672		
Fluorine	8.082e-005	8.082e-005	1.535		
Hydrogen	111.0	111.0	1.118e+005		
Iron	2.362e-005	2.362e-005	1.318		

Magnesium	2.466e-005	2.466e-005	0.5991
Molybdenum	6.125e-007	6.125e-007	0.05873
Nitrogen	9.572e-005	9.572e-005	1.340
Oxygen	55.53	55.53	8.879e+005
Potassium	5.438e-005	5.438e-005	2.125
Rhenium	4.223e-006	4.223e-006	0.7860
Selenium	3.316e-007	3.316e-007	0.02617
Silicon	0.0006834	0.0006834	19.18
Sodium	0.004183	0.004183	96.11
Sulfur	8.760e-005	8.760e-005	2.808

Sample D1119MMT_bs

```

Step #      0          Xi = 0.0000
Temperature = 20.0 C   Pressure = 1.013 bars
pH = 9.380           log fO2 = -0.765
Eh = 0.6736 volts    pe = 11.5812
Ionic strength      = 0.007680
Charge imbalance    = -0.002045 eq/kg (-30.43% error)
Activity of water   = 0.999998
Solvent mass       = 1.000000 kg
Solution mass      = 1.000620 kg
Solution density   = 1.017 g/cm3
Chlorinity         = 0.000048 molal
Dissolved solids   = 619 mg/kg sol'n
Elect. conductivity = 560.53 uS/cm (or umho/cm)
Hardness           = 26.99 mg/kg sol'n as CaCO3
  carbonate        = 26.99 mg/kg sol'n as CaCO3
  non-carbonate    = 0.00 mg/kg sol'n as CaCO3
Rock mass          = 0.000000 kg
Carbonate alkalinity = 357.00 mg/kg sol'n as CaCO3
Water type         = Na-HCO3
  
```

No minerals in system.

Aqueous species	molality	mg/kg sol'n	act. coef.	log act.
HCO3-	0.005527	337.0	0.9131	-2.2970
Na+	0.005317	122.2	0.9131	-2.3138
CO3--	0.0007176	43.04	0.6969	-3.3009
SiO2(aq)	0.0005013	30.10	1.0000	-3.2999
O2(aq)	0.0002406	7.694	1.0000	-3.6187
F-	0.0001578	2.997	0.9120	-3.8418
Ca++	0.0001419	5.684	0.7063	-3.9990
BO2-	0.0001328	5.681	0.9131	-3.9163
HSiO3-	0.0001290	9.942	0.9131	-3.9288
B(OH)3(aq)	0.0001012	6.254	1.0000	-3.9948
CaCO3(aq)	9.675e-005	9.678	1.0000	-4.0143
NO3-	9.223e-005	5.715	0.9109	-4.0756
SO4--	6.496e-005	6.236	0.6937	-4.3462
K+	5.889e-005	2.301	0.9109	-4.2705
Cl-	4.800e-005	1.701	0.9109	-4.3593
NaHCO3(aq)	3.865e-005	3.244	1.0000	-4.4129
AlO2-	3.458e-005	2.038	0.9131	-4.5006
NaHSiO3(aq)	2.857e-005	2.858	1.0000	-4.5441
Fe(OH)3(aq)	2.045e-005	2.184	1.0000	-4.6894
OH-	1.762e-005	0.2995	0.9120	-4.7940
Mg++	1.750e-005	0.4251	0.7179	-4.9009
ReO4-	1.126e-005	2.815	0.9131	-4.9880
NaCO3-	1.004e-005	0.8327	0.9131	-5.0378
HPO4--	9.315e-006	0.8935	0.6937	-5.1897
CaHCO3+	6.289e-006	0.6354	0.9131	-5.2409
MgCO3(aq)	5.730e-006	0.4829	1.0000	-5.2418
CO2(aq)	5.131e-006	0.2257	1.0000	-5.2898
MoO4--	1.826e-006	0.2919	0.6969	-5.8953
MgHCO3+	7.699e-007	0.06565	0.9131	-6.1531
SeO4--	7.417e-007	0.1060	0.6937	-6.2886
CaSO4(aq)	5.709e-007	0.07767	1.0000	-6.2435
Ba++	1.327e-007	0.01821	0.7001	-7.0320
MgSO4(aq)	1.289e-007	0.01550	1.0000	-6.8898
CaF+	7.481e-008	0.004417	0.9131	-7.1655
NaF(aq)	6.772e-008	0.002842	1.0000	-7.1693
H2PO4-	4.972e-008	0.004819	0.9131	-7.3430
HA1O2(aq)	4.880e-008	0.002926	1.0000	-7.3116

MgF+	4.528e-008	0.001959	0.9131	-7.3836
NaCl(aq)	3.461e-008	0.002021	1.0000	-7.4609
NaAlO2(aq)	2.643e-008	0.002165	1.0000	-7.5780
KSO4-	2.012e-008	0.002717	0.9131	-7.7359
BaCO3(aq)	1.853e-008	0.003654	1.0000	-7.7322
PO4---	1.490e-008	0.001415	0.4387	-8.1845
NaOH(aq)	1.288e-008	0.0005147	1.0000	-7.8902

(only species > 1e-8 molal listed)

Mineral saturation states			
	log Q/K		log Q/K
Antigorite	66.7259s/sat	Natrolite	4.3536s/sat
Nontronite-Ca	19.6944s/sat	Smectite-low-Fe-	4.0698s/sat
Nontronite-Mg	19.5744s/sat	Albite_low	3.8988s/sat
Nontronite-Na	19.5548s/sat	Albite	3.8987s/sat
Nontronite-K	19.2630s/sat	Sanidine_high	3.8344s/sat
Nontronite-H	18.2401s/sat	Margarite	3.8011s/sat
Clinoptilolite-h	18.0008s/sat	Clinzoisite	3.7419s/sat
Clinoptilolite-C	17.9718s/sat	Zoisite	3.6959s/sat
Clinoptilolite-h	17.2445s/sat	Chrysotile	3.2544s/sat
Clinoptilolite-N	17.2437s/sat	Witherite	3.1019s/sat
Andradite	14.8590s/sat	Magnetite	2.9364s/sat
Clinoptilolite-K	14.4724s/sat	Anthophyllite	2.6107s/sat
Clinoptilolite-h	14.3626s/sat	Dolomite	2.5806s/sat
Hematite	14.1297s/sat	Dolomite-ord	2.5806s/sat
Fluorapatite	13.5000s/sat	Albite_high	2.5465s/sat
Stilbite	13.2710s/sat	Diaspore	2.0615s/sat
Epidote-ord	12.0445s/sat	Wairakite	2.0050s/sat
Epidote	12.0440s/sat	Smectite-high-Fe	1.6993s/sat
Tremolite	10.2064s/sat	Boehmite	1.6491s/sat
Herschelite	9.7184s/sat	Gibbsite	1.4895s/sat
Muscovite	9.6544s/sat	Jadeite	1.4430s/sat
Clinochlore-14A	9.5081s/sat	Calcite	1.1617s/sat
Mesolite	9.4918s/sat	Aragonite	1.0171s/sat
Amesite-14A	9.2499s/sat	Dolomite-dis	0.9988s/sat
Saponite-Ca	8.2541s/sat	Quartz	0.8319s/sat
Saponite-Mg	8.1345s/sat	Diopside	0.7137s/sat
Saponite-Na	8.1145s/sat	Tridymite	0.6343s/sat
Phlogopite	8.0603s/sat	Dawsonite	0.3706s/sat
Saponite-K	7.8226s/sat	Grossular	0.3575s/sat
Celadonite	7.7711s/sat	Monohydrocalcite	0.3410s/sat
Paragonite	7.5763s/sat	Whitlockite	0.2815s/sat
Scolecite	7.5705s/sat	Cristobalite(alp	0.2699s/sat
Illite	7.5279s/sat	Chalcedony	0.2560s/sat
Montmor-Ca	7.0994s/sat	Kalsilite	0.1715s/sat
Ferrite-Ca	7.0651s/sat	Analcime-K	0.0438s/sat
Montmor-Mg	7.0507s/sat	Corundum	0.0240s/sat
Montmor-Na	7.0277s/sat	Coesite	0.0087s/sat
Talc	6.9187s/sat	Analcime	-0.0777
Saponite-H	6.7998s/sat	Ice	-0.1194
Montmor-K	6.7399s/sat	Anorthite	-0.1591
Beidellite-Ca	6.6265s/sat	Cristobalite(bet	-0.1882
Goethite	6.5903s/sat	Magnesite	-0.2411
Ferrite-Mg	6.5856s/sat	SiO2(am)	-0.4962
Laumontite	6.5754s/sat	Kyanite	-0.5288
Beidellite-Mg	6.5063s/sat	Andalusite	-0.8123
Beidellite-Na	6.4868s/sat	Nepheline	-0.8551
Beidellite-K	6.1950s/sat	Enstatite	-0.9865
Clinochlore-7A	6.0931s/sat	Huntite	-1.1695
Kaolinite	5.3065s/sat	Sillimanite	-1.1858
Pyrophyllite	5.2941s/sat	Barite	-1.3117
Beidellite-H	5.1722s/sat	Fluorite	-1.5957

Maximum_Microcli	5.0675s/sat	Cordierite_hydr	-2.0642
K-Feldspar	5.0664s/sat	Fe(OH)3	-2.0976
Prehnite	4.9544s/sat	Okenite	-2.2209
Mordenite	4.5194s/sat	Wollastonite	-2.5007
Hydroxylapatite	4.4868s/sat	Pseudowollastoni	-2.7488
Lawsonite	4.3820s/sat	Brucite	-2.7778

(only minerals with log Q/K > -3 listed)

Gases	fugacity	log fug.
O2(g)	0.1716	-0.765
H2O(g)	0.01903	-1.721
CO2(g)	0.0001283	-3.892
HF(g)	3.034e-015	-14.518
HCl(g)	5.410e-021	-20.267
NO2(g)	7.110e-022	-21.148
N2(g)	2.067e-023	-22.685
NO(g)	7.189e-028	-27.143
Cl2(g)	3.565e-033	-32.448
BF3(g)	1.134e-041	-40.945
SiF4(g)	8.566e-042	-41.067
H2(g)	9.046e-043	-42.044
CO(g)	3.709e-050	-49.431
SO2(g)	1.031e-060	-59.987
NH3(g)	4.118e-072	-71.385
Na(g)	4.413e-075	-74.355
K(g)	9.784e-078	-77.009
F2(g)	7.221e-086	-85.141
Mg(g)	5.538e-130	-129.257
CH4(g)	4.071e-149	-148.390
H2S(g)	1.511e-149	-148.821
Ca(g)	3.110e-152	-151.507
Al(g)	6.072e-193	-192.217
C(g)	7.073e-194	-193.150
B(g)	1.885e-206	-205.725
Si(g)	2.740e-224	-223.562
S2(g)	1.889e-240	-239.724
C2H4(g)	9.671e-244	-243.015

Original basis	total moles	In fluid moles	mg/kg	Sorbed moles	mg/kg	Kd L/kg
Al+++	3.47e-005	3.47e-005	0.935			
B(OH)3(aq)	0.000234	0.000234	14.5			
Ba++	1.51e-007	1.51e-007	0.0208			
Ca++	0.000246	0.000246	9.84			
Cl-	4.80e-005	4.80e-005	1.70			
F-	0.000158	0.000158	3.00			
Fe++	2.04e-005	2.04e-005	1.14			
H+	-0.00140	-0.00140	-1.41			
H2O	55.5	55.5	9.99e+005			
HCO3-	0.00641	0.00641	391.			
HPO4--	9.38e-006	9.38e-006	0.900			
K+	5.89e-005	5.89e-005	2.30			
Mg++	2.42e-005	2.42e-005	0.587			
MoO4--	1.83e-006	1.83e-006	0.292			
NH3(aq)	9.22e-005	9.22e-005	1.57			
Na+	0.00539	0.00539	124.			
O2(aq)	0.000431	0.000431	13.8			
ReO4-	1.13e-005	1.13e-005	2.82			
SO4--	6.57e-005	6.57e-005	6.31			
SeO3--	7.42e-007	7.42e-007	0.0941			
SiO2(aq)	0.000659	0.000659	39.6			

Elemental composition	In fluid		Sorbed		
	total moles	moles	mg/kg	moles	mg/kg
Aluminum	3.466e-005	3.466e-005	0.9345		
Barium	1.512e-007	1.512e-007	0.02076		
Boron	0.0002340	0.0002340	2.528		
Calcium	0.0002456	0.0002456	9.837		
Carbon	0.006408	0.006408	76.91		
Chlorine	4.803e-005	4.803e-005	1.702		
Fluorine	0.0001580	0.0001580	3.000		
Hydrogen	111.0	111.0	1.118e+005		
Iron	2.045e-005	2.045e-005	1.141		
Magnesium	2.418e-005	2.418e-005	0.5873		
Molybdenum	1.826e-006	1.826e-006	0.1751		
Nitrogen	9.223e-005	9.223e-005	1.291		
Oxygen	55.53	55.53	8.879e+005		
Phosphorus	9.380e-006	9.380e-006	0.2903		
Potassium	5.891e-005	5.891e-005	2.302		
Rhenium	1.126e-005	1.126e-005	2.095		
Selenium	7.417e-007	7.417e-007	0.05853		
Silicon	0.0006589	0.0006589	18.49		
Sodium	0.005395	0.005395	123.9		
Sulfur	6.568e-005	6.568e-005	2.105		

Sample D11NBTW

```

Step #      0          Xi = 0.0000
Temperature = 20.0 C   Pressure = 1.013 bars
pH = 8.200           log fO2 = -0.756
Eh = 0.7424 volts    pe = 12.7636
Ionic strength      = 0.001986
Charge imbalance    = -0.000363 eq/kg (-21.76% error)
Activity of water   = 1.000000
Solvent mass        = 1.000000 kg
Solution mass       = 1.000188 kg
Solution density    = 1.016 g/cm3
Chlorinity          = 0.000000 molal
Dissolved solids    = 188 mg/kg sol'n
Elect. conductivity = 149.80 uS/cm (or umho/cm)
Hardness            = 31.13 mg/kg sol'n as CaCO3
  carbonate         = 31.13 mg/kg sol'n as CaCO3
  non-carbonate     = 0.00 mg/kg sol'n as CaCO3
Rock mass           = 0.000000 kg
Carbonate alkalinity = 88.70 mg/kg sol'n as CaCO3
Water type          = Na-HCO3
  
```

No minerals in system.

Aqueous species	molality	mg/kg sol'n	act. coef.	log act.
HCO3-	0.001735	105.8	0.9523	-2.7819
Na+	0.0008024	18.44	0.9523	-3.1168
SiO2(aq)	0.0004617	27.74	1.0000	-3.3356
O2(aq)	0.0002460	7.871	1.0000	-3.6090
Ca++	0.0002328	9.329	0.8263	-3.7159
NO3-	7.936e-005	4.919	0.9516	-4.1220
K+	7.022e-005	2.745	0.9516	-4.1751
Mg++	6.879e-005	1.672	0.8304	-4.2432
CO2(aq)	2.543e-005	1.119	1.0000	-4.5947
CO3--	1.314e-005	0.7887	0.8230	-4.9658
HSiO3-	7.530e-006	0.5804	0.9523	-5.1445
CaCO3(aq)	4.017e-006	0.4020	1.0000	-5.3961
CaHCO3+	3.790e-006	0.3831	0.9523	-5.4426
Zn++	2.814e-006	0.1840	0.8263	-5.6335
NaHCO3(aq)	1.991e-006	0.1673	1.0000	-5.7008
OH-	1.115e-006	0.01897	0.9520	-5.9740
MgHCO3+	1.099e-006	0.09374	0.9523	-5.9803
MgCO3(aq)	5.636e-007	0.04751	1.0000	-6.2490
NaHSiO3(aq)	2.737e-007	0.02738	1.0000	-6.5628
MoO4--	1.036e-007	0.01657	0.8230	-7.0692
Ba++	6.784e-008	0.009314	0.8241	-7.2526
NaCO3-	3.277e-008	0.002720	0.9523	-7.5057

(only species > 1e-8 molal listed)

Mineral saturation states

	log Q/K		log Q/K
Zn2SiO4	3.9823s/sat	Aragonite	-0.3646
Talc	1.6689s/sat	SiO2(am)	-0.5319
Witherite	1.2164s/sat	Zincite	-0.7120
Quartz	0.7962s/sat	Smithsonite	-0.7663
Tridymite	0.5986s/sat	Monohydrocalcite	-1.0408
Cristobalite(alp)	0.2342s/sat	Zn(OH)2(gamma)	-1.1167
Chalcedony	0.2203s/sat	Zn(OH)2(epsilon)	-1.1420
Dolomite	0.1916s/sat	Magnesite	-1.2483
Dolomite-ord	0.1916s/sat	Dolomite-dis	-1.3902
Coesite	-0.0270	Zn(OH)2(beta)	-1.4179

Ice	-0.1194	Chrysotile	-1.9240
Calcite	-0.2200	Enstatite	-2.7245
Cristobalite(bet	-0.2239	Tremolite	-2.7445

(only minerals with log Q/K > -3 listed)

Gases	fugacity	log fug.
O2(g)	0.1755	-0.756
H2O(g)	0.01903	-1.721
CO2(g)	0.0006359	-3.197
NO2(g)	9.619e-021	-20.017
N2(g)	3.619e-021	-20.441
NO(g)	9.618e-027	-26.017
H2(g)	8.946e-043	-42.048
CO(g)	1.817e-049	-48.741
NH3(g)	5.358e-071	-70.271
Zn(g)	2.942e-075	-74.531
Na(g)	4.563e-077	-76.341
K(g)	8.008e-079	-78.096
Mg(g)	1.087e-131	-130.964
CH4(g)	1.930e-148	-147.715
Ca(g)	2.577e-154	-153.589
C(g)	3.428e-193	-192.465
Si(g)	2.468e-224	-223.608
C2H4(g)	2.221e-242	-241.653

Original basis	total moles	In fluid moles	mg/kg	Sorbed moles	mg/kg	Kd L/kg
Ba++	6.81e-008	6.81e-008	0.00935			
Ca++	0.000241	0.000241	9.64			
H+	-8.06e-005	-8.06e-005	-0.0812			
H2O	55.5	55.5	1.00e+006			
HCO3-	0.00179	0.00179	109.			
K+	7.02e-005	7.02e-005	2.75			
Mg++	7.05e-005	7.05e-005	1.71			
MoO4--	1.04e-007	1.04e-007	0.0166			
NH3(aq)	7.94e-005	7.94e-005	1.35			
Na+	0.000805	0.000805	18.5			
O2(aq)	0.000405	0.000405	12.9			
SiO2(aq)	0.000470	0.000470	28.2			
Zn++	2.81e-006	2.81e-006	0.184			

Elemental composition	total moles	In fluid moles	mg/kg	Sorbed moles	mg/kg
Barium	6.808e-008	6.808e-008	0.009347		
Calcium	0.0002406	0.0002406	9.642		
Carbon	0.001785	0.001785	21.44		
Hydrogen	111.0	111.0	1.119e+005		
Magnesium	7.045e-005	7.045e-005	1.712		
Molybdenum	1.036e-007	1.036e-007	0.009937		
Nitrogen	7.936e-005	7.936e-005	1.111		
Oxygen	55.52	55.52	8.881e+005		
Potassium	7.022e-005	7.022e-005	2.745		
Silicon	0.0004695	0.0004695	13.18		
Sodium	0.0008047	0.0008047	18.50		
Zinc	2.814e-006	2.814e-006	0.1840		

Sample D11NEBOT

```

Step #      0          Xi = 0.0000
Temperature = 20.0 C   Pressure = 1.013 bars
pH = 7.660           log fO2 = -0.756
Eh = 0.7738 volts    pe = 13.3036
Ionic strength = 0.002201
Charge imbalance = -0.000562 eq/kg (-31.31% error)
Activity of water = 0.999999
Solvent mass = 1.000000 kg
Solution mass = 1.000202 kg
Solution density = 1.016 g/cm3
Chlorinity = 0.000021 molal
Dissolved solids = 202 mg/kg sol'n
Elect. conductivity = 166.57 uS/cm (or umho/cm)
Hardness = 33.82 mg/kg sol'n as CaCO3
  carbonate = 33.82 mg/kg sol'n as CaCO3
  non-carbonate = 0.00 mg/kg sol'n as CaCO3
Rock mass = 0.000000 kg
Carbonate alkalinity = 87.80 mg/kg sol'n as CaCO3
Water type = Na-HCO3
  
```

No minerals in system.

Aqueous species	molality	mg/kg sol'n	act. coef.	log act.
HCO3-	0.001739	106.1	0.9500	-2.7820
Na+	0.0007728	17.76	0.9500	-3.1342
SiO2(aq)	0.0004707	28.28	1.0000	-3.3272
Ca++	0.0002510	10.06	0.8187	-3.6873
O2(aq)	0.0002460	7.871	1.0000	-3.6090
NO3-	0.0001255	7.783	0.9493	-3.9238
CO2(aq)	8.815e-005	3.879	1.0000	-4.0548
K+	7.875e-005	3.078	0.9493	-4.1264
Mg++	7.784e-005	1.892	0.8232	-4.1933
SO4--	7.206e-005	6.921	0.8140	-4.2317
F-	3.674e-005	0.6978	0.9496	-4.4574
Cl-	2.120e-005	0.7515	0.9493	-4.6962
CaHCO3+	4.057e-006	0.4100	0.9500	-5.4141
CO3--	3.827e-006	0.2296	0.8152	-5.5059
HSiO3-	2.219e-006	0.1711	0.9500	-5.6761
NaHCO3(aq)	1.913e-006	0.1607	1.0000	-5.7183
CaSO4(aq)	1.523e-006	0.2073	1.0000	-5.8172
CaCO3(aq)	1.237e-006	0.1238	1.0000	-5.9076
MgHCO3+	1.235e-006	0.1054	0.9500	-5.9305
MgSO4(aq)	8.556e-007	0.1030	1.0000	-6.0677
OH-	3.225e-007	0.005483	0.9496	-6.5140
MgCO3(aq)	1.823e-007	0.01537	1.0000	-6.7392
MoO4--	1.344e-007	0.02149	0.8152	-6.9604
NaHSiO3(aq)	7.730e-008	0.007735	1.0000	-7.1118
Ba++	7.660e-008	0.01052	0.8164	-7.2039
MgF+	5.379e-008	0.002329	0.9500	-7.2916
CaF+	3.572e-008	0.002110	0.9500	-7.4693
KSO4-	3.507e-008	0.004740	0.9500	-7.4773
H+	2.295e-008	2.313e-005	0.9533	-7.6600

(only species > 1e-8 molal listed)

Mineral saturation states

	log Q/K		log Q/K
Quartz	0.8046s/sat	Dolomite	-0.8100
Witherite	0.7250s/sat	Dolomite-ord	-0.8100
Tridymite	0.6070s/sat	Aragonite	-0.8761

Cristobalite(alp)	0.2426s/sat	Barite	-1.3692
Chalcedony	0.2287s/sat	Talc	-1.3878
Coesite	-0.0186	Monohydrocalcite	-1.5523
Ice	-0.1194	Magnesite	-1.7385
Cristobalite(bet)	-0.2155	Dolomite-dis	-2.3918
SiO2(am)	-0.5235	Fluorite	-2.5150
Calcite	-0.7315		

(only minerals with log Q/K > -3 listed)

Gases	fugacity	log fug.
O2(g)	0.1755	-0.756
H2O(g)	0.01903	-1.721
CO2(g)	0.002205	-2.657
HF(g)	3.858e-014	-13.414
HCl(g)	1.307e-019	-18.884
N2(g)	1.083e-019	-18.965
NO2(g)	5.263e-020	-19.279
NO(g)	5.263e-026	-25.279
Cl2(g)	2.104e-030	-29.677
SiF4(g)	2.105e-037	-36.677
H2(g)	8.946e-043	-42.048
CO(g)	6.300e-049	-48.201
SO2(g)	3.654e-057	-56.437
NH3(g)	2.932e-070	-69.533
Na(g)	1.264e-077	-76.898
K(g)	2.583e-079	-78.588
F2(g)	1.181e-083	-82.928
Mg(g)	1.014e-132	-131.994
H2S(g)	5.179e-146	-145.286
CH4(g)	6.689e-148	-147.175
Ca(g)	2.289e-155	-154.640
C(g)	1.188e-192	-191.925
Si(g)	2.516e-224	-223.599
S2(g)	2.271e-233	-232.644
C2H4(g)	2.670e-241	-240.574

Original basis	total moles	In fluid moles	mg/kg	Sorbed moles	mg/kg	Kd L/kg
Ba++	7.67e-008	7.67e-008	0.0105			
Ca++	0.000258	0.000258	10.3			
Cl-	2.12e-005	2.12e-005	0.752			
F-	3.68e-005	3.68e-005	0.700			
H+	-4.52e-005	-4.52e-005	-0.0456			
H2O	55.5	55.5	1.00e+006			
HCO3-	0.00184	0.00184	112.			
K+	7.88e-005	7.88e-005	3.08			
Mg++	8.02e-005	8.02e-005	1.95			
MoO4--	1.34e-007	1.34e-007	0.0215			
NH3(aq)	0.000126	0.000126	2.14			
Na+	0.000775	0.000775	17.8			
O2(aq)	0.000497	0.000497	15.9			
SO4--	7.45e-005	7.45e-005	7.15			
SiO2(aq)	0.000473	0.000473	28.4			

Elemental composition	total moles	In fluid moles	mg/kg	Sorbed moles	mg/kg
Barium	7.668e-008	7.668e-008	0.01053		
Calcium	0.0002578	0.0002578	10.33		
Carbon	0.001840	0.001840	22.09		
Chlorine	2.121e-005	2.121e-005	0.7517		

Fluorine	3.683e-005	3.683e-005	0.6995
Hydrogen	111.0	111.0	1.119e+005
Magnesium	8.017e-005	8.017e-005	1.948
Molybdenum	1.344e-007	1.344e-007	0.01289
Nitrogen	0.0001255	0.0001255	1.758
Oxygen	55.52	55.52	8.880e+005
Potassium	7.878e-005	7.878e-005	3.080
Silicon	0.0004730	0.0004730	13.28
Sodium	0.0007748	0.0007748	17.81
Sulfur	7.447e-005	7.447e-005	2.388

Sample D11NWBOT

```

Step #      0          Xi = 0.0000
Temperature = 20.0 C   Pressure = 1.013 bars
pH = 7.790           log fO2 = -0.756
Eh = 0.7662 volts    pe = 13.1736
Ionic strength = 0.002339
Charge imbalance = -0.000656 eq/kg (-34.32% error)
Activity of water = 0.999999
Solvent mass = 1.000000 kg
Solution mass = 1.000212 kg
Solution density = 1.016 g/cm3
Chlorinity = 0.000026 molal
Dissolved solids = 212 mg/kg sol'n
Elect. conductivity = 176.76 uS/cm (or umho/cm)
Hardness = 34.72 mg/kg sol'n as CaCO3
  carbonate = 34.72 mg/kg sol'n as CaCO3
  non-carbonate = 0.00 mg/kg sol'n as CaCO3
Rock mass = 0.000000 kg
Carbonate alkalinity = 93.30 mg/kg sol'n as CaCO3
Water type = Na-HCO3
  
```

No minerals in system.

Aqueous species	molality	mg/kg sol'n	act. coef.	log act.
HCO3-	0.001844	112.5	0.9486	-2.7571
Na+	0.0008239	18.94	0.9486	-3.1071
SiO2(aq)	0.0004490	26.97	1.0000	-3.3477
Ca++	0.0002525	10.12	0.8141	-3.6871
O2(aq)	0.0002460	7.871	1.0000	-3.6090
NO3-	0.0001532	9.495	0.9478	-3.8381
Mg++	8.388e-005	2.038	0.8188	-4.1632
SO4--	8.140e-005	7.818	0.8091	-4.1814
K+	7.698e-005	3.009	0.9478	-4.1369
CO2(aq)	6.920e-005	3.045	1.0000	-4.1599
F-	3.389e-005	0.6437	0.9482	-4.4930
Cl-	2.606e-005	0.9237	0.9478	-4.6073
CO3--	5.499e-006	0.3299	0.8104	-5.3511
ReO4-	5.338e-006	1.335	0.9486	-5.2956
CaHCO3+	4.303e-006	0.4350	0.9486	-5.3891
HSiO3-	2.860e-006	0.2204	0.9486	-5.5665
Zn++	2.474e-006	0.1617	0.8141	-5.6960
NaHCO3(aq)	2.156e-006	0.1811	1.0000	-5.6663
CaCO3(aq)	1.768e-006	0.1769	1.0000	-5.7526
CaSO4(aq)	1.711e-006	0.2329	1.0000	-5.7667
MgHCO3+	1.404e-006	0.1198	0.9486	-5.8755
MgSO4(aq)	1.030e-006	0.1239	1.0000	-5.9872
MoO4--	5.560e-007	0.08890	0.8104	-6.3463
OH-	4.356e-007	0.007408	0.9482	-6.3840
MgCO3(aq)	2.791e-007	0.02353	1.0000	-6.5542
NaHSiO3(aq)	1.059e-007	0.01060	1.0000	-6.9751
Ba++	7.728e-008	0.01061	0.8116	-7.2026
MgF+	5.319e-008	0.002303	0.9486	-7.2971
KSO4-	3.850e-008	0.005203	0.9486	-7.4375
CaF+	3.297e-008	0.001947	0.9486	-7.5049
ZnSO4(aq)	2.455e-008	0.003963	1.0000	-7.6100
H+	1.703e-008	1.717e-005	0.9521	-7.7900
NaCO3-	1.386e-008	0.001150	0.9486	-7.8812

(only species > 1e-8 molal listed)

Mineral saturation states

	log Q/K		log Q/K
Zn2SiO4	2.2053s/sat	Talc	-0.5994
Witherite	0.8812s/sat	Aragonite	-0.7211
Quartz	0.7841s/sat	Smithsonite	-1.2140
Tridymite	0.5865s/sat	Barite	-1.3175
Cristobalite(alp)	0.2221s/sat	Monohydrocalcite	-1.3973
Chalcedony	0.2082s/sat	Magnesite	-1.5535
Coesite	-0.0391	Zincite	-1.5945
Ice	-0.1194	Zn(OH)2(gamma)	-1.9992
Cristobalite(bet)	-0.2359	Zn(OH)2(epsilon)	-2.0245
Dolomite	-0.4700	Dolomite-dis	-2.0518
Dolomite-ord	-0.4700	Zn(OH)2(beta)	-2.3004
SiO2(am)	-0.5440	Fluorite	-2.5862
Calcite	-0.5765		

(only minerals with log Q/K > -3 listed)

Gases	fugacity	log fug.
O2(g)	0.1755	-0.756
H2O(g)	0.01903	-1.721
CO2(g)	0.001731	-2.762
HF(g)	2.635e-014	-13.579
HCl(g)	1.189e-019	-18.925
N2(g)	8.834e-020	-19.054
NO2(g)	4.753e-020	-19.323
NO(g)	4.752e-026	-25.323
Cl2(g)	1.741e-030	-29.759
SiF4(g)	4.366e-038	-37.360
H2(g)	8.946e-043	-42.048
CO(g)	4.946e-049	-48.306
SO2(g)	2.255e-057	-56.647
NH3(g)	2.648e-070	-69.577
Zn(g)	3.856e-076	-75.414
Na(g)	1.816e-077	-76.741
K(g)	3.402e-079	-78.468
F2(g)	5.508e-084	-83.259
Mg(g)	1.978e-132	-131.704
H2S(g)	3.196e-146	-145.495
CH4(g)	5.251e-148	-147.280
Ca(g)	4.167e-155	-154.380
C(g)	9.328e-193	-192.030
Si(g)	2.400e-224	-223.620
S2(g)	8.646e-234	-233.063
C2H4(g)	1.645e-241	-240.784

Original basis	total moles	In fluid		Sorbed		Kd L/kg
		moles	mg/kg	moles	mg/kg	
Ba++	7.74e-008	7.74e-008	0.0106			
Ca++	0.000260	0.000260	10.4			
Cl-	2.61e-005	2.61e-005	0.924			
F-	3.40e-005	3.40e-005	0.645			
H+	-9.49e-005	-9.49e-005	-0.0956			
H2O	55.5	55.5	1.00e+006			
HCO3-	0.00193	0.00193	118.			
K+	7.70e-005	7.70e-005	3.01			
Mg++	8.66e-005	8.66e-005	2.11			
MoO4--	5.56e-007	5.56e-007	0.0889			
NH3(aq)	0.000153	0.000153	2.61			
Na+	0.000826	0.000826	19.0			
O2(aq)	0.000552	0.000552	17.7			

ReO4-	5.34e-006	5.34e-006	1.34
SO4--	8.42e-005	8.42e-005	8.09
SiO2(aq)	0.000452	0.000452	27.2
Zn++	2.50e-006	2.50e-006	0.163

Elemental composition	In fluid			Sorbed	
	total moles	moles	mg/kg	moles	mg/kg
Barium	7.739e-008	7.739e-008	0.01063		
Calcium	0.0002603	0.0002603	10.43		
Carbon	0.001929	0.001929	23.16		
Chlorine	2.606e-005	2.606e-005	0.9239		
Fluorine	3.398e-005	3.398e-005	0.6454		
Hydrogen	111.0	111.0	1.119e+005		
Magnesium	8.665e-005	8.665e-005	2.106		
Molybdenum	5.560e-007	5.560e-007	0.05333		
Nitrogen	0.0001532	0.0001532	2.145		
Oxygen	55.52	55.52	8.880e+005		
Potassium	7.702e-005	7.702e-005	3.011		
Rhenium	5.338e-006	5.338e-006	0.9937		
Silicon	0.0004520	0.0004520	12.69		
Sodium	0.0008262	0.0008262	18.99		
Sulfur	8.421e-005	8.421e-005	2.700		
Zinc	2.498e-006	2.498e-006	0.1633		

Sample D11SEBOT

```

Step #      0          Xi = 0.0000
Temperature = 20.0 C   Pressure = 1.013 bars
pH = 7.820           log fO2 = -0.756
Eh = 0.7645 volts    pe = 13.1436
Ionic strength = 0.002349
Charge imbalance = -0.000634 eq/kg (-33.08% error)
Activity of water = 0.999999
Solvent mass = 1.000000 kg
Solution mass = 1.000210 kg
Solution density = 1.016 g/cm3
Chlorinity = 0.000027 molal
Dissolved solids = 210 mg/kg sol'n
Elect. conductivity = 178.81 uS/cm (or umho/cm)
Hardness = 34.11 mg/kg sol'n as CaCO3
  carbonate = 34.11 mg/kg sol'n as CaCO3
  non-carbonate = 0.00 mg/kg sol'n as CaCO3
Rock mass = 0.000000 kg
Carbonate alkalinity = 90.90 mg/kg sol'n as CaCO3
Water type = Na-HCO3
  
```

No minerals in system.

Aqueous species	molality	mg/kg sol'n	act. coef.	log act.
HCO3-	0.001796	109.6	0.9485	-2.7687
Na+	0.0008495	19.53	0.9485	-3.0938
SiO2(aq)	0.0004210	25.29	1.0000	-3.3757
Ca++	0.0002522	10.11	0.8138	-3.6877
O2(aq)	0.0002460	7.871	1.0000	-3.6090
NO3-	0.0001682	10.43	0.9477	-3.7974
SO4--	9.498e-005	9.122	0.8088	-4.1145
K+	8.477e-005	3.314	0.9477	-4.0951
Mg++	7.787e-005	1.892	0.8185	-4.1956
CO2(aq)	6.288e-005	2.767	1.0000	-4.2015
F-	3.234e-005	0.6144	0.9481	-4.5133
Cl-	2.709e-005	0.9601	0.9477	-4.5906
CO3--	5.739e-006	0.3443	0.8101	-5.3326
ReO4-	5.005e-006	1.252	0.9485	-5.3236
CaHCO3+	4.185e-006	0.4230	0.9485	-5.4013
HSiO3-	2.874e-006	0.2215	0.9485	-5.5646
NaHCO3(aq)	2.165e-006	0.1818	1.0000	-5.6646
CaSO4(aq)	1.993e-006	0.2713	1.0000	-5.7005
CaCO3(aq)	1.842e-006	0.1843	1.0000	-5.7347
MgHCO3+	1.269e-006	0.1083	0.9485	-5.9195
MgSO4(aq)	1.115e-006	0.1341	1.0000	-5.9528
MoO4--	5.057e-007	0.08086	0.8101	-6.3876
OH-	4.668e-007	0.007938	0.9481	-6.3540
MgCO3(aq)	2.703e-007	0.02278	1.0000	-6.5682
NaHSiO3(aq)	1.097e-007	0.01097	1.0000	-6.9599
Ba++	7.656e-008	0.01051	0.8113	-7.2068
KSO4-	4.945e-008	0.006682	0.9485	-7.3288
MgF+	4.711e-008	0.002039	0.9485	-7.3499
CaF+	3.142e-008	0.001856	0.9485	-7.5258
H+	1.590e-008	1.602e-005	0.9520	-7.8200
NaCO3-	1.491e-008	0.001237	0.9485	-7.8495

(only species > 1e-8 molal listed)

Mineral saturation states

	log Q/K		log Q/K
Witherite	0.8953s/sat	Calcite	-0.5587
Quartz	0.7561s/sat	SiO2(am)	-0.5720
Tridymite	0.5585s/sat	Talc	-0.6287
Cristobalite(alp)	0.1941s/sat	Aragonite	-0.7032
Chalcedony	0.1802s/sat	Barite	-1.2549
Coesite	-0.0671	Monohydrocalcite	-1.3794
Ice	-0.1194	Magnesite	-1.5675
Cristobalite(bet)	-0.2640	Dolomite-dis	-2.0480
Dolomite	-0.4662	Fluorite	-2.6274
Dolomite-ord	-0.4662		

(only minerals with log Q/K > -3 listed)

Gases fugacity log fug.

	fugacity	log fug.
O2(g)	0.1755	-0.756
H2O(g)	0.01903	-1.721
CO2(g)	0.001573	-2.803
HF(g)	2.347e-014	-13.630
HCl(g)	1.153e-019	-18.938
N2(g)	9.282e-020	-19.032
NO2(g)	4.872e-020	-19.312
NO(g)	4.871e-026	-25.312
Cl2(g)	1.638e-030	-29.786
SiF4(g)	2.575e-038	-37.589
H2(g)	8.946e-043	-42.048
CO(g)	4.494e-049	-48.347
SO2(g)	2.291e-057	-56.640
NH3(g)	2.714e-070	-69.566
Na(g)	2.006e-077	-76.698
K(g)	4.013e-079	-78.396
F2(g)	4.369e-084	-83.360
Mg(g)	2.107e-132	-131.676
H2S(g)	3.247e-146	-145.489
CH4(g)	4.772e-148	-147.321
Ca(g)	4.778e-155	-154.321
C(g)	8.476e-193	-192.072
Si(g)	2.250e-224	-223.648
S2(g)	8.922e-234	-233.050
C2H4(g)	1.358e-241	-240.867

Original basis total moles In fluid moles mg/kg Sorbed moles mg/kg Kd L/kg

Original basis	total moles	In fluid moles	mg/kg	Sorbed moles	mg/kg	Kd L/kg
Ba++	7.67e-008	7.67e-008	0.0105			
Ca++	0.000260	0.000260	10.4			
Cl-	2.71e-005	2.71e-005	0.960			
F-	3.24e-005	3.24e-005	0.616			
H+	-0.000117	-0.000117	-0.118			
H2O	55.5	55.5	1.00e+006			
HCO3-	0.00187	0.00187	114.			
K+	8.48e-005	8.48e-005	3.32			
Mg++	8.06e-005	8.06e-005	1.96			
MoO4--	5.06e-007	5.06e-007	0.0809			
NH3(aq)	0.000168	0.000168	2.86			
Na+	0.000852	0.000852	19.6			
O2(aq)	0.000583	0.000583	18.6			
ReO4-	5.00e-006	5.00e-006	1.25			
SO4--	9.81e-005	9.81e-005	9.43			
SiO2(aq)	0.000424	0.000424	25.5			

Elemental composition	In fluid			Sorbed	
	total moles	moles	mg/kg	moles	mg/kg
Barium	7.668e-008	7.668e-008	0.01053		
Calcium	0.0002603	0.0002603	10.43		
Carbon	0.001874	0.001874	22.51		
Chlorine	2.709e-005	2.709e-005	0.9603		
Fluorine	3.243e-005	3.243e-005	0.6159		
Hydrogen	111.0	111.0	1.119e+005		
Magnesium	8.057e-005	8.057e-005	1.958		
Molybdenum	5.057e-007	5.057e-007	0.04851		
Nitrogen	0.0001682	0.0001682	2.356		
Oxygen	55.52	55.52	8.880e+005		
Potassium	8.482e-005	8.482e-005	3.316		
Rhenium	5.005e-006	5.005e-006	0.9317		
Silicon	0.0004240	0.0004240	11.91		
Sodium	0.0008518	0.0008518	19.58		
Sulfur	9.814e-005	9.814e-005	3.146		

Sample D11SWBOT

```

Step #      0          Xi = 0.0000
Temperature = 20.0 C   Pressure = 1.013 bars
pH = 7.850           log fO2 = -0.756
Eh = 0.7627 volts    pe = 13.1136
Ionic strength      = 0.002291
Charge imbalance    = -0.000673 eq/kg (-36.1% error)
Activity of water   = 0.999999
Solvent mass        = 1.000000 kg
Solution mass       = 1.000204 kg
Solution density    = 1.016 g/cm3
Chlorinity          = 0.000028 molal
Dissolved solids    = 204 mg/kg sol'n
Elect. conductivity = 174.23 uS/cm (or umho/cm)
Hardness            = 33.20 mg/kg sol'n as CaCO3
  carbonate         = 33.20 mg/kg sol'n as CaCO3
  non-carbonate     = 0.00 mg/kg sol'n as CaCO3
Rock mass           = 0.000000 kg
Carbonate alkalinity = 89.10 mg/kg sol'n as CaCO3
Water type          = Na-HCO3
  
```

No minerals in system.

Aqueous species	molality	mg/kg sol'n	act. coef.	log act.
HCO3-	0.001760	107.3	0.9491	-2.7773
Na+	0.0007983	18.35	0.9491	-3.1205
SiO2(aq)	0.0003860	23.19	1.0000	-3.4134
O2(aq)	0.0002460	7.871	1.0000	-3.6090
Ca++	0.0002378	9.531	0.8157	-3.7122
NO3-	0.0001635	10.13	0.9483	-3.8096
SO4--	9.867e-005	9.477	0.8108	-4.0969
Mg++	8.331e-005	2.024	0.8203	-4.1653
K+	8.100e-005	3.166	0.9483	-4.1146
CO2(aq)	5.754e-005	2.532	1.0000	-4.2400
F-	3.017e-005	0.5731	0.9487	-4.5433
Cl-	2.803e-005	0.9935	0.9483	-4.5754
CO3--	6.015e-006	0.3609	0.8120	-5.3112
CaHCO3+	3.876e-006	0.3918	0.9491	-5.4343
ReO4-	3.256e-006	0.8144	0.9491	-5.5101
HSiO3-	2.821e-006	0.2175	0.9491	-5.5722
NaHCO3(aq)	1.996e-006	0.1676	1.0000	-5.6999
CaSO4(aq)	1.962e-006	0.2670	1.0000	-5.7073
CaCO3(aq)	1.829e-006	0.1830	1.0000	-5.7378
MgHCO3+	1.333e-006	0.1137	0.9491	-5.8978
MoO4--	1.272e-006	0.2034	0.8120	-5.9860
MgSO4(aq)	1.245e-006	0.1498	1.0000	-5.9049
OH-	4.999e-007	0.008501	0.9487	-6.3240
MgCO3(aq)	3.044e-007	0.02566	1.0000	-6.5165
NaHSiO3(aq)	1.013e-007	0.01014	1.0000	-6.9943
Ba++	7.798e-008	0.01071	0.8133	-7.1978
KSO4-	4.921e-008	0.006649	0.9491	-7.3307
MgF+	4.712e-008	0.002040	0.9491	-7.3495
CaF+	2.770e-008	0.001636	0.9491	-7.5802
H+	1.483e-008	1.494e-005	0.9525	-7.8500
NaCO3-	1.472e-008	0.001222	0.9491	-7.8548

(only species > 1e-8 molal listed)

Mineral saturation states

	log Q/K		log Q/K
Witherite	0.9258s/sat	Talc	-0.5086
Quartz	0.7184s/sat	Calcite	-0.5617
Tridymite	0.5208s/sat	SiO2(am)	-0.6097
Cristobalite(alp)	0.1564s/sat	Aragonite	-0.7063
Chalcedony	0.1425s/sat	Barite	-1.2282
Coesite	-0.1048	Monohydrocalcite	-1.3825
Ice	-0.1194	Magnesite	-1.5158
Cristobalite(bet)	-0.3016	Dolomite-dis	-1.9993
Dolomite	-0.4175	Fluorite	-2.7117
Dolomite-ord	-0.4175		

(only minerals with log Q/K > -3 listed)

Gases	fugacity	log fug.
O2(g)	0.1755	-0.756
H2O(g)	0.01903	-1.721
CO2(g)	0.001439	-2.842
HF(g)	2.044e-014	-13.689
HCl(g)	1.114e-019	-18.953
N2(g)	7.643e-020	-19.117
NO2(g)	4.421e-020	-19.355
NO(g)	4.420e-026	-25.355
Cl2(g)	1.530e-030	-29.815
SiF4(g)	1.360e-038	-37.867
H2(g)	8.946e-043	-42.048
CO(g)	4.112e-049	-48.386
SO2(g)	2.078e-057	-56.682
NH3(g)	2.463e-070	-69.609
Na(g)	2.021e-077	-76.694
K(g)	4.112e-079	-78.386
F2(g)	3.315e-084	-83.479
Mg(g)	2.594e-132	-131.586
H2S(g)	2.945e-146	-145.531
CH4(g)	4.366e-148	-147.360
Ca(g)	5.185e-155	-154.285
C(g)	7.756e-193	-192.110
Si(g)	2.063e-224	-223.685
S2(g)	7.341e-234	-233.134
C2H4(g)	1.137e-241	-240.944

Original basis	total moles	In fluid		Sorbed		Kd L/kg
		moles	mg/kg	moles	mg/kg	
Ba++	7.81e-008	7.81e-008	0.0107			
Ca++	0.000246	0.000246	9.84			
Cl-	2.80e-005	2.80e-005	0.994			
F-	3.03e-005	3.03e-005	0.575			
H+	-0.000118	-0.000118	-0.118			
H2O	55.5	55.5	1.00e+006			
HCO3-	0.00183	0.00183	112.			
K+	8.10e-005	8.10e-005	3.17			
Mg++	8.62e-005	8.62e-005	2.10			
MoO4--	1.27e-006	1.27e-006	0.203			
NH3(aq)	0.000163	0.000163	2.78			
Na+	0.000800	0.000800	18.4			
O2(aq)	0.000573	0.000573	18.3			
ReO4-	3.26e-006	3.26e-006	0.814			
SO4--	0.000102	0.000102	9.79			
SiO2(aq)	0.000389	0.000389	23.4			

Elemental composition	In fluid			Sorbed	
	total moles	moles	mg/kg	moles	mg/kg
Barium	7.811e-008	7.811e-008	0.01072		
Calcium	0.0002455	0.0002455	9.839		
Carbon	0.001833	0.001833	22.01		
Chlorine	2.804e-005	2.804e-005	0.9937		
Fluorine	3.025e-005	3.025e-005	0.5746		
Hydrogen	111.0	111.0	1.119e+005		
Magnesium	8.624e-005	8.624e-005	2.096		
Molybdenum	1.272e-006	1.272e-006	0.1220		
Nitrogen	0.0001635	0.0001635	2.289		
Oxygen	55.52	55.52	8.880e+005		
Potassium	8.105e-005	8.105e-005	3.168		
Rhenium	3.256e-006	3.256e-006	0.6061		
Silicon	0.0003889	0.0003889	10.92		
Sodium	0.0008005	0.0008005	18.40		
Sulfur	0.0001019	0.0001019	3.268		

Sample D1119MMB_ts

```

Step #      0          Xi = 0.0000
Temperature = 20.0 C   Pressure = 1.013 bars
pH = 8.330           log fO2 = -0.767
Eh = 0.7347 volts    pe = 12.6309
Ionic strength = 0.002864
Charge imbalance = -0.000333 eq/kg (-13.08% error)
Activity of water = 1.000000
Solvent mass = 1.000000 kg
Solution mass = 1.000274 kg
Solution density = 1.016 g/cm3
Chlorinity = 0.000000 molal
Dissolved solids = 274 mg/kg sol'n
Elect. conductivity = 218.25 uS/cm (or umho/cm)
Hardness = 30.22 mg/kg sol'n as CaCO3
  carbonate = 30.22 mg/kg sol'n as CaCO3
  non-carbonate = 0.00 mg/kg sol'n as CaCO3
Rock mass = 0.000000 kg
Carbonate alkalinity = 134.00 mg/kg sol'n as CaCO3
Water type = Na-HCO3
  
```

No minerals in system.

Aqueous species	molality	mg/kg sol'n	act. coef.	log act.
HCO3-	0.002602	158.7	0.9436	-2.6100
Na+	0.001722	39.58	0.9436	-2.7892
SiO2(aq)	0.0006160	37.00	1.0000	-3.2104
Ca++	0.0002555	10.24	0.7981	-3.6904
O2(aq)	0.0002399	7.675	1.0000	-3.6199
K+	7.350e-005	2.873	0.9427	-4.1593
AlO2-	3.910e-005	2.306	0.9436	-4.4330
Mg++	3.071e-005	0.7461	0.8037	-4.6077
CO2(aq)	2.801e-005	1.232	1.0000	-4.5527
CO3--	2.732e-005	1.639	0.7938	-4.6639
Fe(OH)3(aq)	2.449e-005	2.617	1.0000	-4.6109
HSiO3-	1.368e-005	1.054	0.9436	-4.8892
CaCO3(aq)	8.537e-006	0.8542	1.0000	-5.0687
NaHCO3(aq)	6.291e-006	0.5284	1.0000	-5.2013
CaHCO3+	6.025e-006	0.6089	0.9436	-5.2453
Zn++	2.649e-006	0.1732	0.7981	-5.6749
ReO4-	2.399e-006	0.6002	0.9436	-5.6451
OH-	1.519e-006	0.02582	0.9432	-5.8440
NaHSiO3(aq)	1.047e-006	0.1048	1.0000	-5.9799
MgHCO3+	7.118e-007	0.06072	0.9436	-6.1728
HAlO2(aq)	6.399e-007	0.03837	1.0000	-6.1939
MgCO3(aq)	4.880e-007	0.04114	1.0000	-6.3116
MoO4--	2.790e-007	0.04461	0.7938	-6.6547
Ba++	1.815e-007	0.02492	0.7952	-6.8406
NaCO3-	1.409e-007	0.01170	0.9436	-6.8761
NaAlO2(aq)	1.033e-008	0.0008468	1.0000	-7.9857

(only species > 1e-8 molal listed)

Mineral saturation states

	log Q/K		log Q/K
Nontronite-Ca	20.2531s/sat	Diaspore	3.1791s/sat
Nontronite-Mg	20.1305s/sat	Magnetite	3.1721s/sat
Clinoptilolite-h	20.0535s/sat	Saponite-Mg	3.1133s/sat
Clinoptilolite-C	20.0244s/sat	Phlogopite	3.0872s/sat
Nontronite-Na	19.9057s/sat	Clinochlore-14A	2.9779s/sat
Nontronite-K	19.8074s/sat	Saponite-Na	2.8881s/sat

Nontronite-H	19.0943s/sat	Wairakite	2.8069s/sat
Clinoptilolite-h	17.1140s/sat	Saponite-K	2.7897s/sat
Clinoptilolite-N	17.1132s/sat	Boehmite	2.7667s/sat
Clinoptilolite-K	16.3755s/sat	Gibbsite	2.6072s/sat
Clinoptilolite-h	16.2656s/sat	Albite_high	2.4073s/sat
Hematite	14.2866s/sat	Corundum	2.2593s/sat
Stilbite	14.2794s/sat	Saponite-H	2.0767s/sat
Ferrite-Zn	13.3508s/sat	Witherite	1.9303s/sat
Muscovite	12.3371s/sat	Talc	1.8563s/sat
Epidote-ord	11.0439s/sat	Kyanite	1.7960s/sat
Epidote	11.0435s/sat	Andalusite	1.5125s/sat
Andradite	9.9102s/sat	Jadeite	1.2142s/sat
Mesolite	9.7772s/sat	Sillimanite	1.1390s/sat
Paragonite	9.6723s/sat	Smectite-high-Fe	1.0019s/sat
Herschelite	9.6618s/sat	Quartz	0.9214s/sat
Illite	9.3967s/sat	Tridymite	0.7238s/sat
Beidellite-Ca	9.2635s/sat	Dawsonite	0.6999s/sat
Beidellite-Mg	9.1408s/sat	Anorthite	0.4638s/sat
Beidellite-Na	8.9160s/sat	Dolomite	0.4565s/sat
Beidellite-K	8.8178s/sat	Dolomite-ord	0.4565s/sat
Montmor-Ca	8.4321s/sat	Kalsilite	0.4398s/sat
Montmor-Mg	8.3809s/sat	Analcime-K	0.3981s/sat
Scolecite	8.2829s/sat	Cristobalite(alp)	0.3594s/sat
Montmor-Na	8.1526s/sat	Chalcedony	0.3455s/sat
Beidellite-H	8.1048s/sat	Calcite	0.1073s/sat
Montmor-K	8.0583s/sat	Coesite	0.0982s/sat
Pyrophyllite	7.8874s/sat	Aragonite	-0.0372
Kaolinite	7.7209s/sat	Cristobalite(bet)	-0.0986
Laumontite	7.3774s/sat	Ice	-0.1194
Amesite-14A	6.6724s/sat	Analcime	-0.2866
Goethite	6.6688s/sat	SiO2(am)	-0.4067
Margarite	6.6593s/sat	Clinochlore-7A	-0.4370
Celadonite	6.5012s/sat	Zincite	-0.4933
Maximum_Microcli	5.5149s/sat	Smithsonite	-0.5057
K-Feldspar	5.5137s/sat	Monohydrocalcite	-0.7134
Ferrite-Ca	5.4306s/sat	Cordierite_hydr	-0.7597
Lawsonite	5.0048s/sat	Zn(OH)2(gamma)	-0.8981
Mordenite	4.9536s/sat	Zn(OH)2(epsilon)	-0.9234
Ferrite-Mg	4.9357s/sat	Dolomite-dis	-1.1253
Zn2SiO4	4.5448s/sat	Nepheline	-1.1734
Sanidine_high	4.2818s/sat	Zn(OH)2(beta)	-1.1993
Prehnite	3.8754s/sat	Magnesite	-1.3109
Natrolite	3.8066s/sat	Tremolite	-1.6943
Clinozoisite	3.7805s/sat	Chrysotile	-1.9870
Albite_low	3.7596s/sat	Fe(OH)3	-2.0191
Albite	3.7595s/sat	Grossular	-2.5130
Smectite-low-Fe-	3.7594s/sat	Enstatite	-2.7037
Zoisite	3.7346s/sat	Diopside	-2.7056
Saponite-Ca	3.2354s/sat		
(only minerals with log Q/K > -3 listed)			

Gases	fugacity	log fug.
O2(g)	0.1711	-0.767
H2O(g)	0.01903	-1.721
CO2(g)	0.0007004	-3.155
H2(g)	9.059e-043	-42.043
CO(g)	2.027e-049	-48.693
Zn(g)	4.928e-075	-74.307
Na(g)	1.317e-076	-75.880
K(g)	1.127e-078	-77.948
Mg(g)	8.653e-132	-131.063
CH4(g)	2.235e-148	-147.651

Ca(g)	5.035e-154	-153.298
Al(g)	7.978e-192	-191.098
C(g)	3.871e-193	-192.412
Si(g)	3.376e-224	-223.472
C2H4(g)	2.906e-242	-241.537

Original basis	total moles	In fluid		Sorbed		Kd L/kg
		moles	mg/kg	moles	mg/kg	
Al+++	3.98e-005	3.98e-005	1.07			
Ba++	1.83e-007	1.83e-007	0.0251			
Ca++	0.000270	0.000270	10.8			
Fe++	2.45e-005	2.45e-005	1.37			
H+	-0.000232	-0.000232	-0.234			
H2O	55.5	55.5	1.00e+006			
HCO3-	0.00268	0.00268	163.			
K+	7.35e-005	7.35e-005	2.87			
Mg++	3.19e-005	3.19e-005	0.775			
MoO4--	2.79e-007	2.79e-007	0.0446			
Na+	0.00173	0.00173	39.7			
O2(aq)	0.000246	0.000246	7.87			
ReO4-	2.40e-006	2.40e-006	0.600			
SiO2(aq)	0.000631	0.000631	37.9			
Zn++	2.65e-006	2.65e-006	0.173			

Elemental composition	total moles	In fluid		Sorbed	
		moles	mg/kg	moles	mg/kg
Aluminum	3.976e-005	3.976e-005	1.072		
Barium	1.827e-007	1.827e-007	0.02509		
Calcium	0.0002701	0.0002701	10.82		
Carbon	0.002679	0.002679	32.17		
Hydrogen	111.0	111.0	1.119e+005		
Iron	2.449e-005	2.449e-005	1.368		
Magnesium	3.191e-005	3.191e-005	0.7753		
Molybdenum	2.790e-007	2.790e-007	0.02676		
Oxygen	55.52	55.52	8.880e+005		
Potassium	7.350e-005	7.350e-005	2.873		
Rhenium	2.399e-006	2.399e-006	0.4467		
Silicon	0.0006307	0.0006307	17.71		
Sodium	0.001729	0.001729	39.75		
Zinc	2.649e-006	2.649e-006	0.1732		

Sample D1119MMB_bs

```

Step #      0          Xi = 0.0000
Temperature = 20.0 C   Pressure = 1.013 bars
pH = 8.420           log fO2 = -0.767
Eh = 0.7294 volts    pe = 12.5407
Ionic strength      = 0.003030
Charge imbalance    = -0.000369 eq/kg (-13.9% error)
Activity of water   = 0.999999
Solvent mass        = 1.000000 kg
Solution mass       = 1.000282 kg
Solution density    = 1.016 g/cm3
Chlorinity          = 0.000025 molal
Dissolved solids    = 282 mg/kg sol'n
Elect. conductivity = 231.87 uS/cm (or umho/cm)
Hardness            = 30.99 mg/kg sol'n as CaCO3
  carbonate         = 30.99 mg/kg sol'n as CaCO3
  non-carbonate     = 0.00 mg/kg sol'n as CaCO3
Rock mass           = 0.000000 kg
Carbonate alkalinity = 128.00 mg/kg sol'n as CaCO3
Water type          = Na-HCO3
  
```

No minerals in system.

Aqueous species	molality	mg/kg sol'n	act. coef.	log act.
HCO3-	0.002471	150.7	0.9422	-2.6331
Na+	0.001803	41.44	0.9422	-2.7699
SiO2(aq)	0.0006331	38.03	1.0000	-3.1986
Ca++	0.0002605	10.44	0.7935	-3.6847
O2(aq)	0.0002397	7.666	1.0000	-3.6204
K+	6.920e-005	2.705	0.9412	-4.1862
NO3-	6.269e-005	3.886	0.9412	-4.2291
SO4--	5.144e-005	4.940	0.7873	-4.3926
AlO2-	4.102e-005	2.419	0.9422	-4.4128
F-	4.096e-005	0.7779	0.9417	-4.4138
CO3--	3.206e-005	1.924	0.7889	-4.5970
Mg++	3.070e-005	0.7460	0.7993	-4.6101
Fe(OH)3(aq)	2.555e-005	2.730	1.0000	-4.5926
Cl-	2.489e-005	0.8822	0.9412	-4.6303
CO2(aq)	2.159e-005	0.9498	1.0000	-4.6658
HSiO3-	1.732e-005	1.335	0.9422	-4.7874
CaCO3(aq)	1.009e-005	1.010	1.0000	-4.9960
ReO4-	7.928e-006	1.983	0.9422	-5.1267
NaHCO3(aq)	6.237e-006	0.5238	1.0000	-5.2050
CaHCO3+	5.798e-006	0.5860	0.9422	-5.2626
Zn++	2.977e-006	0.1946	0.7935	-5.6266
OH-	1.871e-006	0.03181	0.9417	-5.7540
NaHSiO3(aq)	1.384e-006	0.1385	1.0000	-5.8588
CaSO4(aq)	1.058e-006	0.1440	1.0000	-5.9755
MoO4--	7.324e-007	0.1171	0.7889	-6.2382
MgHCO3+	6.723e-007	0.05734	0.9422	-6.1983
MgCO3(aq)	5.661e-007	0.04772	1.0000	-6.2471
HAlO2(aq)	5.448e-007	0.03267	1.0000	-6.2638
MgSO4(aq)	2.263e-007	0.02723	1.0000	-6.6454
Ba++	1.891e-007	0.02596	0.7905	-6.8254
NaCO3-	1.722e-007	0.01429	0.9422	-6.7899
CaF+	4.006e-008	0.002366	0.9422	-7.4231
MgF+	2.296e-008	0.0009941	0.9422	-7.6648
KSO4-	2.127e-008	0.002875	0.9422	-7.6980
ZnSO4(aq)	1.771e-008	0.002858	1.0000	-7.7518
NaAlO2(aq)	1.132e-008	0.0009273	1.0000	-7.9463

(only species > 1e-8 molal listed)

Mineral saturation states			
	log Q/K		log Q/K
Nontronite-Ca	20.3410s/sat	Saponite-Mg	3.6958s/sat
Clinoptilolite-h	20.3071s/sat	Phlogopite	3.6487s/sat
Clinoptilolite-C	20.2781s/sat	Saponite-Na	3.4773s/sat
Nontronite-Mg	20.2170s/sat	Saponite-K	3.3637s/sat
Nontronite-Na	19.9990s/sat	Magnetite	3.2273s/sat
Nontronite-K	19.8854s/sat	Diaspore	3.1093s/sat
Nontronite-H	19.1515s/sat	Wairakite	2.9003s/sat
Clinoptilolite-h	17.4245s/sat	Boehmite	2.6968s/sat
Clinoptilolite-N	17.4237s/sat	Saponite-H	2.6298s/sat
Clinoptilolite-K	16.5259s/sat	Gibbsite	2.5373s/sat
Clinoptilolite-h	16.4161s/sat	Albite_high	2.4823s/sat
Stilbite	14.4125s/sat	Talc	2.4364s/sat
Hematite	14.3233s/sat	Corundum	2.1196s/sat
Ferrite-Zn	13.6158s/sat	Witherite	2.0124s/sat
Muscovite	12.2262s/sat	Kyanite	1.6681s/sat
Epidote-ord	11.3297s/sat	Andalusite	1.3846s/sat
Epidote	11.3292s/sat	Jadeite	1.2774s/sat
Andradite	10.5398s/sat	Smectite-high-Fe	1.2013s/sat
Mesolite	9.8698s/sat	Sillimanite	1.0112s/sat
Herschelite	9.7599s/sat	Quartz	0.9333s/sat
Paragonite	9.6076s/sat	Tridymite	0.7356s/sat
Illite	9.3598s/sat	Dawsonite	0.6263s/sat
Beidellite-Ca	9.1749s/sat	Dolomite	0.5937s/sat
Beidellite-Mg	9.0508s/sat	Dolomite-ord	0.5937s/sat
Beidellite-Na	8.8328s/sat	Anorthite	0.5336s/sat
Beidellite-K	8.7194s/sat	Kalsilite	0.4449s/sat
Montmor-Ca	8.4521s/sat	Analcime-K	0.4158s/sat
Montmor-Mg	8.3995s/sat	Cristobalite(alp)	0.3713s/sat
Scolecite	8.3645s/sat	Chalcedony	0.3573s/sat
Montmor-Na	8.1780s/sat	Clinochlore-7A	0.3466s/sat
Montmor-K	8.0685s/sat	Calcite	0.1800s/sat
Beidellite-H	7.9855s/sat	Coesite	0.1100s/sat
Pyrophyllite	7.7951s/sat	Aragonite	0.0355s/sat
Kaolinite	7.6048s/sat	Cristobalite(bet)	-0.0868
Laumontite	7.4708s/sat	Ice	-0.1194
Amesite-14A	7.1268s/sat	Analcime	-0.2245
Celadonite	6.7194s/sat	Zincite	-0.2651
Goethite	6.6871s/sat	Tremolite	-0.3401
Margarite	6.5893s/sat	Smithsonite	-0.3905
Ferrite-Ca	5.6531s/sat	SiO2(am)	-0.3949
Maximum_Microcli	5.5437s/sat	Cordierite_hydr	-0.6247
K-Feldspar	5.5425s/sat	Monohydrocalcite	-0.6407
Ferrite-Mg	5.1500s/sat	Zn(OH)2(gamma)	-0.6698
Lawsonite	5.0746s/sat	Zn(OH)2(epsilon)	-0.6952
Mordenite	5.0412s/sat	Zn(OH)2(beta)	-0.9711
Zn2SiO4	5.0131s/sat	Dolomite-dis	-0.9881
Sanidine_high	4.3106s/sat	Nepheline	-1.1221
Prehnite	4.1428s/sat	Barite	-1.1515
Clinzoisite	3.9780s/sat	Magnesite	-1.2464
Zoisite	3.9321s/sat	Chrysotile	-1.4306
Natrolite	3.9211s/sat	Fe(OH)3	-2.0008
Smectite-low-Fe-	3.9173s/sat	Grossular	-2.0598
Albite_low	3.8346s/sat	Diopside	-2.3185
Albite	3.8345s/sat	Fluorite	-2.4252
Saponite-Ca	3.8192s/sat	Enstatite	-2.5143
Clinochlore-14A	3.7615s/sat		

(only minerals with log Q/K > -3 listed)

Gases	fugacity	log fug.
O2(g)	0.1710	-0.767
H2O(g)	0.01903	-1.721
CO2(g)	0.0005399	-3.268
HF(g)	7.413e-015	-14.130
HCl(g)	2.644e-020	-19.578
NO2(g)	4.559e-021	-20.341
N2(g)	8.566e-022	-21.067
NO(g)	4.618e-027	-26.336
Cl2(g)	8.498e-032	-31.071
SiF4(g)	3.857e-040	-39.414
H2(g)	9.064e-043	-42.043
CO(g)	1.563e-049	-48.806
SO2(g)	7.720e-059	-58.112
NH3(g)	2.659e-071	-70.575
Zn(g)	8.340e-075	-74.079
Na(g)	1.695e-076	-75.771
K(g)	1.304e-078	-77.885
F2(g)	4.303e-085	-84.366
Mg(g)	1.303e-131	-130.885
H2S(g)	1.138e-147	-146.944
CH4(g)	1.726e-148	-147.763
Ca(g)	7.727e-154	-153.112
Al(g)	6.798e-192	-191.168
C(g)	2.987e-193	-192.525
Si(g)	3.474e-224	-223.459
S2(g)	1.068e-236	-235.971
C2H4(g)	1.732e-242	-241.761

Original basis	total moles	In fluid		Sorbed		Kd L/kg
		moles	mg/kg	moles	mg/kg	
Al+++	4.16e-005	4.16e-005	1.12			
Ba++	1.91e-007	1.91e-007	0.0262			
Ca++	0.000277	0.000277	11.1			
Cl-	2.49e-005	2.49e-005	0.883			
F-	4.10e-005	4.10e-005	0.779			
Fe++	2.56e-005	2.56e-005	1.43			
H+	-0.000321	-0.000321	-0.324			
H2O	55.5	55.5	1.00e+006			
HCO3-	0.00255	0.00255	155.			
K+	6.92e-005	6.92e-005	2.71			
Mg++	3.22e-005	3.22e-005	0.782			
MoO4--	7.32e-007	7.32e-007	0.117			
NH3(aq)	6.27e-005	6.27e-005	1.07			
Na+	0.00181	0.00181	41.6			
O2(aq)	0.000371	0.000371	11.9			
ReO4-	7.93e-006	7.93e-006	1.98			
SO4--	5.28e-005	5.28e-005	5.07			
SiO2(aq)	0.000652	0.000652	39.1			
Zn++	2.99e-006	2.99e-006	0.196			

Elemental composition	total moles	In fluid		Sorbed	
		moles	mg/kg	moles	mg/kg
Aluminum	4.158e-005	4.158e-005	1.122		
Barium	1.906e-007	1.906e-007	0.02617		
Calcium	0.0002775	0.0002775	11.12		
Carbon	0.002548	0.002548	30.59		
Chlorine	2.490e-005	2.490e-005	0.8825		
Fluorine	4.103e-005	4.103e-005	0.7792		
Hydrogen	111.0	111.0	1.119e+005		

Iron	2.555e-005	2.555e-005	1.427
Magnesium	3.219e-005	3.219e-005	0.7822
Molybdenum	7.324e-007	7.324e-007	0.07025
Nitrogen	6.269e-005	6.269e-005	0.8779
Oxygen	55.52	55.52	8.880e+005
Potassium	6.922e-005	6.922e-005	2.706
Rhenium	7.928e-006	7.928e-006	1.476
Silicon	0.0006518	0.0006518	18.30
Sodium	0.001811	0.001811	41.62
Sulfur	5.276e-005	5.276e-005	1.691
Zinc	2.995e-006	2.995e-006	0.1958

Sample D11NEND

```

Step #      0          Xi = 0.0000
Temperature = 20.0 C   Pressure = 1.013 bars
pH = 8.140           log fO2 = -0.756
Eh = 0.7459 volts    pe = 12.8236
Ionic strength = 0.002579
Charge imbalance = -0.000744 eq/kg (-35.22% error)
Activity of water = 0.999999
Solvent mass = 1.000000 kg
Solution mass = 1.000234 kg
Solution density = 1.016 g/cm3
Chlorinity = 0.000026 molal
Dissolved solids = 234 mg/kg sol'n
Elect. conductivity = 195.01 uS/cm (or umho/cm)
Hardness = 35.52 mg/kg sol'n as CaCO3
  carbonate = 35.52 mg/kg sol'n as CaCO3
  non-carbonate = 0.00 mg/kg sol'n as CaCO3
Rock mass = 0.000000 kg
Carbonate alkalinity = 101.00 mg/kg sol'n as CaCO3
Water type = Na-HCO3
  
```

No minerals in system.

Aqueous species	molality	mg/kg sol'n	act. coef.	log act.
HCO3-	0.001979	120.7	0.9462	-2.7277
Na+	0.0009686	22.26	0.9462	-3.0378
SiO2(aq)	0.0005213	31.32	1.0000	-3.2829
O2(aq)	0.0002460	7.871	1.0000	-3.6090
Ca++	0.0002446	9.800	0.8065	-3.7050
NO3-	0.0001619	10.04	0.9454	-3.8152
SO4--	0.0001129	10.84	0.8011	-4.0437
Mg++	9.548e-005	2.320	0.8116	-4.1107
K+	8.476e-005	3.313	0.9454	-4.0962
F-	4.117e-005	0.7820	0.9458	-4.4096
CO2(aq)	3.308e-005	1.456	1.0000	-4.4804
Cl-	2.595e-005	0.9197	0.9454	-4.6103
CO3--	1.330e-005	0.7982	0.8025	-4.9716
ReO4-	1.311e-005	3.279	0.9462	-4.9065
HSiO3-	7.452e-006	0.5744	0.9462	-5.1517
CaHCO3+	4.431e-006	0.4479	0.9462	-5.3775
CaCO3(aq)	4.065e-006	0.4068	1.0000	-5.3909
NaHCO3(aq)	2.706e-006	0.2273	1.0000	-5.5676
CaSO4(aq)	2.255e-006	0.3069	1.0000	-5.6469
MgHCO3+	1.700e-006	0.1450	0.9462	-5.7936
MgSO4(aq)	1.595e-006	0.1920	1.0000	-5.7972
MoO4--	1.169e-006	0.1870	0.8025	-6.0276
OH-	9.777e-007	0.01662	0.9458	-6.0340
MgCO3(aq)	7.545e-007	0.06360	1.0000	-6.1223
NaHSiO3(aq)	3.228e-007	0.03230	1.0000	-6.4911
Ba++	9.355e-008	0.01284	0.8038	-7.1238
MgF+	7.290e-008	0.003156	0.9462	-7.1613
KSO4-	5.820e-008	0.007864	0.9462	-7.2591
NaCO3-	3.904e-008	0.003239	0.9462	-7.4325
CaF+	3.843e-008	0.002270	0.9462	-7.4393

(only species > 1e-8 molal listed)

Mineral saturation states

	log Q/K		log Q/K
Talc	1.9172s/sat	Calcite	-0.2149
Witherite	1.3394s/sat	Aragonite	-0.3594

Quartz	0.8489s/sat	SiO2(am)	-0.4792
Tridymite	0.6513s/sat	Monohydrocalcite	-1.0356
Dolomite	0.3235s/sat	Barite	-1.1010
Dolomite-ord	0.3235s/sat	Magnesite	-1.1216
Cristobalite(alp)	0.2869s/sat	Dolomite-dis	-1.2583
Chalcedony	0.2730s/sat	Chrysotile	-1.7812
Coesite	0.0257s/sat	Fluorite	-2.4373
Ice	-0.1194	Tremolite	-2.4785
Cristobalite(bet)	-0.1711	Enstatite	-2.6593

(only minerals with log Q/K > -3 listed)

Gases	fugacity	log fug.
O2(g)	0.1755	-0.756
H2O(g)	0.01903	-1.721
CO2(g)	0.0008273	-3.082
HF(g)	1.426e-014	-13.846
HCl(g)	5.275e-020	-19.278
NO2(g)	2.238e-020	-19.650
N2(g)	1.959e-020	-19.708
NO(g)	2.238e-026	-25.650
Cl2(g)	3.427e-031	-30.465
SiF4(g)	4.350e-039	-38.361
H2(g)	8.945e-043	-42.048
CO(g)	2.364e-049	-48.626
SO2(g)	6.177e-058	-57.209
NH3(g)	1.247e-070	-69.904
Na(g)	4.767e-077	-76.322
K(g)	8.364e-079	-78.078
F2(g)	1.614e-084	-83.792
Mg(g)	1.118e-131	-130.951
H2S(g)	8.755e-147	-146.058
CH4(g)	2.510e-148	-147.600
Ca(g)	2.004e-154	-153.698
C(g)	4.459e-193	-192.351
Si(g)	2.786e-224	-223.555
S2(g)	6.488e-235	-234.188
C2H4(g)	3.759e-242	-241.425

Original basis	total moles	In fluid		Sorbed		Kd L/kg
		moles	mg/kg	moles	mg/kg	
Ba++	9.39e-008	9.39e-008	0.0129			
Ca++	0.000255	0.000255	10.2			
Cl-	2.60e-005	2.60e-005	0.920			
F-	4.13e-005	4.13e-005	0.784			
H+	-0.000156	-0.000156	-0.157			
H2O	55.5	55.5	1.00e+006			
HCO3-	0.00204	0.00204	124.			
K+	8.48e-005	8.48e-005	3.32			
Mg++	9.96e-005	9.96e-005	2.42			
MoO4--	1.17e-006	1.17e-006	0.187			
NH3(aq)	0.000162	0.000162	2.76			
Na+	0.000972	0.000972	22.3			
O2(aq)	0.000570	0.000570	18.2			
ReO4-	1.31e-005	1.31e-005	3.28			
SO4--	0.000117	0.000117	11.2			
SiO2(aq)	0.000529	0.000529	31.8			

Elemental composition	In fluid			Sorbed	
	total moles	moles	mg/kg	moles	mg/kg
Barium	9.388e-008	9.388e-008	0.01289		
Calcium	0.0002554	0.0002554	10.23		
Carbon	0.002039	0.002039	24.48		
Chlorine	2.595e-005	2.595e-005	0.9199		
Fluorine	4.128e-005	4.128e-005	0.7841		
Hydrogen	111.0	111.0	1.119e+005		
Magnesium	9.961e-005	9.961e-005	2.420		
Molybdenum	1.169e-006	1.169e-006	0.1122		
Nitrogen	0.0001619	0.0001619	2.267		
Oxygen	55.52	55.52	8.880e+005		
Potassium	8.482e-005	8.482e-005	3.316		
Rhenium	1.311e-005	1.311e-005	2.440		
Silicon	0.0005291	0.0005291	14.86		
Sodium	0.0009717	0.0009717	22.33		
Sulfur	0.0001168	0.0001168	3.744		

Sample D14BG

```

Step #      0          Xi = 0.0000
Temperature = 20.0 C   Pressure = 1.013 bars
pH = 8.020           log fO2 = -0.756
Eh = 0.7528 volts    pe = 12.9436
Ionic strength      = 0.002623
Charge imbalance    = -0.000658 eq/kg (-32.65% error)
Activity of water   = 0.999997
Solvent mass        = 1.000000 kg
Solution mass       = 1.000218 kg
Solution density    = 1.016 g/cm3
Chlorinity          = 0.000087 molal
Dissolved solids    = 218 mg/kg sol'n
Elect. conductivity = 194.66 uS/cm (or umho/cm)
Hardness            = 40.46 mg/kg sol'n as CaCO3
  carbonate         = 40.46 mg/kg sol'n as CaCO3
  non-carbonate     = 0.00 mg/kg sol'n as CaCO3
Rock mass           = 0.000000 kg
Carbonate alkalinity = 84.00 mg/kg sol'n as CaCO3
Water type          = Na-HCO3
  
```

No minerals in system.

Aqueous species	molality	mg/kg sol'n	act. coef.	log act.
HCO3-	0.001651	100.7	0.9458	-2.8065
Na+	0.0008411	19.33	0.9458	-3.0994
SiO2(aq)	0.0005163	31.01	1.0000	-3.2871
Ca++	0.0002778	11.13	0.8052	-3.6503
O2(aq)	0.0002460	7.871	1.0000	-3.6090
SO4--	0.0002110	20.26	0.7997	-3.7728
NO3-	0.0001267	7.851	0.9450	-3.9220
Mg++	0.0001090	2.648	0.8104	-4.0540
Cl-	8.686e-005	3.079	0.9450	-4.0857
K+	6.661e-005	2.604	0.9450	-4.2010
CO2(aq)	3.637e-005	1.600	1.0000	-4.4392
F-	3.382e-005	0.6424	0.9454	-4.4952
CO3--	8.432e-006	0.5059	0.8011	-5.1704
HSiO3-	5.601e-006	0.4317	0.9458	-5.2759
CaSO4(aq)	4.771e-006	0.6494	1.0000	-5.3214
CaHCO3+	4.193e-006	0.4238	0.9458	-5.4016
MgSO4(aq)	3.392e-006	0.4081	1.0000	-5.4696
CaCO3(aq)	2.917e-006	0.2919	1.0000	-5.5351
ReO4-	2.135e-006	0.5341	0.9458	-5.6948
NaHCO3(aq)	1.959e-006	0.1646	1.0000	-5.7079
MgHCO3+	1.616e-006	0.1379	0.9458	-5.8157
OH-	7.420e-007	0.01262	0.9454	-6.1540
MgCO3(aq)	5.440e-007	0.04585	1.0000	-6.2644
NaHSiO3(aq)	2.105e-007	0.02106	1.0000	-6.6768
Ba++	1.037e-007	0.01424	0.8025	-7.0799
KSO4-	8.534e-008	0.01153	0.9458	-7.0931
MgF+	6.823e-008	0.002954	0.9458	-7.1902
MoO4--	5.334e-008	0.008529	0.8011	-7.3693
CaF+	3.581e-008	0.002115	0.9458	-7.4702
NaCO3-	2.145e-008	0.001780	0.9458	-7.6928
NaCl(aq)	1.065e-008	0.0006220	1.0000	-7.9728
H+	1.006e-008	1.013e-005	0.9497	-8.0200
(only species > 1e-8 molal listed)				

Mineral saturation states

	log Q/K		log Q/K
Talc	1.3503s/sat	Calcite	-0.3591
Witherite	1.1845s/sat	SiO2(am)	-0.4834
Quartz	0.8447s/sat	Aragonite	-0.5036
Tridymite	0.6471s/sat	Barite	-0.7863
Cristobalite(alp)	0.2827s/sat	Monohydrocalcite	-1.1798
Chalcedony	0.2688s/sat	Magnesite	-1.2637
Dolomite	0.0372s/sat	Dolomite-dis	-1.5446
Dolomite-ord	0.0372s/sat	Chrysotile	-2.3396
Coesite	0.0215s/sat	Fluorite	-2.5538
Ice	-0.1194	Enstatite	-2.8468
Cristobalite(bet)	-0.1753	Gypsum	-2.9328

(only minerals with log Q/K > -3 listed)

Gases	fugacity	log fug.
O2(g)	0.1755	-0.756
H2O(g)	0.01903	-1.721
CO2(g)	0.0009097	-3.041
HF(g)	1.544e-014	-13.811
HCl(g)	2.327e-019	-18.633
NO2(g)	2.307e-020	-19.637
N2(g)	2.082e-020	-19.681
NO(g)	2.307e-026	-25.637
Cl2(g)	6.668e-030	-29.176
SiF4(g)	5.916e-039	-38.228
H2(g)	8.945e-043	-42.048
CO(g)	2.600e-049	-48.585
SO2(g)	2.003e-057	-56.698
NH3(g)	1.285e-070	-69.891
Na(g)	3.139e-077	-76.503
K(g)	4.984e-079	-78.302
F2(g)	1.891e-084	-83.723
Mg(g)	7.333e-132	-131.135
H2S(g)	2.839e-146	-145.547
CH4(g)	2.760e-148	-147.559
Ca(g)	1.308e-154	-153.883
C(g)	4.903e-193	-192.310
Si(g)	2.759e-224	-223.559
S2(g)	6.821e-234	-233.166
C2H4(g)	4.545e-242	-241.342

Original basis	total moles	In fluid		Sorbed		Kd L/kg
		moles	mg/kg	moles	mg/kg	
Ba++	1.04e-007	1.04e-007	0.0143			
Ca++	0.000290	0.000290	11.6			
Cl-	8.69e-005	8.69e-005	3.08			
F-	3.39e-005	3.39e-005	0.644			
H+	-0.000109	-0.000109	-0.110			
H2O	55.5	55.5	1.00e+006			
HCO3-	0.00171	0.00171	104.			
K+	6.67e-005	6.67e-005	2.61			
Mg++	0.000115	0.000115	2.78			
MoO4--	5.33e-008	5.33e-008	0.00853			
NH3(aq)	0.000127	0.000127	2.16			
Na+	0.000843	0.000843	19.4			
O2(aq)	0.000499	0.000499	16.0			
ReO4-	2.14e-006	2.14e-006	0.534			
SO4--	0.000219	0.000219	21.1			
SiO2(aq)	0.000522	0.000522	31.4			

Elemental composition	In fluid		Sorbed	
	total moles	moles	mg/kg	moles
Barium	1.039e-007	1.039e-007	0.01427	
Calcium	0.0002897	0.0002897	11.61	
Carbon	0.001707	0.001707	20.50	
Chlorine	8.688e-005	8.688e-005	3.080	
Fluorine	3.393e-005	3.393e-005	0.6444	
Hydrogen	111.0	111.0	1.119e+005	
Magnesium	0.0001146	0.0001146	2.784	
Molybdenum	5.334e-008	5.334e-008	0.005116	
Nitrogen	0.0001267	0.0001267	1.774	
Oxygen	55.52	55.52	8.880e+005	
Potassium	6.670e-005	6.670e-005	2.607	
Rhenium	2.135e-006	2.135e-006	0.3975	
Silicon	0.0005221	0.0005221	14.66	
Sodium	0.0008433	0.0008433	19.38	
Sulfur	0.0002192	0.0002192	7.028	

Sample D11SWTOP

```

Step #      0          Xi = 0.0000
Temperature = 20.0 C   Pressure = 1.013 bars
pH = 8.090           log fO2 = -0.756
Eh = 0.7488 volts    pe = 12.8736
Ionic strength = 0.002336
Charge imbalance = -0.000350 eq/kg (-19.09% error)
Activity of water = 0.999999
Solvent mass = 1.000000 kg
Solution mass = 1.000205 kg
Solution density = 1.016 g/cm3
Chlorinity = 0.000030 molal
Dissolved solids = 205 mg/kg sol'n
Elect. conductivity = 168.52 uS/cm (or umho/cm)
Hardness = 39.99 mg/kg sol'n as CaCO3
  carbonate = 39.99 mg/kg sol'n as CaCO3
  non-carbonate = 0.00 mg/kg sol'n as CaCO3
Rock mass = 0.000000 kg
Carbonate alkalinity = 85.20 mg/kg sol'n as CaCO3
Water type = Na-HCO3
  
```

No minerals in system.

Aqueous species	molality	mg/kg sol'n	act. coef.	log act.
HCO3-	0.001671	101.9	0.9486	-2.8000
Na+	0.0008751	20.11	0.9486	-3.0809
SiO2(aq)	0.0006225	37.39	1.0000	-3.2059
Ca++	0.0002936	11.76	0.8142	-3.6215
O2(aq)	0.0002460	7.871	1.0000	-3.6090
SO4--	0.0001055	10.14	0.8092	-4.0685
Mg++	9.167e-005	2.228	0.8189	-4.1245
F-	4.560e-005	0.8662	0.9482	-4.3641
CO2(aq)	3.142e-005	1.383	1.0000	-4.5027
Cl-	2.997e-005	1.062	0.9479	-4.5466
NO3-	1.857e-005	1.151	0.9479	-4.7545
CO3--	9.939e-006	0.5963	0.8105	-5.0939
HSiO3-	7.911e-006	0.6097	0.9486	-5.1247
CaHCO3+	4.535e-006	0.4583	0.9486	-5.3664
CaCO3(aq)	3.717e-006	0.3719	1.0000	-5.4298
Zn++	2.674e-006	0.1748	0.8142	-5.6620
CaSO4(aq)	2.581e-006	0.3512	1.0000	-5.5883
ReO4-	2.135e-006	0.5341	0.9486	-5.6935
NaHCO3(aq)	2.075e-006	0.1743	1.0000	-5.6829
MgSO4(aq)	1.460e-006	0.1756	1.0000	-5.8358
MgHCO3+	1.391e-006	0.1186	0.9486	-5.8797
OH-	8.692e-007	0.01478	0.9482	-6.0840
MgCO3(aq)	5.515e-007	0.04649	1.0000	-6.2584
NaHSiO3(aq)	3.111e-007	0.03113	1.0000	-6.5071
Ba++	8.791e-008	0.01207	0.8117	-7.1465
MgF+	7.823e-008	0.003387	0.9486	-7.1296
MoO4--	5.334e-008	0.008529	0.8105	-7.3642
CaF+	5.159e-008	0.003047	0.9486	-7.3103
ZnSO4(aq)	3.442e-008	0.005556	1.0000	-7.4632
NaCO3-	2.661e-008	0.002208	0.9486	-7.5978

(only species > 1e-8 molal listed)

Mineral saturation states

	log Q/K		log Q/K
Zn2SiO4	3.6150s/sat	SiO2(am)	-0.4022
Talc	1.8839s/sat	Smithsonite	-0.9229

Witherite	1.1943s/sat	Zincite	-0.9605
Quartz	0.9259s/sat	Monohydrocalcite	-1.0745
Tridymite	0.7283s/sat	Barite	-1.1486
Cristobalite(alp)	0.3639s/sat	Magnesite	-1.2577
Chalcedony	0.3500s/sat	Zn(OH)2(gamma)	-1.3652
Dolomite	0.1485s/sat	Zn(OH)2(epsilon)	-1.3906
Dolomite-ord	0.1485s/sat	Dolomite-dis	-1.4333
Coesite	0.1027s/sat	Zn(OH)2(beta)	-1.6665
Cristobalite(bet)	-0.0941	Chrysotile	-1.9685
Ice	-0.1194	Fluorite	-2.2627
Calcite	-0.2538	Tremolite	-2.4645
Aragonite	-0.3983	Enstatite	-2.6961

(only minerals with log Q/K > -3 listed)

Gases	fugacity	log fug.
O2(g)	0.1755	-0.756
H2O(g)	0.01903	-1.721
CO2(g)	0.0007859	-3.105
HF(g)	1.777e-014	-13.750
HCl(g)	6.854e-020	-19.164
NO2(g)	2.888e-021	-20.539
N2(g)	3.262e-022	-21.486
NO(g)	2.888e-027	-26.539
Cl2(g)	5.786e-031	-30.238
SiF4(g)	1.252e-038	-37.902
H2(g)	8.946e-043	-42.048
CO(g)	2.246e-049	-48.649
SO2(g)	7.344e-058	-57.134
NH3(g)	1.609e-071	-70.793
Zn(g)	1.660e-075	-74.780
Na(g)	3.848e-077	-76.415
F2(g)	2.505e-084	-83.601
Mg(g)	8.606e-132	-131.065
H2S(g)	1.041e-146	-145.983
CH4(g)	2.384e-148	-147.623
Ca(g)	1.929e-154	-153.715
C(g)	4.236e-193	-192.373
Si(g)	3.327e-224	-223.478
S2(g)	9.172e-235	-234.038
C2H4(g)	3.392e-242	-241.469

Original basis	total moles	In fluid		Sorbed		Kd L/kg
		moles	mg/kg	moles	mg/kg	
Ba++	8.81e-008	8.81e-008	0.0121			
Ca++	0.000304	0.000304	12.2			
Cl-	3.00e-005	3.00e-005	1.06			
F-	4.57e-005	4.57e-005	0.869			
H+	-1.05e-005	-1.05e-005	-0.0105			
H2O	55.5	55.5	1.00e+006			
HCO3-	0.00172	0.00172	105.			
Mg++	9.51e-005	9.51e-005	2.31			
MoO4--	5.33e-008	5.33e-008	0.00853			
NH3(aq)	1.86e-005	1.86e-005	0.316			
Na+	0.000878	0.000878	20.2			
O2(aq)	0.000283	0.000283	9.06			
ReO4-	2.14e-006	2.14e-006	0.534			
SO4--	0.000110	0.000110	10.5			
SiO2(aq)	0.000631	0.000631	37.9			
Zn++	2.71e-006	2.71e-006	0.177			

Elemental composition	In fluid			Sorbed	
	total moles	moles	mg/kg	moles	mg/kg
Barium	8.814e-008	8.814e-008	0.01210		
Calcium	0.0003045	0.0003045	12.20		
Carbon	0.001724	0.001724	20.71		
Chlorine	2.998e-005	2.998e-005	1.063		
Fluorine	4.574e-005	4.574e-005	0.8688		
Hydrogen	111.0	111.0	1.119e+005		
Magnesium	9.515e-005	9.515e-005	2.312		
Molybdenum	5.334e-008	5.334e-008	0.005116		
Nitrogen	1.857e-005	1.857e-005	0.2600		
Oxygen	55.52	55.52	8.880e+005		
Rhenium	2.135e-006	2.135e-006	0.3975		
Silicon	0.0006307	0.0006307	17.71		
Sodium	0.0008775	0.0008775	20.17		
Sulfur	0.0001096	0.0001096	3.514		
Zinc	2.709e-006	2.709e-006	0.1771		

Sample D11NWTOP

```

Step #      0          Xi = 0.0000
Temperature = 20.0 C   Pressure = 1.013 bars
pH = 8.080           log fO2 = -0.756
Eh = 0.7494 volts    pe = 12.8836
Ionic strength      = 0.002307
Charge imbalance    = -0.000468 eq/kg (-25.74% error)
Activity of water   = 0.999999
Solvent mass        = 1.000000 kg
Solution mass       = 1.000204 kg
Solution density    = 1.016 g/cm3
Chlorinity          = 0.000041 molal
Dissolved solids    = 204 mg/kg sol'n
Elect. conductivity = 169.73 uS/cm (or umho/cm)
Hardness            = 36.79 mg/kg sol'n as CaCO3
  carbonate         = 36.79 mg/kg sol'n as CaCO3
  non-carbonate     = 0.00 mg/kg sol'n as CaCO3
Rock mass           = 0.000000 kg
Carbonate alkalinity = 82.30 mg/kg sol'n as CaCO3
Water type          = Na-HCO3
  
```

No minerals in system.

Aqueous species	molality	mg/kg sol'n	act. coef.	log act.
HCO3-	0.001615	98.54	0.9489	-2.8145
Na+	0.0008709	20.02	0.9489	-3.0828
SiO2(aq)	0.0005915	35.53	1.0000	-3.2280
Ca++	0.0002603	10.43	0.8151	-3.6732
O2(aq)	0.0002460	7.871	1.0000	-3.6090
SO4--	0.0001246	11.97	0.8102	-3.9959
Mg++	9.381e-005	2.280	0.8198	-4.1140
NO3-	7.126e-005	4.418	0.9481	-4.1703
F-	4.742e-005	0.9006	0.9485	-4.3470
Cl-	4.052e-005	1.436	0.9481	-4.4155
CO2(aq)	3.110e-005	1.368	1.0000	-4.5073
CO3--	9.382e-006	0.5629	0.8115	-5.1184
HSiO3-	7.344e-006	0.5660	0.9489	-5.1568
CaHCO3+	3.892e-006	0.3934	0.9489	-5.4326
CaCO3(aq)	3.118e-006	0.3120	1.0000	-5.5061
CaSO4(aq)	2.708e-006	0.3686	1.0000	-5.5674
ReO4-	2.135e-006	0.5341	0.9489	-5.6934
NaHCO3(aq)	1.998e-006	0.1678	1.0000	-5.6994
MgSO4(aq)	1.768e-006	0.2127	1.0000	-5.7526
MgHCO3+	1.377e-006	0.1175	0.9489	-5.8837
OH-	8.491e-007	0.01444	0.9485	-6.0940
MgCO3(aq)	5.340e-007	0.04501	1.0000	-6.2725
NaHSiO3(aq)	2.876e-007	0.02878	1.0000	-6.5412
Ba++	8.578e-008	0.01178	0.8127	-7.1567
MgF+	8.333e-008	0.003608	0.9489	-7.1020
MoO4--	5.334e-008	0.008529	0.8115	-7.3637
CaF+	4.762e-008	0.002813	0.9489	-7.3450
NaCO3-	2.503e-008	0.002077	0.9489	-7.6243

(only species > 1e-8 molal listed)

Mineral saturation states

	log Q/K		log Q/K
Talc	1.7669s/sat	Calcite	-0.3300
Witherite	1.1596s/sat	SiO2(am)	-0.4243
Quartz	0.9038s/sat	Aragonite	-0.4746
Tridymite	0.7062s/sat	Barite	-1.0861

Cristobalite(alp)	0.3418s/sat	Monohydrocalcite	-1.1508
Chalcedony	0.3279s/sat	Magnesite	-1.2718
Coesite	0.0806s/sat	Dolomite-dis	-1.5236
Dolomite	0.0582s/sat	Chrysotile	-2.0413
Dolomite-ord	0.0582s/sat	Fluorite	-2.2803
Cristobalite(bet)	-0.1162	Enstatite	-2.7277
Ice	-0.1194	Tremolite	-2.8325

(only minerals with log Q/K > -3 listed)

Gases	fugacity	log fug.
O2(g)	0.1755	-0.756
H2O(g)	0.01903	-1.721
CO2(g)	0.0007777	-3.109
HF(g)	1.891e-014	-13.723
HCl(g)	9.485e-020	-19.023
NO2(g)	1.135e-020	-19.945
N2(g)	5.034e-021	-20.298
NO(g)	1.134e-026	-25.945
Cl2(g)	1.108e-030	-29.955
SiF4(g)	1.527e-038	-37.816
H2(g)	8.946e-043	-42.048
CO(g)	2.223e-049	-48.653
SO2(g)	9.091e-058	-57.041
NH3(g)	6.320e-071	-70.199
Na(g)	3.744e-077	-76.427
F2(g)	2.838e-084	-83.547
Mg(g)	8.420e-132	-131.075
H2S(g)	1.289e-146	-145.890
CH4(g)	2.360e-148	-147.627
Ca(g)	1.636e-154	-153.786
C(g)	4.192e-193	-192.378
Si(g)	3.162e-224	-223.500
S2(g)	1.405e-234	-233.852
C2H4(g)	3.322e-242	-241.479

Original basis	total moles	In fluid moles	mg/kg	Sorbed moles	mg/kg	Kd L/kg
Ba++	8.60e-008	8.60e-008	0.0118			
Ca++	0.000270	0.000270	10.8			
Cl-	4.05e-005	4.05e-005	1.44			
F-	4.76e-005	4.76e-005	0.903			
H+	-6.17e-005	-6.17e-005	-0.0622			
H2O	55.5	55.5	1.00e+006			
HCO3-	0.00167	0.00167	102.			
Mg++	9.76e-005	9.76e-005	2.37			
MoO4--	5.33e-008	5.33e-008	0.00853			
NH3(aq)	7.13e-005	7.13e-005	1.21			
Na+	0.000873	0.000873	20.1			
O2(aq)	0.000389	0.000389	12.4			
ReO4-	2.14e-006	2.14e-006	0.534			
SO4--	0.000129	0.000129	12.4			
SiO2(aq)	0.000599	0.000599	36.0			

Elemental composition	total moles	In fluid moles	mg/kg	Sorbed moles	mg/kg
Barium	8.599e-008	8.599e-008	0.01181		
Calcium	0.0002701	0.0002701	10.82		
Carbon	0.001667	0.001667	20.02		
Chlorine	4.053e-005	4.053e-005	1.436		
Fluorine	4.755e-005	4.755e-005	0.9032		

Hydrogen	111.0	111.0	1.119e+005
Magnesium	9.758e-005	9.758e-005	2.371
Molybdenum	5.334e-008	5.334e-008	0.005116
Nitrogen	7.126e-005	7.126e-005	0.9979
Oxygen	55.52	55.52	8.880e+005
Rhenium	2.135e-006	2.135e-006	0.3975
Silicon	0.0005992	0.0005992	16.82
Sodium	0.0008732	0.0008732	20.07
Sulfur	0.0001291	0.0001291	4.138

Sample D11NETOP

```

Step #      0          Xi = 0.0000
Temperature = 20.0 C   Pressure = 1.013 bars
pH = 8.070          log fO2 = -0.756
Eh = 0.7499 volts    pe = 12.8936
Ionic strength      = 0.002422
Charge imbalance    = -0.000586 eq/kg (-30.8% error)
Activity of water   = 0.999999
Solvent mass        = 1.000000 kg
Solution mass       = 1.000212 kg
Solution density    = 1.016 g/cm3
Chlorinity          = 0.000036 molal
Dissolved solids    = 212 mg/kg sol'n
Elect. conductivity = 178.76 uS/cm (or umho/cm)
Hardness            = 37.69 mg/kg sol'n as CaCO3
  carbonate         = 37.69 mg/kg sol'n as CaCO3
  non-carbonate     = 0.00 mg/kg sol'n as CaCO3
Rock mass           = 0.000000 kg
Carbonate alkalinity = 85.00 mg/kg sol'n as CaCO3
Water type          = Na-HCO3
  
```

No minerals in system.

Aqueous species	molality	mg/kg sol'n	act. coef.	log act.
HCO3-	0.001669	101.8	0.9478	-2.8010
Na+	0.0008794	20.21	0.9478	-3.0791
SiO2(aq)	0.0005848	35.13	1.0000	-3.2330
Ca++	0.0002668	10.69	0.8114	-3.6645
O2(aq)	0.0002460	7.871	1.0000	-3.6090
SO4--	0.0001483	14.24	0.8063	-3.9224
NO3-	0.0001219	7.556	0.9470	-3.9377
Mg++	9.503e-005	2.309	0.8163	-4.1103
F-	4.220e-005	0.8015	0.9474	-4.3982
Cl-	3.635e-005	1.289	0.9470	-4.4631
CO2(aq)	3.283e-005	1.445	1.0000	-4.4837
CO3--	9.505e-006	0.5702	0.8076	-5.1149
HSiO3-	7.103e-006	0.5475	0.9478	-5.1718
CaHCO3+	4.102e-006	0.4146	0.9478	-5.4103
CaSO4(aq)	3.272e-006	0.4454	1.0000	-5.4852
CaCO3(aq)	3.208e-006	0.3210	1.0000	-5.4938
ReO4-	2.135e-006	0.5341	0.9478	-5.6939
MgSO4(aq)	2.111e-006	0.2541	1.0000	-5.6754
NaHCO3(aq)	2.079e-006	0.1746	1.0000	-5.6822
MgHCO3+	1.435e-006	0.1224	0.9478	-5.8664
OH-	8.308e-007	0.01413	0.9474	-6.1040
MgCO3(aq)	5.430e-007	0.04578	1.0000	-6.2652
NaHSiO3(aq)	2.802e-007	0.02804	1.0000	-6.5525
Ba++	9.150e-008	0.01256	0.8089	-7.1307
MgF+	7.480e-008	0.003238	0.9478	-7.1494
MoO4--	5.334e-008	0.008529	0.8076	-7.3658
CaF+	4.324e-008	0.002554	0.9478	-7.3874
NaCO3-	2.548e-008	0.002115	0.9478	-7.6171

(only species > 1e-8 molal listed)

Mineral saturation states

	log Q/K		log Q/K
Talc	1.6981s/sat	Calcite	-0.3177
Witherite	1.1892s/sat	SiO2(am)	-0.4293
Quartz	0.8988s/sat	Aragonite	-0.4623
Tridymite	0.7012s/sat	Barite	-0.9867

Cristobalite(alp)	0.3368s/sat	Monohydrocalcite	-1.1385
Chalcedony	0.3229s/sat	Magnesite	-1.2645
Dolomite	0.0778s/sat	Dolomite-dis	-1.5040
Dolomite-ord	0.0778s/sat	Chrysotile	-2.1001
Coesite	0.0756s/sat	Fluorite	-2.3739
Ice	-0.1194	Enstatite	-2.7490
Cristobalite(bet)	-0.1212	Tremolite	-2.9763

(only minerals with log Q/K > -3 listed)

Gases	fugacity	log fug.
O2(g)	0.1755	-0.756
H2O(g)	0.01903	-1.721
CO2(g)	0.0008211	-3.086
HF(g)	1.720e-014	-13.764
HCl(g)	8.698e-020	-19.061
NO2(g)	1.983e-020	-19.703
N2(g)	1.538e-020	-19.813
NO(g)	1.983e-026	-25.703
Cl2(g)	9.318e-031	-30.031
SiF4(g)	1.033e-038	-37.986
H2(g)	8.946e-043	-42.048
CO(g)	2.347e-049	-48.630
SO2(g)	1.127e-057	-56.948
NH3(g)	1.105e-070	-69.957
Na(g)	3.690e-077	-76.433
F2(g)	2.348e-084	-83.629
Mg(g)	8.111e-132	-131.091
H2S(g)	1.598e-146	-145.796
CH4(g)	2.491e-148	-147.604
Ca(g)	1.594e-154	-153.798
C(g)	4.425e-193	-192.354
Si(g)	3.126e-224	-223.505
S2(g)	2.161e-234	-233.665
C2H4(g)	3.703e-242	-241.431

Original basis	total moles	In fluid moles	mg/kg	Sorbed moles	mg/kg	Kd L/kg
Ba++	9.17e-008	9.17e-008	0.0126			
Ca++	0.000277	0.000277	11.1			
Cl-	3.64e-005	3.64e-005	1.29			
F-	4.23e-005	4.23e-005	0.804			
H+	-0.000111	-0.000111	-0.111			
H2O	55.5	55.5	1.00e+006			
HCO3-	0.00172	0.00172	105.			
Mg++	9.92e-005	9.92e-005	2.41			
MoO4--	5.33e-008	5.33e-008	0.00853			
NH3(aq)	0.000122	0.000122	2.08			
Na+	0.000882	0.000882	20.3			
O2(aq)	0.000490	0.000490	15.7			
ReO4-	2.14e-006	2.14e-006	0.534			
SO4--	0.000154	0.000154	14.8			
SiO2(aq)	0.000592	0.000592	35.6			

Elemental composition	total moles	In fluid moles	mg/kg	Sorbed moles	mg/kg
Barium	9.173e-008	9.173e-008	0.01259		
Calcium	0.0002775	0.0002775	11.12		
Carbon	0.001722	0.001722	20.68		
Chlorine	3.636e-005	3.636e-005	1.289		
Fluorine	4.232e-005	4.232e-005	0.8038		

Hydrogen	111.0	111.0	1.119e+005
Magnesium	9.920e-005	9.920e-005	2.411
Molybdenum	5.334e-008	5.334e-008	0.005116
Nitrogen	0.0001219	0.0001219	1.707
Oxygen	55.52	55.52	8.880e+005
Rhenium	2.135e-006	2.135e-006	0.3975
Silicon	0.0005922	0.0005922	16.63
Sodium	0.0008818	0.0008818	20.27
Sulfur	0.0001537	0.0001537	4.926

Sample D11SETOP

```

Step #      0          Xi = 0.0000
Temperature = 20.0 C   Pressure = 1.013 bars
pH = 8.110           log fO2 = -0.756
Eh = 0.7476 volts    pe = 12.8536
Ionic strength = 0.002444
Charge imbalance = -0.000546 eq/kg (-28.4% error)
Activity of water = 0.999998
Solvent mass = 1.000000 kg
Solution mass = 1.000213 kg
Solution density = 1.016 g/cm3
Chlorinity = 0.000056 molal
Dissolved solids = 213 mg/kg sol'n
Elect. conductivity = 181.58 uS/cm (or umho/cm)
Hardness = 38.01 mg/kg sol'n as CaCO3
  carbonate = 38.01 mg/kg sol'n as CaCO3
  non-carbonate = 0.00 mg/kg sol'n as CaCO3
Rock mass = 0.000000 kg
Carbonate alkalinity = 82.50 mg/kg sol'n as CaCO3
Water type = Na-HCO3
  
```

No minerals in system.

Aqueous species	molality	mg/kg sol'n	act. coef.	log act.
HCO3-	0.001617	98.66	0.9475	-2.8146
Na+	0.0009093	20.90	0.9475	-3.0647
SiO2(aq)	0.0005841	35.09	1.0000	-3.2335
Ca++	0.0002598	10.41	0.8107	-3.6764
O2(aq)	0.0002460	7.871	1.0000	-3.6090
NO3-	0.0001666	10.33	0.9467	-3.8020
SO4--	0.0001422	13.66	0.8056	-3.9411
Mg++	0.0001052	2.557	0.8156	-4.0664
Cl-	5.606e-005	1.987	0.9467	-4.2751
F-	4.111e-005	0.7808	0.9471	-4.4097
CO2(aq)	2.902e-005	1.277	1.0000	-4.5374
CO3--	1.011e-005	0.6065	0.8069	-5.0885
HSiO3-	7.781e-006	0.5997	0.9475	-5.1324
CaHCO3+	3.868e-006	0.3910	0.9475	-5.4359
CaCO3(aq)	3.316e-006	0.3318	1.0000	-5.4794
CaSO4(aq)	3.050e-006	0.4151	1.0000	-5.5157
Zn++	2.619e-006	0.1712	0.8107	-5.6730
MgSO4(aq)	2.238e-006	0.2693	1.0000	-5.6502
ReO4-	2.135e-006	0.5341	0.9475	-5.6940
NaHCO3(aq)	2.083e-006	0.1749	1.0000	-5.6814
MgHCO3+	1.539e-006	0.1313	0.9475	-5.8362
OH-	9.112e-007	0.01549	0.9471	-6.0640
MgCO3(aq)	6.384e-007	0.05381	1.0000	-6.1949
NaHSiO3(aq)	3.173e-007	0.03175	1.0000	-6.4986
Ba++	1.093e-007	0.01501	0.8082	-7.0537
MgF+	8.061e-008	0.003490	0.9475	-7.1170
MoO4--	5.334e-008	0.008529	0.8069	-7.3662
ZnSO4(aq)	4.501e-008	0.007265	1.0000	-7.3467
CaF+	4.098e-008	0.002420	0.9475	-7.4108
NaCO3-	2.800e-008	0.002323	0.9475	-7.5763
(only species > 1e-8 molal listed)				

Mineral saturation states

	log Q/K		log Q/K
Zn2SiO4	3.6453s/sat	Aragonite	-0.4479
Talc	2.0677s/sat	Barite	-0.9283

Witherite	1.2926s/sat	Smithsonite	-0.9285
Quartz	0.8983s/sat	Zincite	-0.9315
Tridymite	0.7006s/sat	Monohydrocalcite	-1.1241
Cristobalite(alp)	0.3363s/sat	Magnesite	-1.1942
Chalcedony	0.3224s/sat	Zn(OH)2(gamma)	-1.3363
Dolomite	0.1625s/sat	Zn(OH)2(epsilon)	-1.3616
Dolomite-ord	0.1625s/sat	Dolomite-dis	-1.4193
Coesite	0.0750s/sat	Zn(OH)2(beta)	-1.6375
Ice	-0.1194	Chrysotile	-1.7294
Cristobalite(bet)	-0.1218	Tremolite	-2.2249
Calcite	-0.3033	Fluorite	-2.4088
SiO2(am)	-0.4298	Enstatite	-2.6256

(only minerals with log Q/K > -3 listed)

Gases	fugacity	log fug.
O2(g)	0.1755	-0.756
H2O(g)	0.01903	-1.721
CO2(g)	0.0007257	-3.139
HF(g)	1.528e-014	-13.816
HCl(g)	1.223e-019	-18.913
NO2(g)	2.472e-020	-19.607
N2(g)	2.391e-020	-19.621
NO(g)	2.472e-026	-25.607
Cl2(g)	1.842e-030	-29.735
SiF4(g)	6.422e-039	-38.192
H2(g)	8.946e-043	-42.048
CO(g)	2.074e-049	-48.683
SO2(g)	8.983e-058	-57.047
NH3(g)	1.377e-070	-69.861
Zn(g)	1.774e-075	-74.751
Na(g)	4.182e-077	-76.379
F2(g)	1.852e-084	-83.732
Mg(g)	1.079e-131	-130.967
H2S(g)	1.273e-146	-145.895
CH4(g)	2.202e-148	-147.657
Ca(g)	1.864e-154	-153.729
C(g)	3.911e-193	-192.408
Si(g)	3.122e-224	-223.506
S2(g)	1.372e-234	-233.863
C2H4(g)	2.892e-242	-241.539

Original basis	total moles	In fluid		Sorbed		Kd L/kg
		moles	mg/kg	moles	mg/kg	
Ba++	1.10e-007	1.10e-007	0.0151			
Ca++	0.000270	0.000270	10.8			
Cl-	5.61e-005	5.61e-005	1.99			
F-	4.12e-005	4.12e-005	0.783			
H+	-0.000161	-0.000161	-0.162			
H2O	55.5	55.5	1.00e+006			
HCO3-	0.00167	0.00167	102.			
Mg++	0.000110	0.000110	2.67			
MoO4--	5.33e-008	5.33e-008	0.00853			
NH3(aq)	0.000167	0.000167	2.84			
Na+	0.000912	0.000912	21.0			
O2(aq)	0.000579	0.000579	18.5			
ReO4-	2.14e-006	2.14e-006	0.534			
SO4--	0.000148	0.000148	14.2			
SiO2(aq)	0.000592	0.000592	35.6			
Zn++	2.66e-006	2.66e-006	0.174			

Elemental composition	In fluid			Sorbed	
	total moles	moles	mg/kg	moles	mg/kg
Barium	1.096e-007	1.096e-007	0.01505		
Calcium	0.0002701	0.0002701	10.82		
Carbon	0.001668	0.001668	20.03		
Chlorine	5.607e-005	5.607e-005	1.987		
Fluorine	4.123e-005	4.123e-005	0.7832		
Hydrogen	111.0	111.0	1.119e+005		
Magnesium	0.0001097	0.0001097	2.666		
Molybdenum	5.334e-008	5.334e-008	0.005116		
Nitrogen	0.0001666	0.0001666	2.334		
Oxygen	55.52	55.52	8.880e+005		
Rhenium	2.135e-006	2.135e-006	0.3975		
Silicon	0.0005922	0.0005922	16.63		
Sodium	0.0009118	0.0009118	20.96		
Sulfur	0.0001475	0.0001475	4.729		
Zinc	2.664e-006	2.664e-006	0.1741		

Sample D1419MMT_ts

```

Step #      0          Xi = 0.0000
Temperature = 20.0 C   Pressure = 1.013 bars
pH = 7.830           log fO2 = -0.756
Eh = 0.7639 volts    pe = 13.1336
Ionic strength = 0.003674
Charge imbalance = -0.000497 eq/kg (-18.71% error)
Activity of water = 0.999994
Solvent mass = 1.000000 kg
Solution mass = 1.000266 kg
Solution density = 1.016 g/cm3
Chlorinity = 0.000169 molal
Dissolved solids = 265 mg/kg sol'n
Elect. conductivity = 263.76 uS/cm (or umho/cm)
Hardness = 70.54 mg/kg sol'n as CaCO3
  carbonate = 70.54 mg/kg sol'n as CaCO3
  non-carbonate = 0.00 mg/kg sol'n as CaCO3
Rock mass = 0.000000 kg
Carbonate alkalinity = 83.90 mg/kg sol'n as CaCO3
Water type = Na-HCO3
  
```

No minerals in system.

Aqueous species	molality	mg/kg sol'n	act. coef.	log act.
HCO3-	0.001651	100.7	0.9370	-2.8106
Na+	0.0009864	22.67	0.9370	-3.0342
SiO2(aq)	0.0005009	30.09	1.0000	-3.3003
Ca++	0.0004763	19.08	0.7771	-3.4316
NO3-	0.0003889	24.10	0.9358	-3.4390
SO4--	0.0003372	32.38	0.7699	-3.5857
O2(aq)	0.0002460	7.871	1.0000	-3.6090
Mg++	0.0001941	4.716	0.7839	-3.8177
Cl-	0.0001687	5.980	0.9358	-3.8017
K+	6.732e-005	2.632	0.9358	-4.2006
CO2(aq)	5.580e-005	2.455	1.0000	-4.2534
CaSO4(aq)	1.215e-005	1.653	1.0000	-4.9155
MgSO4(aq)	8.993e-006	1.082	1.0000	-5.0461
ReO4-	8.562e-006	2.142	0.9370	-5.0957
CaHCO3+	6.936e-006	0.7011	0.9370	-5.1871
CO3--	5.597e-006	0.3358	0.7718	-5.3646
HSiO3-	3.541e-006	0.2729	0.9370	-5.4791
CaCO3(aq)	3.086e-006	0.3088	1.0000	-5.5106
MgHCO3+	2.784e-006	0.2375	0.9370	-5.5835
Zn++	2.452e-006	0.1603	0.7771	-5.7201
NaHCO3(aq)	2.254e-006	0.1893	1.0000	-5.6470
MgCO3(aq)	5.994e-007	0.05052	1.0000	-6.2223
OH-	4.837e-007	0.008224	0.9364	-6.3440
Ba++	1.553e-007	0.02132	0.7736	-6.9203
NaHSiO3(aq)	1.532e-007	0.01533	1.0000	-6.8148
MoO4--	1.364e-007	0.02181	0.7718	-6.9776
KSO4-	1.327e-007	0.01793	0.9370	-6.9055
ZnSO4(aq)	9.154e-008	0.01478	1.0000	-7.0384
NaCl(aq)	2.379e-008	0.001390	1.0000	-7.6236
MgCl+	1.948e-008	0.001164	0.9370	-7.7386
NaCO3-	1.608e-008	0.001335	0.9370	-7.8219
H+	1.570e-008	1.582e-005	0.9422	-7.8300
CaCl+	1.264e-008	0.0009542	0.9370	-7.9267

(only species > 1e-8 molal listed)

Mineral saturation states

	log Q/K		log Q/K
Zn2SiO4	2.3645s/sat	Aragonite	-0.4791
Witherite	1.1499s/sat	SiO2(am)	-0.4966
Talc	0.8668s/sat	Monohydrocalcite	-1.1553
Quartz	0.8316s/sat	Magnesite	-1.2216
Tridymite	0.6339s/sat	Smithsonite	-1.2515
Cristobalite(alp)	0.2696s/sat	Dolomite-dis	-1.4779
Chalcedony	0.2556s/sat	Zincite	-1.5385
Dolomite	0.1039s/sat	Zn(OH)2(gamma)	-1.9433
Dolomite-ord	0.1039s/sat	Zn(OH)2(epsilon)	-1.9686
Coesite	0.0083s/sat	Zn(OH)2(beta)	-2.2445
Ice	-0.1194	Gypsum	-2.5269
Cristobalite(bet)	-0.1885	Anhydrite	-2.7517
Calcite	-0.3346	Chrysotile	-2.7969
Barite	-0.4396		

(only minerals with log Q/K > -3 listed)

Gases	fugacity	log fug.
O2(g)	0.1755	-0.756
H2O(g)	0.01903	-1.721
CO2(g)	0.001395	-2.855
HCl(g)	6.932e-019	-18.159
N2(g)	4.617e-019	-18.336
NO2(g)	1.087e-019	-18.964
NO(g)	1.086e-025	-24.964
Cl2(g)	5.919e-029	-28.228
H2(g)	8.945e-043	-42.048
CO(g)	3.988e-049	-48.399
SO2(g)	7.393e-057	-56.131
NH3(g)	6.052e-070	-69.218
Zn(g)	4.385e-076	-75.358
Na(g)	2.354e-077	-76.628
K(g)	3.221e-079	-78.492
Mg(g)	5.268e-132	-131.278
H2S(g)	1.048e-145	-144.980
CH4(g)	4.234e-148	-147.373
Ca(g)	9.022e-155	-154.045
C(g)	7.520e-193	-192.124
Si(g)	2.677e-224	-223.572
S2(g)	9.293e-233	-232.032
C2H4(g)	1.069e-241	-240.971

Original basis	total moles	In fluid		Sorbed		Kd L/kg
		moles	mg/kg	moles	mg/kg	
Ba++	1.56e-007	1.56e-007	0.0213			
Ca++	0.000498	0.000498	20.0			
Cl-	0.000169	0.000169	5.98			
H+	-0.000347	-0.000347	-0.349			
H2O	55.5	55.5	1.00e+006			
HCO3-	0.00173	0.00173	105.			
K+	6.75e-005	6.75e-005	2.64			
Mg++	0.000207	0.000207	5.02			
MoO4--	1.36e-007	1.36e-007	0.0218			
NH3(aq)	0.000389	0.000389	6.62			
Na+	0.000989	0.000989	22.7			
O2(aq)	0.00102	0.00102	32.8			
ReO4-	8.56e-006	8.56e-006	2.14			
SO4--	0.000359	0.000359	34.4			
SiO2(aq)	0.000505	0.000505	30.3			
Zn++	2.54e-006	2.54e-006	0.166			

Elemental composition	total moles	In fluid		Sorbed	
		moles	mg/kg	moles	mg/kg
Barium	1.555e-007	1.555e-007	0.02135		
Calcium	0.0004985	0.0004985	19.97		
Carbon	0.001728	0.001728	20.74		
Chlorine	0.0001688	0.0001688	5.982		
Hydrogen	111.0	111.0	1.119e+005		
Magnesium	0.0002065	0.0002065	5.018		
Molybdenum	1.364e-007	1.364e-007	0.01309		
Nitrogen	0.0003889	0.0003889	5.445		
Oxygen	55.52	55.52	8.880e+005		
Potassium	6.746e-005	6.746e-005	2.637		
Rhenium	8.562e-006	8.562e-006	1.594		
Silicon	0.0005046	0.0005046	14.17		
Sodium	0.0009888	0.0009888	22.73		
Sulfur	0.0003586	0.0003586	11.49		
Zinc	2.543e-006	2.543e-006	0.1663		

Sample D1419MMT_bs

```

Step #      0          Xi = 0.0000
Temperature = 20.0 C   Pressure = 1.013 bars
pH = 8.330           log fO2 = -0.758
Eh = 0.7348 volts    pe = 12.6329
Ionic strength = 0.003451
Charge imbalance = -0.001012 eq/kg (-33.84% error)
Activity of water = 0.999998
Solvent mass = 1.000000 kg
Solution mass = 1.000316 kg
Solution density = 1.016 g/cm3
Chlorinity = 0.000054 molal
Dissolved solids = 316 mg/kg sol'n
Elect. conductivity = 261.94 uS/cm (or umho/cm)
Hardness = 37.81 mg/kg sol'n as CaCO3
  carbonate = 37.81 mg/kg sol'n as CaCO3
  non-carbonate = 0.00 mg/kg sol'n as CaCO3
Rock mass = 0.000000 kg
Carbonate alkalinity = 156.00 mg/kg sol'n as CaCO3
Water type = Na-HCO3
  
```

No minerals in system.

Aqueous species	molality	mg/kg sol'n	act. coef.	log act.
HCO3-	0.003024	184.5	0.9387	-2.5469
Na+	0.001768	40.63	0.9387	-2.7800
SiO2(aq)	0.0005954	35.76	1.0000	-3.2252
Ca++	0.0003165	12.68	0.7826	-3.6061
O2(aq)	0.0002446	7.824	1.0000	-3.6116
NO3-	0.0001354	8.392	0.9376	-3.8964
SO4--	7.384e-005	7.091	0.7757	-4.2420
Cl-	5.356e-005	1.898	0.9376	-4.2991
F-	4.172e-005	0.7924	0.9382	-4.4074
Mg++	3.698e-005	0.8985	0.7890	-4.5350
CO2(aq)	3.239e-005	1.425	1.0000	-4.4896
CO3--	3.225e-005	1.935	0.7775	-4.6008
HSiO3-	1.329e-005	1.024	0.9387	-4.9040
CaCO3(aq)	1.199e-005	1.199	1.0000	-4.9213
AlO2-	1.005e-005	0.5923	0.9387	-5.0255
CaHCO3+	8.505e-006	0.8595	0.9387	-5.0978
NaHCO3(aq)	7.430e-006	0.6240	1.0000	-5.1290
Fe(OH)3(aq)	5.868e-006	0.6269	1.0000	-5.2315
ReO4-	4.350e-006	1.088	0.9387	-5.3890
CaSO4(aq)	1.794e-006	0.2441	1.0000	-5.7463
OH-	1.527e-006	0.02596	0.9382	-5.8440
NaHSiO3(aq)	1.034e-006	0.1034	1.0000	-5.9856
MgHCO3+	9.782e-007	0.08344	0.9387	-6.0370
MgCO3(aq)	6.671e-007	0.05623	1.0000	-6.1758
MgSO4(aq)	3.805e-007	0.04578	1.0000	-6.4197
MoO4--	1.898e-007	0.03034	0.7775	-6.8311
NaCO3-	1.673e-007	0.01388	0.9387	-6.8039
HAlO2(aq)	1.635e-007	0.009807	1.0000	-6.7864
Ba++	1.081e-007	0.01484	0.7792	-7.0746
CaF+	4.890e-008	0.002888	0.9387	-7.3381
MgF+	2.781e-008	0.001204	0.9387	-7.5833
NaCl(aq)	1.359e-008	0.0007938	1.0000	-7.8669
(only species > 1e-8 molal listed)				

Mineral saturation states			
	log Q/K		log Q/K
Nontronite-Ca	18.7762s/sat	Clinochlore-14A	2.1121s/sat
Nontronite-Mg	18.6516s/sat	Zoisite	2.0815s/sat
Nontronite-Na	18.4179s/sat	Saponite-H	2.0450s/sat
Clinoptilolite-h	17.9303s/sat	Talc	2.0153s/sat
Clinoptilolite-C	17.9013s/sat	Gibbsite	2.0147s/sat
Nontronite-H	17.6035s/sat	Albite_high	1.7796s/sat
Clinoptilolite-h	14.8764s/sat	Witherite	1.7594s/sat
Clinoptilolite-N	14.8755s/sat	Wairakite	1.6471s/sat
Hematite	13.0455s/sat	Magnetite	1.3084s/sat
Epidote-ord	9.3628s/sat	Corundum	1.0743s/sat
Epidote	9.3623s/sat	Quartz	0.9066s/sat
Andradite	8.8779s/sat	Dolomite	0.7397s/sat
Mesolite	8.6153s/sat	Dolomite-ord	0.7397s/sat
Paragonite	7.8597s/sat	Tridymite	0.7090s/sat
Beidellite-Ca	7.8427s/sat	Jadeite	0.6014s/sat
Beidellite-Mg	7.7180s/sat	Kyanite	0.5962s/sat
Beidellite-Na	7.4843s/sat	Cristobalite(alp)	0.3446s/sat
Montmor-Ca	7.4215s/sat	Chalcedony	0.3307s/sat
Montmor-Mg	7.3683s/sat	Andalusite	0.3127s/sat
Scolecite	7.1380s/sat	Calcite	0.2548s/sat
Montmor-Na	7.1310s/sat	Dawsonite	0.1797s/sat
Beidellite-H	6.6700s/sat	Aragonite	0.1102s/sat
Pyrophyllite	6.6433s/sat	Coesite	0.0834s/sat
Kaolinite	6.5063s/sat	Sillimanite	-0.0607
Laumontite	6.2176s/sat	Cristobalite(bet)	-0.1134
Goethite	6.0482s/sat	Ice	-0.1194
Amesite-14A	4.5636s/sat	SiO2(am)	-0.4215
Mordenite	4.3496s/sat	Monohydrocalcite	-0.5660
Margarite	4.3441s/sat	Anorthite	-0.6663
Ferrite-Ca	4.2739s/sat	Dolomite-dis	-0.8421
Lawsonite	3.8747s/sat	Analcime	-0.8767
Ferrite-Mg	3.7673s/sat	Magnesite	-1.1751
Saponite-Ca	3.2177s/sat	Barite	-1.2501
Albite_low	3.1319s/sat	Tremolite	-1.2803
Albite	3.1318s/sat	Clinochlore-7A	-1.3029
Saponite-Mg	3.0937s/sat	Nepheline	-1.7715
Saponite-Na	2.8594s/sat	Chrysotile	-1.7985
Prehnite	2.8148s/sat	Fluorite	-2.3338
Natrolite	2.5957s/sat	Diopside	-2.5780
Diaspore	2.5866s/sat	Fe(OH)3	-2.6397
Boehmite	2.1742s/sat	Enstatite	-2.6458
Clinozoisite	2.1274s/sat		

(only minerals with log Q/K > -3 listed)

Gases	fugacity	log fug.
O2(g)	0.1745	-0.758
H2O(g)	0.01903	-1.721
CO2(g)	0.0008099	-3.092
HF(g)	9.256e-015	-14.034
HCl(g)	6.972e-020	-19.157
NO2(g)	1.200e-020	-19.921
N2(g)	5.703e-021	-20.244
NO(g)	1.204e-026	-25.919
Cl2(g)	5.970e-031	-30.224
SiF4(g)	8.815e-040	-39.055
H2(g)	8.972e-043	-42.047
CO(g)	2.322e-049	-48.634
SO2(g)	1.636e-058	-57.786
NH3(g)	6.757e-071	-70.170

Na(g)	1.339e-076	-75.873
F2(g)	6.777e-085	-84.169
Mg(g)	1.013e-131	-130.994
H2S(g)	2.340e-147	-146.631
CH4(g)	2.487e-148	-147.604
Ca(g)	6.056e-154	-153.218
Al(g)	2.010e-192	-191.697
C(g)	4.391e-193	-192.357
Si(g)	3.201e-224	-223.495
S2(g)	4.605e-236	-235.337
C2H4(g)	3.668e-242	-241.436

Original basis	total moles	In fluid		Sorbed		Kd L/kg
		moles	mg/kg	moles	mg/kg	
Al+++	1.02e-005	1.02e-005	0.275			
Ba++	1.09e-007	1.09e-007	0.0150			
Ca++	0.000339	0.000339	13.6			
Cl-	5.36e-005	5.36e-005	1.90			
F-	4.18e-005	4.18e-005	0.794			
Fe++	5.87e-006	5.87e-006	0.328			
H+	-0.000216	-0.000216	-0.218			
H2O	55.5	55.5	1.00e+006			
HCO3-	0.00312	0.00312	190.			
Mg++	3.90e-005	3.90e-005	0.948			
MoO4--	1.90e-007	1.90e-007	0.0303			
NH3(aq)	0.000135	0.000135	2.31			
Na+	0.00178	0.00178	40.8			
O2(aq)	0.000517	0.000517	16.5			
ReO4-	4.35e-006	4.35e-006	1.09			
SO4--	7.60e-005	7.60e-005	7.30			
SiO2(aq)	0.000610	0.000610	36.6			

Elemental composition	total moles	In fluid		Sorbed	
		moles	mg/kg	moles	mg/kg
Aluminum	1.021e-005	1.021e-005	0.2755		
Barium	1.089e-007	1.089e-007	0.01495		
Calcium	0.0003389	0.0003389	13.58		
Carbon	0.003118	0.003118	37.44		
Chlorine	5.358e-005	5.358e-005	1.899		
Fluorine	4.180e-005	4.180e-005	0.7940		
Hydrogen	111.0	111.0	1.119e+005		
Iron	5.868e-006	5.868e-006	0.3276		
Magnesium	3.903e-005	3.903e-005	0.9484		
Molybdenum	1.898e-007	1.898e-007	0.01820		
Nitrogen	0.0001354	0.0001354	1.896		
Oxygen	55.52	55.52	8.880e+005		
Rhenium	4.350e-006	4.350e-006	0.8097		
Silicon	0.0006097	0.0006097	17.12		
Sodium	0.001777	0.001777	40.83		
Sulfur	7.602e-005	7.602e-005	2.437		

Sample D14NEBOT

```

Step #      0          Xi = 0.0000
Temperature = 20.0 C   Pressure = 1.013 bars
pH = 8.060           log fO2 = -0.756
Eh = 0.7505 volts    pe = 12.9036
Ionic strength      = 0.002980
Charge imbalance    = -0.000700 eq/kg (-30% error)
Activity of water   = 0.999998
Solvent mass       = 1.000000 kg
Solution mass      = 1.000252 kg
Solution density   = 1.016 g/cm3
Chlorinity         = 0.000060 molal
Dissolved solids   = 252 mg/kg sol'n
Elect. conductivity = 221.86 uS/cm (or umho/cm)
Hardness           = 45.52 mg/kg sol'n as CaCO3
  carbonate        = 45.52 mg/kg sol'n as CaCO3
  non-carbonate    = 0.00 mg/kg sol'n as CaCO3
Rock mass          = 0.000000 kg
Carbonate alkalinity = 96.60 mg/kg sol'n as CaCO3
Water type         = Na-HCO3
  
```

No minerals in system.

Aqueous species	molality	mg/kg sol'n	act. coef.	log act.
HCO3-	0.001895	115.6	0.9426	-2.7482
Na+	0.001050	24.13	0.9426	-3.0045
SiO2(aq)	0.0006091	36.59	1.0000	-3.2153
Ca++	0.0003075	12.32	0.7949	-3.6119
NO3-	0.0002524	15.64	0.9417	-3.6241
O2(aq)	0.0002460	7.871	1.0000	-3.6090
SO4--	0.0002014	19.34	0.7888	-3.7990
Mg++	0.0001265	3.075	0.8006	-3.9943
Cl-	5.966e-005	2.115	0.9417	-4.2504
K+	5.832e-005	2.280	0.9417	-4.2603
F-	3.990e-005	0.7578	0.9421	-4.4249
CO2(aq)	3.794e-005	1.669	1.0000	-4.4209
CO3--	1.072e-005	0.6430	0.7903	-5.0721
HSiO3-	7.270e-006	0.5603	0.9426	-5.1641
CaHCO3+	5.257e-006	0.5313	0.9426	-5.3049
ReO4-	5.227e-006	1.307	0.9426	-5.3074
CaSO4(aq)	4.907e-006	0.6679	1.0000	-5.3092
CaCO3(aq)	3.996e-006	0.3998	1.0000	-5.3984
MgSO4(aq)	3.664e-006	0.4409	1.0000	-5.4361
NaHCO3(aq)	2.787e-006	0.2341	1.0000	-5.5548
MgHCO3+	2.128e-006	0.1815	0.9426	-5.6977
OH-	8.164e-007	0.01388	0.9421	-6.1140
MgCO3(aq)	7.827e-007	0.06597	1.0000	-6.1064
NaHSiO3(aq)	3.387e-007	0.03389	1.0000	-6.4702
Ba++	1.215e-007	0.01668	0.7919	-7.0168
MgF+	9.235e-008	0.003998	0.9426	-7.0602
KSO4-	7.033e-008	0.009504	0.9426	-7.1785
MoO4--	6.052e-008	0.009677	0.7903	-7.3203
CaF+	4.614e-008	0.002725	0.9426	-7.3616
NaCO3-	3.357e-008	0.002786	0.9426	-7.4997
(only species > 1e-8 molal listed)				

Mineral saturation states

	log Q/K		log Q/K
Talc	2.0567s/sat	Aragonite	-0.3669
Witherite	1.3459s/sat	SiO2(am)	-0.4116

Quartz	0.9165s/sat	Barite	-0.7494
Tridymite	0.7189s/sat	Monohydrocalcite	-1.0431
Cristobalite(alp)	0.3545s/sat	Magnesite	-1.1057
Chalcedony	0.3406s/sat	Dolomite-dis	-1.2498
Dolomite	0.3320s/sat	Chrysotile	-1.7768
Dolomite-ord	0.3320s/sat	Tremolite	-2.2898
Coesite	0.0933s/sat	Fluorite	-2.3748
Cristobalite(bet)	-0.1035	Enstatite	-2.6353
Ice	-0.1194	Gypsum	-2.9205
Calcite	-0.2223		
(only minerals with log Q/K > -3 listed)			

Gases	fugacity	log fug.
O2(g)	0.1755	-0.756
H2O(g)	0.01903	-1.721
CO2(g)	0.0009488	-3.023
HF(g)	1.655e-014	-13.781
HCl(g)	1.452e-019	-18.838
N2(g)	6.827e-020	-19.166
NO2(g)	4.178e-020	-19.379
NO(g)	4.178e-026	-25.379
Cl2(g)	2.599e-030	-29.585
SiF4(g)	9.223e-039	-38.035
H2(g)	8.945e-043	-42.048
CO(g)	2.712e-049	-48.567
SO2(g)	1.568e-057	-56.805
NH3(g)	2.327e-070	-69.633
Na(g)	4.281e-077	-76.368
K(g)	4.768e-079	-78.322
F2(g)	2.174e-084	-83.663
Mg(g)	1.012e-131	-130.995
H2S(g)	2.223e-146	-145.653
CH4(g)	2.879e-148	-147.541
Ca(g)	1.718e-154	-153.765
C(g)	5.114e-193	-192.291
Si(g)	3.256e-224	-223.487
S2(g)	4.182e-234	-233.379
C2H4(g)	4.944e-242	-241.306

Original basis	total moles	In fluid moles	mg/kg	Sorbed moles	mg/kg	Kd L/kg
Ba++	1.22e-007	1.22e-007	0.0167			
Ca++	0.000322	0.000322	12.9			
Cl-	5.97e-005	5.97e-005	2.12			
F-	4.00e-005	4.00e-005	0.761			
H+	-0.000238	-0.000238	-0.240			
H2O	55.5	55.5	1.00e+006			
HCO3-	0.00196	0.00196	119.			
K+	5.84e-005	5.84e-005	2.28			
Mg++	0.000133	0.000133	3.24			
MoO4--	6.05e-008	6.05e-008	0.00968			
NH3(aq)	0.000252	0.000252	4.30			
Na+	0.00105	0.00105	24.2			
O2(aq)	0.000751	0.000751	24.0			
ReO4-	5.23e-006	5.23e-006	1.31			
SO4--	0.000210	0.000210	20.2			
SiO2(aq)	0.000617	0.000617	37.0			

Elemental composition	In fluid			Sorbed	
	total moles	moles	mg/kg	moles	mg/kg
Barium	1.218e-007	1.218e-007	0.01673		
Calcium	0.0003217	0.0003217	12.89		
Carbon	0.001958	0.001958	23.51		
Chlorine	5.968e-005	5.968e-005	2.115		
Fluorine	4.004e-005	4.004e-005	0.7605		
Hydrogen	111.0	111.0	1.119e+005		
Magnesium	0.0001332	0.0001332	3.237		
Molybdenum	6.052e-008	6.052e-008	0.005805		
Nitrogen	0.0002524	0.0002524	3.534		
Oxygen	55.52	55.52	8.880e+005		
Potassium	5.840e-005	5.840e-005	2.283		
Rhenium	5.227e-006	5.227e-006	0.9730		
Silicon	0.0006167	0.0006167	17.32		
Sodium	0.001053	0.001053	24.20		
Sulfur	0.0002100	0.0002100	6.733		

Sample D14NWBOT

```

Step #      0          Xi = 0.0000
Temperature = 20.0 C   Pressure = 1.013 bars
pH = 8.010           log fO2 = -0.756
Eh = 0.7534 volts    pe = 12.9536
Ionic strength      = 0.003093
Charge imbalance    = -0.000842 eq/kg (-34.51% error)
Activity of water   = 0.999998
Solvent mass        = 1.000000 kg
Solution mass       = 1.000265 kg
Solution density    = 1.016 g/cm3
Chlorinity          = 0.000054 molal
Dissolved solids    = 265 mg/kg sol'n
Elect. conductivity = 229.31 uS/cm (or umho/cm)
Hardness            = 46.33 mg/kg sol'n as CaCO3
  carbonate         = 46.33 mg/kg sol'n as CaCO3
  non-carbonate     = 0.00 mg/kg sol'n as CaCO3
Rock mass           = 0.000000 kg
Carbonate alkalinity = 107.00 mg/kg sol'n as CaCO3
Water type          = Na-HCO3
  
```

No minerals in system.

Aqueous species	molality	mg/kg sol'n	act. coef.	log act.
HCO3-	0.002101	128.2	0.9416	-2.7036
Na+	0.001067	24.52	0.9416	-2.9981
SiO2(aq)	0.0006238	37.47	1.0000	-3.2050
Ca++	0.0003117	12.49	0.7918	-3.6076
O2(aq)	0.0002460	7.871	1.0000	-3.6090
NO3-	0.0002270	14.07	0.9407	-3.6706
SO4--	0.0002013	19.33	0.7855	-3.8010
Mg++	0.0001294	3.145	0.7977	-3.9861
K+	6.109e-005	2.388	0.9407	-4.2406
Cl-	5.384e-005	1.908	0.9407	-4.2955
CO2(aq)	4.717e-005	2.075	1.0000	-4.3264
F-	4.284e-005	0.8137	0.9412	-4.3945
CO3--	1.063e-005	0.6376	0.7871	-5.0775
HSiO3-	6.642e-006	0.5119	0.9416	-5.2038
CaHCO3+	5.889e-006	0.5952	0.9416	-5.2561
CaSO4(aq)	4.933e-006	0.6714	1.0000	-5.3069
ReO4-	4.202e-006	1.051	0.9416	-5.4027
CaCO3(aq)	3.986e-006	0.3988	1.0000	-5.3995
MgSO4(aq)	3.717e-006	0.4473	1.0000	-5.4298
NaHCO3(aq)	3.135e-006	0.2633	1.0000	-5.5038
MgHCO3+	2.406e-006	0.2052	0.9416	-5.6449
MgCO3(aq)	7.877e-007	0.06640	1.0000	-6.1036
OH-	7.284e-007	0.01238	0.9412	-6.1640
NaHSiO3(aq)	3.138e-007	0.03139	1.0000	-6.5034
Ba++	1.158e-007	0.01590	0.7887	-7.0394
MgF+	1.011e-007	0.004375	0.9416	-7.0215
MoO4--	7.591e-008	0.01214	0.7871	-7.2237
KSO4-	7.333e-008	0.009909	0.9416	-7.1608
CaF+	5.004e-008	0.002955	0.9416	-7.3268
NaCO3-	3.369e-008	0.002795	0.9416	-7.4987
H+	1.033e-008	1.041e-005	0.9461	-8.0100

(only species > 1e-8 molal listed)

Mineral saturation states

	log Q/K		log Q/K
Talc	1.8228s/sat	Aragonite	-0.3680
Witherite	1.3178s/sat	SiO2(am)	-0.4013
Quartz	0.9268s/sat	Barite	-0.7740
Tridymite	0.7292s/sat	Monohydrocalcite	-1.0442
Cristobalite(alp)	0.3648s/sat	Magnesite	-1.1029
Chalcedony	0.3509s/sat	Dolomite-dis	-1.2482
Dolomite	0.3336s/sat	Chrysotile	-2.0314
Dolomite-ord	0.3336s/sat	Fluorite	-2.3097
Coesite	0.1036s/sat	Enstatite	-2.7167
Cristobalite(bet)	-0.0932	Tremolite	-2.8573
Ice	-0.1194	Gypsum	-2.9182
Calcite	-0.2235		

(only minerals with log Q/K > -3 listed)

Gases	fugacity	log fug.
O2(g)	0.1755	-0.756
H2O(g)	0.01903	-1.721
CO2(g)	0.001180	-2.928
HF(g)	1.992e-014	-13.701
HCl(g)	1.469e-019	-18.833
N2(g)	6.937e-020	-19.159
NO2(g)	4.212e-020	-19.376
NO(g)	4.211e-026	-25.376
Cl2(g)	2.658e-030	-29.575
SiF4(g)	1.981e-038	-37.703
H2(g)	8.945e-043	-42.048
CO(g)	3.371e-049	-48.472
SO2(g)	1.965e-057	-56.707
NH3(g)	2.346e-070	-69.630
Na(g)	3.873e-077	-76.412
K(g)	4.446e-079	-78.352
F2(g)	3.148e-084	-83.502
Mg(g)	8.189e-132	-131.087
H2S(g)	2.786e-146	-145.555
CH4(g)	3.579e-148	-147.446
Ca(g)	1.378e-154	-153.861
C(g)	6.358e-193	-192.197
Si(g)	3.334e-224	-223.477
S2(g)	6.568e-234	-233.183
C2H4(g)	7.643e-242	-241.117

Original basis	total moles	In fluid		Sorbed		Kd L/kg
		moles	mg/kg	moles	mg/kg	
Ba ⁺⁺	1.16e-007	1.16e-007	0.0159			
Ca ⁺⁺	0.000327	0.000327	13.1			
Cl ⁻	5.39e-005	5.39e-005	1.91			
F ⁻	4.30e-005	4.30e-005	0.817			
H ⁺	-0.000203	-0.000203	-0.204			
H ₂ O	55.5	55.5	1.00e+006			
HCO ₃ ⁻	0.00218	0.00218	133.			
K ⁺	6.12e-005	6.12e-005	2.39			
Mg ⁺⁺	0.000136	0.000136	3.32			
MoO ₄ ⁻⁻	7.59e-008	7.59e-008	0.0121			
NH ₃ (aq)	0.000227	0.000227	3.86			
Na ⁺	0.00107	0.00107	24.6			
O ₂ (aq)	0.000700	0.000700	22.4			
ReO ₄ ⁻	4.20e-006	4.20e-006	1.05			
SO ₄ ⁻⁻	0.000210	0.000210	20.2			
SiO ₂ (aq)	0.000631	0.000631	37.9			

Elemental composition	total moles	In fluid		Sorbed	
		moles	mg/kg	moles	mg/kg
Barium	1.161e-007	1.161e-007	0.01594		
Calcium	0.0003266	0.0003266	13.09		
Carbon	0.002175	0.002175	26.12		
Chlorine	5.385e-005	5.385e-005	1.909		
Fluorine	4.299e-005	4.299e-005	0.8166		
Hydrogen	111.0	111.0	1.119e+005		
Magnesium	0.0001365	0.0001365	3.316		
Molybdenum	7.591e-008	7.591e-008	0.007281		
Nitrogen	0.0002270	0.0002270	3.178		
Oxygen	55.52	55.52	8.880e+005		
Potassium	6.116e-005	6.116e-005	2.391		
Rhenium	4.202e-006	4.202e-006	0.7822		
Silicon	0.0006307	0.0006307	17.71		
Sodium	0.001070	0.001070	24.60		
Sulfur	0.0002100	0.0002100	6.732		

Sample D14SEBOT

```

Step #      0          Xi = 0.0000
Temperature = 20.0 C   Pressure = 1.013 bars
pH = 7.980           log fO2 = -0.756
Eh = 0.7552 volts    pe = 12.9836
Ionic strength = 0.003083
Charge imbalance = -0.000772 eq/kg (-31.79% error)
Activity of water = 0.999998
Solvent mass = 1.000000 kg
Solution mass = 1.000262 kg
Solution density = 1.016 g/cm3
Chlorinity = 0.000063 molal
Dissolved solids = 262 mg/kg sol'n
Elect. conductivity = 229.23 uS/cm (or umho/cm)
Hardness = 46.53 mg/kg sol'n as CaCO3
  carbonate = 46.53 mg/kg sol'n as CaCO3
  non-carbonate = 0.00 mg/kg sol'n as CaCO3
Rock mass = 0.000000 kg
Carbonate alkalinity= 103.00 mg/kg sol'n as CaCO3
Water type = Na-HCO3
  
```

No minerals in system.

Aqueous species	molality	mg/kg sol'n	act. coef.	log act.
HCO3-	0.002024	123.5	0.9417	-2.7198
Na+	0.001075	24.72	0.9417	-2.9945
SiO2(aq)	0.0006069	36.45	1.0000	-3.2169
Ca++	0.0003101	12.42	0.7921	-3.6098
NO3-	0.0002619	16.23	0.9407	-3.6084
O2(aq)	0.0002460	7.871	1.0000	-3.6090
SO4--	0.0001962	18.84	0.7858	-3.8120
Mg++	0.0001339	3.254	0.7980	-3.9712
K+	6.587e-005	2.575	0.9407	-4.2078
Cl-	6.272e-005	2.223	0.9407	-4.2291
CO2(aq)	4.869e-005	2.142	1.0000	-4.3125
F-	4.325e-005	0.8214	0.9412	-4.3903
CO3--	9.552e-006	0.5731	0.7874	-5.1237
HSiO3-	6.031e-006	0.4648	0.9417	-5.2457
CaHCO3+	5.645e-006	0.5706	0.9417	-5.2744
ReO4-	5.497e-006	1.375	0.9417	-5.2860
CaSO4(aq)	4.787e-006	0.6515	1.0000	-5.3200
MgSO4(aq)	3.751e-006	0.4514	1.0000	-5.4259
CaCO3(aq)	3.566e-006	0.3568	1.0000	-5.4478
Zn++	3.046e-006	0.1991	0.7921	-5.6175
NaHCO3(aq)	3.045e-006	0.2558	1.0000	-5.5164
MgHCO3+	2.399e-006	0.2046	0.9417	-5.6461
MgCO3(aq)	7.330e-007	0.06179	1.0000	-6.1349
OH-	6.797e-007	0.01156	0.9412	-6.1940
NaHSiO3(aq)	2.872e-007	0.02874	1.0000	-6.5418
Ba++	1.137e-007	0.01561	0.7890	-7.0473
MoO4--	1.057e-007	0.01689	0.7874	-7.0799
MgF+	1.056e-007	0.004571	0.9417	-7.0025
KSO4-	7.710e-008	0.01042	0.9417	-7.1390
ZnSO4(aq)	6.886e-008	0.01111	1.0000	-7.1620
CaF+	5.026e-008	0.002969	0.9417	-7.3248
NaCO3-	3.054e-008	0.002534	0.9417	-7.5413
H+	1.107e-008	1.115e-005	0.9462	-7.9800

(only species > 1e-8 molal listed)

Mineral saturation states

	log Q/K		log Q/K
Zn2SiO4	3.2531s/sat	Aragonite	-0.4163
Talc	1.6398s/sat	Barite	-0.7928
Witherite	1.2638s/sat	Smithsonite	-0.9081
Quartz	0.9149s/sat	Monohydrocalcite	-1.0925
Tridymite	0.7173s/sat	Magnesite	-1.1342
Cristobalite(alp)	0.3529s/sat	Zincite	-1.1359
Chalcedony	0.3390s/sat	Dolomite-dis	-1.3278
Dolomite	0.2541s/sat	Zn(OH)2(gamma)	-1.5407
Dolomite-ord	0.2540s/sat	Zn(OH)2(epsilon)	-1.5660
Coesite	0.0917s/sat	Zn(OH)2(beta)	-1.8419
Cristobalite(bet)	-0.1051	Chrysotile	-2.1905
Ice	-0.1194	Fluorite	-2.3035
Calcite	-0.2718	Enstatite	-2.7737
SiO2(am)	-0.4132	Gypsum	-2.9313

(only minerals with log Q/K > -3 listed)

Gases	fugacity	log fug.
O2(g)	0.1755	-0.756
H2O(g)	0.01903	-1.721
CO2(g)	0.001218	-2.914
HF(g)	2.155e-014	-13.667
HCl(g)	1.834e-019	-18.737
N2(g)	1.061e-019	-18.974
NO2(g)	5.208e-020	-19.283
NO(g)	5.207e-026	-25.283
Cl2(g)	4.142e-030	-29.383
SiF4(g)	2.640e-038	-37.578
H2(g)	8.945e-043	-42.048
CO(g)	3.480e-049	-48.458
SO2(g)	2.200e-057	-56.657
NH3(g)	2.901e-070	-69.537
Zn(g)	1.108e-075	-74.955
Na(g)	3.644e-077	-76.438
K(g)	4.474e-079	-78.349
F2(g)	3.684e-084	-83.434
Mg(g)	7.382e-132	-131.132
H2S(g)	3.119e-146	-145.506
CH4(g)	3.695e-148	-147.432
Ca(g)	1.194e-154	-153.923
C(g)	6.563e-193	-192.183
Si(g)	3.244e-224	-223.489
S2(g)	8.233e-234	-233.084
C2H4(g)	8.145e-242	-241.089

Original basis	total moles	In fluid		Sorbed		Kd L/kg
		moles	mg/kg	moles	mg/kg	
Ba++	1.14e-007	1.14e-007	0.0156			
Ca++	0.000324	0.000324	13.0			
Cl-	6.27e-005	6.27e-005	2.22			
F-	4.34e-005	4.34e-005	0.824			
H+	-0.000234	-0.000234	-0.236			
H2O	55.5	55.5	1.00e+006			
HCO3-	0.00210	0.00210	128.			
K+	6.59e-005	6.59e-005	2.58			
Mg++	0.000141	0.000141	3.42			
MoO4--	1.06e-007	1.06e-007	0.0169			
NH3(aq)	0.000262	0.000262	4.46			
Na+	0.00108	0.00108	24.8			

O2(aq)	0.000770	0.000770	24.6
ReO4-	5.50e-006	5.50e-006	1.37
SO4--	0.000205	0.000205	19.7
SiO2(aq)	0.000613	0.000613	36.8
Zn++	3.12e-006	3.12e-006	0.204

Elemental composition	In fluid			Sorbed	
	total moles	moles	mg/kg	moles	mg/kg
Barium	1.139e-007	1.139e-007	0.01564		
Calcium	0.0003241	0.0003241	12.99		
Carbon	0.002098	0.002098	25.19		
Chlorine	6.273e-005	6.273e-005	2.224		
Fluorine	4.341e-005	4.341e-005	0.8245		
Hydrogen	111.0	111.0	1.119e+005		
Magnesium	0.0001409	0.0001409	3.424		
Molybdenum	1.057e-007	1.057e-007	0.01013		
Nitrogen	0.0002619	0.0002619	3.667		
Oxygen	55.52	55.52	8.880e+005		
Potassium	6.595e-005	6.595e-005	2.578		
Rhenium	5.497e-006	5.497e-006	1.023		
Silicon	0.0006132	0.0006132	17.22		
Sodium	0.001079	0.001079	24.79		
Sulfur	0.0002049	0.0002049	6.568		
Zinc	3.115e-006	3.115e-006	0.2037		

Sample D14SBOT

```

Step #      0          Xi = 0.0000
Temperature = 20.0 C   Pressure = 1.013 bars
pH = 8.060           log fO2 = -0.756
Eh = 0.7505 volts    pe = 12.9036
Ionic strength = 0.003071
Charge imbalance = -0.000576 eq/kg (-24.04% error)
Activity of water = 0.999998
Solvent mass = 1.000000 kg
Solution mass = 1.000257 kg
Solution density = 1.016 g/cm3
Chlorinity = 0.000056 molal
Dissolved solids = 257 mg/kg sol'n
Elect. conductivity = 227.19 uS/cm (or umho/cm)
Hardness = 48.37 mg/kg sol'n as CaCO3
  carbonate = 48.37 mg/kg sol'n as CaCO3
  non-carbonate = 0.00 mg/kg sol'n as CaCO3
Rock mass = 0.000000 kg
Carbonate alkalinity = 96.90 mg/kg sol'n as CaCO3
Water type = Na-HCO3
  
```

No minerals in system.

Aqueous species	molality	mg/kg sol'n	act. coef.	log act.
HCO3-	0.001900	115.9	0.9418	-2.7474
Na+	0.001110	25.50	0.9418	-2.9809
SiO2(aq)	0.0006402	38.46	1.0000	-3.1937
Ca++	0.0003239	12.98	0.7924	-3.5907
O2(aq)	0.0002460	7.871	1.0000	-3.6090
NO3-	0.0002412	14.95	0.9409	-3.6440
SO4--	0.0002038	19.57	0.7862	-3.7953
Mg++	0.0001373	3.336	0.7983	-3.9602
K+	6.712e-005	2.624	0.9409	-4.1996
Cl-	5.550e-005	1.967	0.9409	-4.2822
F-	4.319e-005	0.8204	0.9413	-4.3909
CO2(aq)	3.801e-005	1.672	1.0000	-4.4201
CO3--	1.077e-005	0.6463	0.7878	-5.0713
HSiO3-	7.648e-006	0.5894	0.9418	-5.1425
ReO4-	5.655e-006	1.415	0.9418	-5.2736
CaHCO3+	5.535e-006	0.5594	0.9418	-5.2829
CaSO4(aq)	5.198e-006	0.7074	1.0000	-5.2842
CaCO3(aq)	4.204e-006	0.4206	1.0000	-5.3764
MgSO4(aq)	3.997e-006	0.4810	1.0000	-5.3982
NaHCO3(aq)	2.949e-006	0.2477	1.0000	-5.5303
MgHCO3+	2.308e-006	0.1969	0.9418	-5.6628
MgCO3(aq)	8.481e-007	0.07149	1.0000	-6.0715
OH-	8.171e-007	0.01389	0.9413	-6.1140
NaHSiO3(aq)	3.759e-007	0.03762	1.0000	-6.4249
Ba++	1.251e-007	0.01717	0.7893	-7.0056
MoO4--	1.190e-007	0.01903	0.7878	-7.0281
MgF+	1.081e-007	0.004682	0.9418	-6.9920
KSO4-	8.165e-008	0.01103	0.9418	-7.1141
CaF+	5.245e-008	0.003098	0.9418	-7.3063
NaCO3-	3.555e-008	0.002950	0.9418	-7.4752
(only species > 1e-8 molal listed)				

Mineral saturation states

	log Q/K		log Q/K
Talc	2.2456s/sat	Aragonite	-0.3449
Witherite	1.3579s/sat	SiO2(am)	-0.3900

Quartz	0.9381s/sat	Barite	-0.7344
Tridymite	0.7405s/sat	Monohydrocalcite	-1.0211
Dolomite	0.3889s/sat	Magnesite	-1.0708
Dolomite-ord	0.3889s/sat	Dolomite-dis	-1.1929
Cristobalite(alp)	0.3761s/sat	Chrysotile	-1.6312
Chalcedony	0.3622s/sat	Tremolite	-1.9037
Coesite	0.1149s/sat	Fluorite	-2.2854
Cristobalite(bet)	-0.0819	Enstatite	-2.5796
Ice	-0.1194	Gypsum	-2.8956
Calcite	-0.2003		
(only minerals with log Q/K > -3 listed)			

Gases	fugacity	log fug.
O2(g)	0.1755	-0.756
H2O(g)	0.01903	-1.721
CO2(g)	0.0009505	-3.022
HF(g)	1.790e-014	-13.747
HCl(g)	1.350e-019	-18.870
N2(g)	6.228e-020	-19.206
NO2(g)	3.991e-020	-19.399
NO(g)	3.990e-026	-25.399
Cl2(g)	2.245e-030	-29.649
SiF4(g)	1.327e-038	-37.877
H2(g)	8.945e-043	-42.048
CO(g)	2.716e-049	-48.566
SO2(g)	1.582e-057	-56.801
NH3(g)	2.223e-070	-69.653
Na(g)	4.521e-077	-76.345
K(g)	5.482e-079	-78.261
F2(g)	2.543e-084	-83.595
Mg(g)	1.094e-131	-130.961
H2S(g)	2.242e-146	-145.649
CH4(g)	2.884e-148	-147.540
Ca(g)	1.804e-154	-153.744
C(g)	5.123e-193	-192.290
Si(g)	3.422e-224	-223.466
S2(g)	4.256e-234	-233.371
C2H4(g)	4.962e-242	-241.304

Original basis	total moles	In fluid moles	mg/kg	Sorbed moles	mg/kg	Kd L/kg
Ba++	1.25e-007	1.25e-007	0.0172			
Ca++	0.000339	0.000339	13.6			
Cl-	5.55e-005	5.55e-005	1.97			
F-	4.34e-005	4.34e-005	0.823			
H+	-0.000228	-0.000228	-0.230			
H2O	55.5	55.5	1.00e+006			
HCO3-	0.00196	0.00196	120.			
K+	6.72e-005	6.72e-005	2.63			
Mg++	0.000145	0.000145	3.51			
MoO4--	1.19e-007	1.19e-007	0.0190			
NH3(aq)	0.000241	0.000241	4.11			
Na+	0.00111	0.00111	25.6			
O2(aq)	0.000729	0.000729	23.3			
ReO4-	5.66e-006	5.66e-006	1.41			
SO4--	0.000213	0.000213	20.5			
SiO2(aq)	0.000648	0.000648	38.9			

Elemental composition	In fluid			Sorbed	
	total moles	moles	mg/kg	moles	mg/kg
Barium	1.254e-007	1.254e-007	0.01722		
Calcium	0.0003389	0.0003389	13.58		
Carbon	0.001964	0.001964	23.59		
Chlorine	5.552e-005	5.552e-005	1.968		
Fluorine	4.336e-005	4.336e-005	0.8235		
Hydrogen	111.0	111.0	1.119e+005		
Magnesium	0.0001446	0.0001446	3.512		
Molybdenum	1.190e-007	1.190e-007	0.01141		
Nitrogen	0.0002412	0.0002412	3.378		
Oxygen	55.52	55.52	8.880e+005		
Potassium	6.720e-005	6.720e-005	2.627		
Rhenium	5.655e-006	5.655e-006	1.053		
Silicon	0.0006482	0.0006482	18.20		
Sodium	0.001113	0.001113	25.58		
Sulfur	0.0002131	0.0002131	6.831		

Sample D1419MMB_ts

```

Step #      0          Xi = 0.0000
Temperature = 20.0 C   Pressure = 1.013 bars
pH = 7.970           log fO2 = -0.756
Eh = 0.7557 volts    pe = 12.9936
Ionic strength = 0.003038
Charge imbalance = -0.000473 eq/kg (-20.47% error)
Activity of water = 0.999995
Solvent mass = 1.000000 kg
Solution mass = 1.000251 kg
Solution density = 1.016 g/cm3
Chlorinity = 0.000126 molal
Dissolved solids = 251 mg/kg sol'n
Elect. conductivity = 222.33 uS/cm (or umho/cm)
Hardness = 55.75 mg/kg sol'n as CaCO3
  carbonate = 55.75 mg/kg sol'n as CaCO3
  non-carbonate = 0.00 mg/kg sol'n as CaCO3
Rock mass = 0.000000 kg
Carbonate alkalinity = 83.80 mg/kg sol'n as CaCO3
Water type = Na-HCO3
  
```

No minerals in system.

Aqueous species	molality	mg/kg sol'n	act. coef.	log act.
HCO3-	0.001646	100.4	0.9421	-2.8095
Na+	0.0009350	21.49	0.9421	-3.0551
SiO2(aq)	0.0005654	33.97	1.0000	-3.2476
Ca++	0.0004019	16.10	0.7933	-3.4964
NO3-	0.0003333	20.66	0.9411	-3.5035
O2(aq)	0.0002460	7.871	1.0000	-3.6090
SO4--	0.0001852	17.78	0.7871	-3.8364
Mg++	0.0001336	3.247	0.7991	-3.9716
Cl-	0.0001263	4.475	0.9411	-3.9251
K+	5.833e-005	2.280	0.9411	-4.2604
ReO4-	4.677e-005	11.70	0.9421	-4.3559
CO2(aq)	4.052e-005	1.783	1.0000	-4.3923
CO3--	7.579e-006	0.4547	0.7887	-5.2235
CaHCO3+	5.958e-006	0.6021	0.9421	-5.2508
CaSO4(aq)	5.874e-006	0.7995	1.0000	-5.2311
HSiO3-	5.489e-006	0.4230	0.9421	-5.2864
CaCO3(aq)	3.679e-006	0.3681	1.0000	-5.4343
MgSO4(aq)	3.543e-006	0.4263	1.0000	-5.4507
NaHCO3(aq)	2.154e-006	0.1809	1.0000	-5.6667
MgHCO3+	1.948e-006	0.1662	0.9421	-5.7363
MoO4--	7.673e-007	0.1227	0.7887	-6.2181
OH-	6.640e-007	0.01129	0.9416	-6.2040
MgCO3(aq)	5.821e-007	0.04906	1.0000	-6.2350
NaHSiO3(aq)	2.275e-007	0.02276	1.0000	-6.6430
Ba++	1.330e-007	0.01827	0.7902	-6.9783
KSO4-	6.454e-008	0.008721	0.9421	-7.2161
NaCO3-	2.110e-008	0.001751	0.9421	-7.7016
NaCl(aq)	1.707e-008	0.0009971	1.0000	-7.7679
H+	1.132e-008	1.141e-005	0.9465	-7.9700
MgCl+	1.023e-008	0.0006114	0.9421	-8.0159
(only species > 1e-8 molal listed)				

Mineral saturation states

	log Q/K		log Q/K
Talc	1.4558s/sat	Calcite	-0.2582
Witherite	1.2331s/sat	Aragonite	-0.4028

Quartz	0.8842s/sat	SiO2(am)	-0.4439
Tridymite	0.6866s/sat	Barite	-0.7482
Cristobalite(alp)	0.3222s/sat	Monohydrocalcite	-1.0790
Chalcedony	0.3083s/sat	Magnesite	-1.2343
Dolomite	0.1675s/sat	Dolomite-dis	-1.4144
Dolomite-ord	0.1674s/sat	Chrysotile	-2.3131
Coesite	0.0610s/sat	Enstatite	-2.8248
Ice	-0.1194	Gypsum	-2.8424
Cristobalite(bet)	-0.1358		

(only minerals with log Q/K > -3 listed)

Gases	fugacity	log fug.
O2(g)	0.1755	-0.756
H2O(g)	0.01903	-1.721
CO2(g)	0.001013	-2.994
HCl(g)	3.780e-019	-18.423
N2(g)	1.801e-019	-18.745
NO2(g)	6.785e-020	-19.168
NO(g)	6.784e-026	-25.168
Cl2(g)	1.760e-029	-28.755
H2(g)	8.945e-043	-42.048
CO(g)	2.896e-049	-48.538
SO2(g)	2.178e-057	-56.662
NH3(g)	3.780e-070	-69.423
Na(g)	3.098e-077	-76.509
K(g)	3.874e-079	-78.412
Mg(g)	7.044e-132	-131.152
H2S(g)	3.087e-146	-145.510
CH4(g)	3.075e-148	-147.512
Ca(g)	1.481e-154	-153.829
C(g)	5.462e-193	-192.263
Si(g)	3.022e-224	-223.520
S2(g)	8.066e-234	-233.093
C2H4(g)	5.641e-242	-241.249

Original basis	total moles	In fluid moles	mg/kg	Sorbed moles	mg/kg	Kd L/kg
Ba++	1.33e-007	1.33e-007	0.0183			
Ca++	0.000417	0.000417	16.7			
Cl-	0.000126	0.000126	4.48			
H+	-0.000311	-0.000311	-0.313			
H2O	55.5	55.5	1.00e+006			
HCO3-	0.00171	0.00171	104.			
K+	5.84e-005	5.84e-005	2.28			
Mg++	0.000140	0.000140	3.39			
MoO4--	7.67e-007	7.67e-007	0.123			
NH3(aq)	0.000333	0.000333	5.67			
Na+	0.000937	0.000937	21.5			
O2(aq)	0.000913	0.000913	29.2			
ReO4-	4.68e-005	4.68e-005	11.7			
SO4--	0.000195	0.000195	18.7			
SiO2(aq)	0.000571	0.000571	34.3			

Elemental composition	total moles	In fluid moles	mg/kg	Sorbed moles	mg/kg
Barium	1.333e-007	1.333e-007	0.01830		
Calcium	0.0004174	0.0004174	16.73		
Carbon	0.001708	0.001708	20.51		
Chlorine	0.0001263	0.0001263	4.477		
Hydrogen	111.0	111.0	1.119e+005		

Magnesium	0.0001397	0.0001397	3.394
Molybdenum	7.673e-007	7.673e-007	0.07359
Nitrogen	0.0003333	0.0003333	4.667
Oxygen	55.52	55.52	8.880e+005
Potassium	5.840e-005	5.840e-005	2.283
Rhenium	4.677e-005	4.677e-005	8.707
Silicon	0.0005712	0.0005712	16.04
Sodium	0.0009375	0.0009375	21.55
Sulfur	0.0001946	0.0001946	6.240

Sample D1419MMB_bs

```

Step #      0          Xi = 0.0000
Temperature = 20.0 C   Pressure = 1.013 bars
pH = 8.020           log fO2 = -0.756
Eh = 0.7528 volts    pe = 12.9436
Ionic strength = 0.003305
Charge imbalance = -0.000699 eq/kg (-26.79% error)
Activity of water = 0.999996
Solvent mass = 1.000000 kg
Solution mass = 1.000282 kg
Solution density = 1.016 g/cm3
Chlorinity = 0.000109 molal
Dissolved solids = 282 mg/kg sol'n
Elect. conductivity = 246.00 uS/cm (or umho/cm)
Hardness = 51.90 mg/kg sol'n as CaCO3
  carbonate = 51.90 mg/kg sol'n as CaCO3
  non-carbonate = 0.00 mg/kg sol'n as CaCO3
Rock mass = 0.000000 kg
Carbonate alkalinity= 100.00 mg/kg sol'n as CaCO3
Water type = Na-HCO3
  
```

No minerals in system.

Aqueous species	molality	mg/kg sol'n	act. coef.	log act.
HCO3-	0.001962	119.7	0.9399	-2.7343
Na+	0.001195	27.46	0.9399	-2.9496
SiO2(aq)	0.0005127	30.80	1.0000	-3.2901
NO3-	0.0004206	26.07	0.9388	-3.4035
Ca++	0.0003645	14.61	0.7862	-3.5427
O2(aq)	0.0002460	7.871	1.0000	-3.6090
SO4--	0.0001868	17.94	0.7796	-3.8367
Mg++	0.0001316	3.197	0.7925	-3.9818
Cl-	0.0001093	3.875	0.9388	-3.9886
ReO4-	6.501e-005	16.26	0.9399	-4.2140
K+	5.808e-005	2.270	0.9388	-4.2634
CO2(aq)	4.294e-005	1.889	1.0000	-4.3671
CO3--	1.021e-005	0.6124	0.7813	-5.0983
CaHCO3+	6.383e-006	0.6451	0.9399	-5.2219
HSiO3-	5.597e-006	0.4314	0.9399	-5.2790
CaSO4(aq)	5.277e-006	0.7182	1.0000	-5.2776
CaCO3(aq)	4.412e-006	0.4415	1.0000	-5.3553
MgSO4(aq)	3.458e-006	0.4161	1.0000	-5.4612
NaHCO3(aq)	3.266e-006	0.2743	1.0000	-5.4860
Zn++	2.490e-006	0.1628	0.7862	-5.7082
MgHCO3+	2.268e-006	0.1934	0.9399	-5.6713
MgCO3(aq)	7.584e-007	0.06393	1.0000	-6.1201
OH-	7.468e-007	0.01270	0.9394	-6.1540
MoO4--	5.037e-007	0.08053	0.7813	-6.4050
NaHSiO3(aq)	2.951e-007	0.02953	1.0000	-6.5300
Ba++	1.079e-007	0.01482	0.7830	-7.0731
KSO4-	6.422e-008	0.008677	0.9399	-7.2193
ZnSO4(aq)	5.279e-008	0.008520	1.0000	-7.2775
NaCO3-	3.598e-008	0.002985	0.9399	-7.4709
NaCl(aq)	1.880e-008	0.001098	1.0000	-7.7260
H+	1.011e-008	1.019e-005	0.9446	-8.0200

(only species > 1e-8 molal listed)

Mineral saturation states

	log Q/K		log Q/K
Zn2SiO4	3.1585s/sat	SiO2(am)	-0.4864
Talc	1.5550s/sat	Barite	-0.8433
Witherite	1.2635s/sat	Smithsonite	-0.9733
Quartz	0.8417s/sat	Monohydrocalcite	-1.0000
Tridymite	0.6441s/sat	Magnesite	-1.1194
Dolomite	0.3613s/sat	Zincite	-1.1466
Dolomite-ord	0.3613s/sat	Dolomite-dis	-1.2205
Cristobalite(alp)	0.2797s/sat	Zn(OH)2(gamma)	-1.5514
Chalcedony	0.2658s/sat	Zn(OH)2(epsilon)	-1.5767
Coesite	0.0184s/sat	Zn(OH)2(beta)	-1.8526
Ice	-0.1194	Chrysotile	-2.1289
Cristobalite(bet)	-0.1784	Enstatite	-2.7776
Calcite	-0.1793	Gypsum	-2.8890
Aragonite	-0.3239		

(only minerals with log Q/K > -3 listed)

Gases	fugacity	log fug.
O2(g)	0.1755	-0.756
H2O(g)	0.01903	-1.721
CO2(g)	0.001074	-2.969
HCl(g)	2.910e-019	-18.536
N2(g)	2.266e-019	-18.645
NO2(g)	7.613e-020	-19.118
NO(g)	7.612e-026	-25.119
Cl2(g)	1.043e-029	-28.982
H2(g)	8.945e-043	-42.048
CO(g)	3.069e-049	-48.513
SO2(g)	1.729e-057	-56.762
NH3(g)	4.240e-070	-69.373
Zn(g)	1.081e-075	-74.966
Na(g)	4.431e-077	-76.353
K(g)	4.317e-079	-78.365
Mg(g)	8.660e-132	-131.062
H2S(g)	2.451e-146	-145.611
CH4(g)	3.258e-148	-147.487
Ca(g)	1.676e-154	-153.776
C(g)	5.788e-193	-192.237
Si(g)	2.740e-224	-223.562
S2(g)	5.083e-234	-233.294
C2H4(g)	6.335e-242	-241.198

Original basis	total moles	In fluid		Sorbed		Kd L/kg
		moles	mg/kg	moles	mg/kg	
Ba++	1.08e-007	1.08e-007	0.0149			
Ca++	0.000381	0.000381	15.2			
Cl-	0.000109	0.000109	3.88			
H+	-0.000400	-0.000400	-0.403			
H2O	55.5	55.5	1.00e+006			
HCO3-	0.00203	0.00203	124.			
K+	5.81e-005	5.81e-005	2.27			
Mg++	0.000138	0.000138	3.35			
MoO4--	5.04e-007	5.04e-007	0.0805			
NH3(aq)	0.000421	0.000421	7.16			
Na+	0.00120	0.00120	27.5			
O2(aq)	0.00109	0.00109	34.8			
ReO4-	6.50e-005	6.50e-005	16.3			
SO4--	0.000196	0.000196	18.8			
SiO2(aq)	0.000519	0.000519	31.2			
Zn++	2.54e-006	2.54e-006	0.166			

Elemental composition	total moles	In fluid		Sorbed	
		moles	mg/kg	moles	mg/kg
Barium	1.082e-007	1.082e-007	0.01486		
Calcium	0.0003806	0.0003806	15.25		
Carbon	0.002032	0.002032	24.40		
Chlorine	0.0001094	0.0001094	3.876		
Hydrogen	111.0	111.0	1.119e+005		
Magnesium	0.0001381	0.0001381	3.355		
Molybdenum	5.037e-007	5.037e-007	0.04831		
Nitrogen	0.0004206	0.0004206	5.890		
Oxygen	55.52	55.52	8.880e+005		
Potassium	5.814e-005	5.814e-005	2.273		
Rhenium	6.501e-005	6.501e-005	12.10		
Silicon	0.0005186	0.0005186	14.56		
Sodium	0.001199	0.001199	27.55		
Sulfur	0.0001957	0.0001957	6.273		
Zinc	2.543e-006	2.543e-006	0.1663		

Sample D14SEND

```

Step #      0                Xi = 0.0000
Temperature = 20.0 C       Pressure = 1.013 bars
pH = 8.030                log fO2 = -0.758
Eh = 0.7522 volts         pe = 12.9330
Ionic strength = 0.002409
Charge imbalance = -0.000403 eq/kg (-20.76% error)
Activity of water = 1.000000
Solvent mass = 1.000000 kg
Solution mass = 1.000218 kg
Solution density = 1.016 g/cm3
Chlorinity = 0.000000 molal
Dissolved solids = 218 mg/kg sol'n
Elect. conductivity = 177.09 uS/cm (or umho/cm)
Hardness = 34.37 mg/kg sol'n as CaCO3
  carbonate = 34.37 mg/kg sol'n as CaCO3
  non-carbonate = 0.00 mg/kg sol'n as CaCO3
Rock mass = 0.000000 kg
Carbonate alkalinity = 93.60 mg/kg sol'n as CaCO3
Water type = Na-HCO3
  
```

No minerals in system.

Aqueous species	molality	mg/kg sol'n	act. coef.	log act.
HCO3-	0.001840	112.2	0.9479	-2.7584
Na+	0.001003	23.05	0.9479	-3.0219
SiO2(aq)	0.0005577	33.50	1.0000	-3.2536
Ca++	0.0002646	10.60	0.8118	-3.6680
O2(aq)	0.0002448	7.830	1.0000	-3.6113
SO4--	0.0001251	12.01	0.8067	-3.9962
K+	7.017e-005	2.743	0.9471	-4.1775
Mg++	6.572e-005	1.597	0.8167	-4.2702
CO2(aq)	3.970e-005	1.747	1.0000	-4.4012
ReO4-	1.126e-005	2.816	0.9479	-4.9718
CO3--	9.555e-006	0.5733	0.8080	-5.1123
AlO2-	9.213e-006	0.5433	0.9479	-5.0588
HSiO3-	6.177e-006	0.4761	0.9479	-5.2324
Fe(OH)3(aq)	5.128e-006	0.5479	1.0000	-5.2901
CaHCO3+	4.487e-006	0.4536	0.9479	-5.3712
CaCO3(aq)	3.201e-006	0.3203	1.0000	-5.4947
MoO4--	2.923e-006	0.4675	0.8080	-5.6267
CaSO4(aq)	2.739e-006	0.3728	1.0000	-5.5624
NaHCO3(aq)	2.615e-006	0.2197	1.0000	-5.5825
MgSO4(aq)	1.233e-006	0.1483	1.0000	-5.9091
MgHCO3+	1.095e-006	0.09340	0.9479	-5.9838
OH-	7.576e-007	0.01288	0.9475	-6.1440
MgCO3(aq)	3.779e-007	0.03186	1.0000	-6.4226
HALO2(aq)	3.022e-007	0.01812	1.0000	-6.5198
NaHSiO3(aq)	2.780e-007	0.02782	1.0000	-6.5559
Ba++	1.037e-007	0.01423	0.8093	-7.0763
KSO4-	5.375e-008	0.007264	0.9479	-7.2929
NaCO3-	2.923e-008	0.002426	0.9479	-7.5574

(only species > 1e-8 molal listed)

Mineral saturation states

	log Q/K		log Q/K
Nontronite-Ca	18.5335s/sat	Gibbsite	2.2813s/sat
Nontronite-Mg	18.4628s/sat	Saponite-Ca	2.0863s/sat
Nontronite-Na	18.1056s/sat	Saponite-Mg	2.0162s/sat
Nontronite-K	18.0781s/sat	Natrolite	1.9598s/sat

Nontronite-H	17.4700s/sat	Prehnite	1.9390s/sat
Clinoptilolite-h	17.2887s/sat	Saponite-Na	1.6584s/sat
Clinoptilolite-C	17.2597s/sat	Saponite-K	1.6310s/sat
Clinoptilolite-K	13.5090s/sat	Corundum	1.6076s/sat
Clinoptilolite-h	13.5034s/sat	Phlogopite	1.5259s/sat
Clinoptilolite-N	13.5025s/sat	Clinozoisite	1.5182s/sat
Clinoptilolite-h	13.3992s/sat	Zoisite	1.4723s/sat
Hematite	12.9283s/sat	Albite_high	1.4190s/sat
Stilbite	12.6115s/sat	Wairakite	1.4048s/sat
Muscovite	10.9118s/sat	Witherite	1.2461s/sat
Epidote-ord	8.4284s/sat	Magnetite	1.1326s/sat
Epidote	8.4279s/sat	Kyanite	1.1011s/sat
Mesolite	8.2592s/sat	Saponite-H	1.0229s/sat
Beidellite-Ca	8.2504s/sat	Talc	0.8958s/sat
Illite	8.2395s/sat	Clinocllore-14A	0.8837s/sat
Beidellite-Mg	8.1797s/sat	Quartz	0.8782s/sat
Paragonite	8.0324s/sat	Andalusite	0.8175s/sat
Beidellite-Na	7.8224s/sat	Tridymite	0.6806s/sat
Beidellite-K	7.7951s/sat	Sillimanite	0.4441s/sat
Herschelite	7.7304s/sat	Cristobalite(alp	0.3162s/sat
Montmor-Mg	7.5339s/sat	Chalcedony	0.3023s/sat
Montmor-Ca	7.5332s/sat	Jadeite	0.2692s/sat
Beidellite-H	7.1870s/sat	Coesite	0.0550s/sat
Montmor-Na	7.1731s/sat	Dawsonite	-0.0071
Montmor-K	7.1497s/sat	Dolomite	-0.0805
Pyrophyllite	7.0629s/sat	Dolomite-ord	-0.0805
Kaolinite	6.9827s/sat	Ice	-0.1194
Scolecite	6.9240s/sat	Cristobalite(bet	-0.1418
Andradite	6.6897s/sat	Kalsilite	-0.2474
Goethite	5.9896s/sat	Analcime-K	-0.3083
Laumontite	5.9753s/sat	Calcite	-0.3187
Celadonite	5.4218s/sat	SiO2(am)	-0.4499
Maximum_Microcli	4.7413s/sat	Aragonite	-0.4632
K-Feldspar	4.7401s/sat	Smectite-high-Fe	-0.4665
Margarite	4.6919s/sat	Anorthite	-0.8518
Amesite-14A	4.2322s/sat	Barite	-1.0061
Mordenite	4.0692s/sat	Monohydrocalcite	-1.1394
Lawsonite	3.6892s/sat	Analcime	-1.1990
Sanidine_high	3.5082s/sat	Magnesite	-1.4219
Ferrite-Ca	3.4948s/sat	Dolomite-dis	-1.6623
Ferrite-Mg	3.3149s/sat	Nepheline	-2.0752
Diaspore	2.8533s/sat	Clinocllore-7A	-2.5312
Albite_low	2.7714s/sat	Fe(OH)3	-2.6982
Albite	2.7713s/sat	Cordierite_hydr	-2.8043
Smectite-low-Fe-	2.4924s/sat	Chrysotile	-2.8611
Boehmite	2.4408s/sat		

(only minerals with log Q/K > -3 listed)

Gases	fugacity	log fug.
O2(g)	0.1746	-0.758
H2O(g)	0.01903	-1.721
CO2(g)	0.0009929	-3.003
H2(g)	8.969e-043	-42.047
CO(g)	2.845e-049	-48.546
SO2(g)	1.147e-057	-56.941
Na(g)	3.843e-077	-76.415
K(g)	5.391e-079	-78.268
Mg(g)	4.680e-132	-131.330
H2S(g)	1.638e-146	-145.786
CH4(g)	3.044e-148	-147.517
Ca(g)	1.319e-154	-153.880
Al(g)	3.711e-192	-191.430

C(g)	5.380e-193	-192.269
Si(g)	2.996e-224	-223.523
S2(g)	2.259e-234	-233.646
C2H4(g)	5.501e-242	-241.260

Original basis	total moles	In fluid		Sorbed		Kd L/kg
		moles	mg/kg	moles	mg/kg	
Al+++	9.52e-006	9.52e-006	0.257			
Ba++	1.04e-007	1.04e-007	0.0143			
Ca++	0.000275	0.000275	11.0			
Fe++	5.13e-006	5.13e-006	0.286			
H+	-2.87e-005	-2.87e-005	-0.0289			
H2O	55.5	55.5	1.00e+006			
HCO3-	0.00190	0.00190	116.			
K+	7.02e-005	7.02e-005	2.75			
Mg++	6.84e-005	6.84e-005	1.66			
MoO4--	2.92e-006	2.92e-006	0.467			
Na+	0.00101	0.00101	23.1			
O2(aq)	0.000246	0.000246	7.87			
ReO4-	1.13e-005	1.13e-005	2.82			
SO4--	0.000129	0.000129	12.4			
SiO2(aq)	0.000564	0.000564	33.9			

Elemental composition	total moles	In fluid		Sorbed	
		moles	mg/kg	moles	mg/kg
Aluminum	9.519e-006	9.519e-006	0.2568		
Barium	1.039e-007	1.039e-007	0.01427		
Calcium	0.0002750	0.0002750	11.02		
Carbon	0.001901	0.001901	22.83		
Hydrogen	111.0	111.0	1.119e+005		
Iron	5.128e-006	5.128e-006	0.2863		
Magnesium	6.843e-005	6.843e-005	1.663		
Molybdenum	2.923e-006	2.923e-006	0.2804		
Oxygen	55.52	55.52	8.880e+005		
Potassium	7.022e-005	7.022e-005	2.745		
Rhenium	1.126e-005	1.126e-005	2.096		
Silicon	0.0005641	0.0005641	15.84		
Sodium	0.001006	0.001006	23.12		
Sulfur	0.0001291	0.0001291	4.138		

Sample D14NTOP

```

Step #      0          Xi = 0.0000
Temperature = 20.0 C   Pressure = 1.013 bars
pH = 8.140          log fO2 = -0.793
Eh = 0.7453 volts    pe = 12.8142
Ionic strength      = 0.007648
Charge imbalance    = 0.001126 eq/kg (19.22% error)
Activity of water   = 0.999993
Solvent mass        = 1.000000 kg
Solution mass       = 1.000540 kg
Solution density    = 1.017 g/cm3
Chlorinity          = 0.000200 molal
Dissolved solids    = 540 mg/kg sol'n
Elect. conductivity = 522.67 uS/cm (or umho/cm)
Hardness            = 115.40 mg/kg sol'n as CaCO3
  carbonate         = 115.40 mg/kg sol'n as CaCO3
  non-carbonate     = 0.00 mg/kg sol'n as CaCO3
Rock mass           = 0.000000 kg
Carbonate alkalinity = 182.00 mg/kg sol'n as CaCO3
Water type          = Na-HCO3
  
```

No minerals in system.

Aqueous species	molality	mg/kg sol'n	act. coef.	log act.
Na+	0.004187	96.22	0.9133	-2.4175
HCO3-	0.003514	214.3	0.9133	-2.4936
Ca++	0.0008601	34.45	0.7067	-3.2162
SO4--	0.0006983	67.04	0.6942	-3.3145
SiO2(aq)	0.0005443	32.68	1.0000	-3.2642
B(OH)3(aq)	0.0003412	21.08	1.0000	-3.4671
O2(aq)	0.0002256	7.216	1.0000	-3.6466
Cl-	0.0001995	7.067	0.9111	-3.7406
Mg++	0.0001881	4.570	0.7183	-3.8693
K+	0.0001006	3.930	0.9111	-4.0379
Fe(OH)3(aq)	8.178e-005	8.735	1.0000	-4.0874
CO2(aq)	5.671e-005	2.494	1.0000	-4.2464
ReO4-	5.656e-005	14.14	0.9133	-4.2869
CaSO4(aq)	3.724e-005	5.067	1.0000	-4.4290
CO3--	2.624e-005	1.574	0.6974	-4.7375
BO2-	2.575e-005	1.102	0.9133	-4.6286
CaHCO3+	2.425e-005	2.450	0.9133	-4.6547
CaCO3(aq)	2.147e-005	2.148	1.0000	-4.6681
NaHCO3(aq)	1.936e-005	1.625	1.0000	-4.7132
AlO2-	1.633e-005	0.9627	0.9133	-4.8264
MgSO4(aq)	1.491e-005	1.794	1.0000	-4.8265
MoO4--	1.231e-005	1.968	0.6974	-5.0662
HSiO3-	8.061e-006	0.6211	0.9133	-5.1330
MgHCO3+	5.265e-006	0.4489	0.9133	-5.3180
Zn++	3.566e-006	0.2331	0.7067	-5.5985
MgCO3(aq)	2.255e-006	0.1901	1.0000	-5.6468
NaHSiO3(aq)	1.406e-006	0.1406	1.0000	-5.8520
OH-	1.014e-006	0.01723	0.9122	-6.0340
HAlO2(aq)	4.006e-007	0.02402	1.0000	-6.3973
KSO4-	3.696e-007	0.04993	0.9133	-6.4717
Ba++	3.052e-007	0.04189	0.7006	-6.6700
NaCO3-	2.893e-007	0.02400	0.9133	-6.5781
ZnSO4(aq)	2.261e-007	0.03649	1.0000	-6.6457
NaCl(aq)	1.133e-007	0.006617	1.0000	-6.9458
CaCl+	2.450e-008	0.001850	0.9133	-7.6502
MgCl+	2.043e-008	0.001220	0.9133	-7.7291

(only species > 1e-8 molal listed)

Mineral saturation states			
	log Q/K		log Q/K
Nontronite-Ca	21.0513s/sat	Prehnite	3.4956s/sat
Nontronite-Mg	20.9723s/sat	Clinozoisite	3.1973s/sat
Nontronite-Na	20.7483s/sat	Zoisite	3.1514s/sat
Nontronite-K	20.5674s/sat	Diaspore	2.9757s/sat
Nontronite-H	19.8770s/sat	Saponite-H	2.8874s/sat
Clinoptilolite-h	18.7422s/sat	Talc	2.7164s/sat
Clinoptilolite-C	18.7132s/sat	Boehmite	2.5633s/sat
Clinoptilolite-h	16.2695s/sat	Gibbsite	2.4037s/sat
Clinoptilolite-N	16.2687s/sat	Wairakite	2.2791s/sat
Hematite	15.3337s/sat	Albite_high	2.2242s/sat
Clinoptilolite-K	14.6631s/sat	Witherite	2.0273s/sat
Clinoptilolite-h	14.5532s/sat	Corundum	1.8525s/sat
Ferrite-Zn	14.0943s/sat	Dolomite	1.5218s/sat
Stilbite	13.5894s/sat	Dolomite-ord	1.5218s/sat
Muscovite	11.4969s/sat	Smectite-high-Fe	1.3481s/sat
Epidote-ord	11.1877s/sat	Kyanite	1.3354s/sat
Epidote	11.1873s/sat	Jadeite	1.0850s/sat
Andradite	11.0786s/sat	Andalusite	1.0518s/sat
Mesolite	9.3953s/sat	Dawsonite	0.9846s/sat
Herschelite	9.2470s/sat	Quartz	0.8676s/sat
Paragonite	9.0825s/sat	Clinochlore-7A	0.7868s/sat
Illite	8.7891s/sat	Sillimanite	0.6784s/sat
Beidellite-Ca	8.6077s/sat	Tridymite	0.6700s/sat
Beidellite-Mg	8.5286s/sat	Calcite	0.5079s/sat
Beidellite-Na	8.3047s/sat	Aragonite	0.3634s/sat
Beidellite-K	8.1238s/sat	Cristobalite(alp)	0.3056s/sat
Montmor-Ca	8.0111s/sat	Chalcedony	0.2917s/sat
Montmor-Mg	8.0035s/sat	Kalsilite	0.1140s/sat
Scolecite	7.8089s/sat	Barite	0.0819s/sat
Montmor-Na	7.7760s/sat	Coesite	0.0444s/sat
Montmor-K	7.5991s/sat	Anorthite	0.0436s/sat
Beidellite-H	7.4334s/sat	Analcime-K	0.0272s/sat
Pyrophyllite	7.2654s/sat	Dolomite-dis	-0.0600
Kaolinite	7.2064s/sat	Ice	-0.1194
Goethite	7.1923s/sat	Tremolite	-0.1442
Amesite-14A	7.1847s/sat	Cristobalite(bet)	-0.1524
Laumontite	6.8496s/sat	Monohydrocalcite	-0.3128
Ferrite-Ca	6.5720s/sat	Analcime	-0.4171
Celadonite	6.3724s/sat	SiO2(am)	-0.4605
Ferrite-Mg	6.3413s/sat	Smithsonite	-0.5030
Margarite	5.8323s/sat	Magnesite	-0.6461
Maximum_Microcli	5.0815s/sat	Zincite	-0.7970
K-Feldspar	5.0803s/sat	Chrysotile	-1.0194
Magnetite	4.7495s/sat	Cordierite_hydr	-1.1254
Lawsonite	4.5847s/sat	Zn(OH)2(gamma)	-1.2017
Mordenite	4.5831s/sat	Zn(OH)2(epsilon)	-1.2271
Clinochlore-14A	4.2017s/sat	Nepheline	-1.2488
Saponite-Ca	4.0617s/sat	Fe(OH)3	-1.4955
Saponite-Mg	3.9832s/sat	Zn(OH)2(beta)	-1.5030
Zn2SiO4	3.8837s/sat	Antigorite	-1.5827
Smectite-low-Fe-	3.8789s/sat	Gypsum	-2.0403
Sanidine_high	3.8484s/sat	Anhydrite	-2.2652
Saponite-Na	3.7587s/sat	Diopside	-2.3605
Phlogopite	3.7290s/sat	Enstatite	-2.3991
Natrolite	3.6019s/sat	Jarosite	-2.5407
Saponite-K	3.5778s/sat	Grossular	-2.7985
Albite_low	3.5765s/sat	Bassanite	-2.9116
Albite	3.5764s/sat		

(only minerals with log Q/K > -3 listed)

Gases	fugacity	log fug.
O2(g)	0.1610	-0.793
H2O(g)	0.01903	-1.721
CO2(g)	0.001418	-2.848
HCl(g)	3.908e-019	-18.408
Cl2(g)	1.801e-029	-28.744
H2(g)	9.341e-043	-42.030
CO(g)	4.232e-049	-48.373
SO2(g)	3.458e-057	-56.461
Zn(g)	2.526e-075	-74.598
Na(g)	2.032e-076	-75.692
K(g)	9.773e-079	-78.010
Mg(g)	2.037e-131	-130.691
H2S(g)	5.580e-146	-145.253
CH4(g)	5.116e-148	-147.291
Ca(g)	6.449e-154	-153.190
Al(g)	5.230e-192	-191.282
C(g)	8.335e-193	-192.079
B(g)	6.669e-206	-205.176
Si(g)	3.172e-224	-223.499
S2(g)	2.417e-233	-232.617
C2H4(g)	1.432e-241	-240.844

Original basis	total moles	In fluid moles	mg/kg	Sorbed moles	mg/kg	Kd L/kg
Al+++	1.67e-005	1.67e-005	0.452			
B(OH)3(aq)	0.000367	0.000367	22.7			
Ba++	3.07e-007	3.07e-007	0.0421			
Ca++	0.000943	0.000943	37.8			
Cl-	0.000200	0.000200	7.07			
Fe++	8.18e-005	8.18e-005	4.56			
H+	-0.000260	-0.000260	-0.262			
H2O	55.5	55.5	9.99e+005			
HCO3-	0.00367	0.00367	224.			
K+	0.000101	0.000101	3.94			
Mg++	0.000211	0.000211	5.12			
MoO4--	1.23e-005	1.23e-005	1.97			
Na+	0.00421	0.00421	96.7			
O2(aq)	0.000246	0.000246	7.87			
ReO4-	5.66e-005	5.66e-005	14.1			
SO4--	0.000751	0.000751	72.1			
SiO2(aq)	0.000554	0.000554	33.3			
Zn++	3.79e-006	3.79e-006	0.248			

Elemental composition	total moles	In fluid moles	mg/kg	Sorbed moles	mg/kg
Aluminum	1.674e-005	1.674e-005	0.4515		
Barium	3.068e-007	3.068e-007	0.04210		
Boron	0.0003669	0.0003669	3.964		
Calcium	0.0009431	0.0009431	37.78		
Carbon	0.003670	0.003670	44.05		
Chlorine	0.0001996	0.0001996	7.073		
Hydrogen	111.0	111.0	1.118e+005		
Iron	8.178e-005	8.178e-005	4.565		
Magnesium	0.0002106	0.0002106	5.115		
Molybdenum	1.231e-005	1.231e-005	1.180		
Oxygen	55.53	55.53	8.879e+005		
Potassium	0.0001009	0.0001009	3.945		
Rhenium	5.656e-005	5.656e-005	10.53		

Silicon	0.0005537	0.0005537	15.54
Sodium	0.004209	0.004209	96.70
Sulfur	0.0007510	0.0007510	24.07
Zinc	3.793e-006	3.793e-006	0.2479

Sample D14SEBOT

```

Step #      0          Xi = 0.0000
Temperature = 20.0 C   Pressure = 1.013 bars
pH = 7.980           log fO2 = -0.756
Eh = 0.7552 volts    pe = 12.9836
Ionic strength = 0.003083
Charge imbalance = -0.000772 eq/kg (-31.79% error)
Activity of water = 0.999998
Solvent mass = 1.000000 kg
Solution mass = 1.000262 kg
Solution density = 1.016 g/cm3
Chlorinity = 0.000063 molal
Dissolved solids = 262 mg/kg sol'n
Elect. conductivity = 229.23 uS/cm (or umho/cm)
Hardness = 46.53 mg/kg sol'n as CaCO3
  carbonate = 46.53 mg/kg sol'n as CaCO3
  non-carbonate = 0.00 mg/kg sol'n as CaCO3
Rock mass = 0.000000 kg
Carbonate alkalinity = 103.00 mg/kg sol'n as CaCO3
Water type = Na-HCO3
  
```

No minerals in system.

Aqueous species	molality	mg/kg sol'n	act. coef.	log act.
HCO3-	0.002024	123.5	0.9417	-2.7198
Na+	0.001075	24.72	0.9417	-2.9945
SiO2(aq)	0.0006069	36.45	1.0000	-3.2169
Ca++	0.0003101	12.42	0.7921	-3.6098
NO3-	0.0002619	16.23	0.9407	-3.6084
O2(aq)	0.0002460	7.871	1.0000	-3.6090
SO4--	0.0001962	18.84	0.7858	-3.8120
Mg++	0.0001339	3.254	0.7980	-3.9712
K+	6.587e-005	2.575	0.9407	-4.2078
Cl-	6.272e-005	2.223	0.9407	-4.2291
CO2(aq)	4.869e-005	2.142	1.0000	-4.3125
F-	4.325e-005	0.8214	0.9412	-4.3903
CO3--	9.552e-006	0.5731	0.7874	-5.1237
HSiO3-	6.031e-006	0.4648	0.9417	-5.2457
CaHCO3+	5.645e-006	0.5706	0.9417	-5.2744
ReO4-	5.497e-006	1.375	0.9417	-5.2860
CaSO4(aq)	4.787e-006	0.6515	1.0000	-5.3200
MgSO4(aq)	3.751e-006	0.4514	1.0000	-5.4259
CaCO3(aq)	3.566e-006	0.3568	1.0000	-5.4478
Zn++	3.046e-006	0.1991	0.7921	-5.6175
NaHCO3(aq)	3.045e-006	0.2558	1.0000	-5.5164
MgHCO3+	2.399e-006	0.2046	0.9417	-5.6461
MgCO3(aq)	7.330e-007	0.06179	1.0000	-6.1349
OH-	6.797e-007	0.01156	0.9412	-6.1940
NaHSiO3(aq)	2.872e-007	0.02874	1.0000	-6.5418
Ba++	1.137e-007	0.01561	0.7890	-7.0473
MoO4--	1.057e-007	0.01689	0.7874	-7.0799
MgF+	1.056e-007	0.004571	0.9417	-7.0025
KSO4-	7.710e-008	0.01042	0.9417	-7.1390
ZnSO4(aq)	6.886e-008	0.01111	1.0000	-7.1620
CaF+	5.026e-008	0.002969	0.9417	-7.3248
NaCO3-	3.054e-008	0.002534	0.9417	-7.5413
H+	1.107e-008	1.115e-005	0.9462	-7.9800

(only species > 1e-8 molal listed)

Mineral saturation states

	log Q/K		log Q/K
Zn2SiO4	3.2531s/sat	Aragonite	-0.4163
Talc	1.6398s/sat	Barite	-0.7928
Witherite	1.2638s/sat	Smithsonite	-0.9081
Quartz	0.9149s/sat	Monohydrocalcite	-1.0925
Tridymite	0.7173s/sat	Magnesite	-1.1342
Cristobalite(alp)	0.3529s/sat	Zincite	-1.1359
Chalcedony	0.3390s/sat	Dolomite-dis	-1.3278
Dolomite	0.2541s/sat	Zn(OH)2(gamma)	-1.5407
Dolomite-ord	0.2540s/sat	Zn(OH)2(epsilon)	-1.5660
Coesite	0.0917s/sat	Zn(OH)2(beta)	-1.8419
Cristobalite(bet)	-0.1051	Chrysotile	-2.1905
Ice	-0.1194	Fluorite	-2.3035
Calcite	-0.2718	Enstatite	-2.7737
SiO2(am)	-0.4132	Gypsum	-2.9313

(only minerals with log Q/K > -3 listed)

Gases	fugacity	log fug.
O2(g)	0.1755	-0.756
H2O(g)	0.01903	-1.721
CO2(g)	0.001218	-2.914
HF(g)	2.155e-014	-13.667
HCl(g)	1.834e-019	-18.737
N2(g)	1.061e-019	-18.974
NO2(g)	5.208e-020	-19.283
NO(g)	5.207e-026	-25.283
Cl2(g)	4.142e-030	-29.383
SiF4(g)	2.640e-038	-37.578
H2(g)	8.945e-043	-42.048
CO(g)	3.480e-049	-48.458
SO2(g)	2.200e-057	-56.657
NH3(g)	2.901e-070	-69.537
Zn(g)	1.108e-075	-74.955
Na(g)	3.644e-077	-76.438
K(g)	4.474e-079	-78.349
F2(g)	3.684e-084	-83.434
Mg(g)	7.382e-132	-131.132
H2S(g)	3.119e-146	-145.506
CH4(g)	3.695e-148	-147.432
Ca(g)	1.194e-154	-153.923
C(g)	6.563e-193	-192.183
Si(g)	3.244e-224	-223.489
S2(g)	8.233e-234	-233.084
C2H4(g)	8.145e-242	-241.089

Original basis	total moles	In fluid		Sorbed		Kd L/kg
		moles	mg/kg	moles	mg/kg	
Ba++	1.14e-007	1.14e-007	0.0156			
Ca++	0.000324	0.000324	13.0			
Cl-	6.27e-005	6.27e-005	2.22			
F-	4.34e-005	4.34e-005	0.824			
H+	-0.000234	-0.000234	-0.236			
H2O	55.5	55.5	1.00e+006			
HCO3-	0.00210	0.00210	128.			
K+	6.59e-005	6.59e-005	2.58			
Mg++	0.000141	0.000141	3.42			
MoO4--	1.06e-007	1.06e-007	0.0169			
NH3(aq)	0.000262	0.000262	4.46			
Na+	0.00108	0.00108	24.8			

O2(aq)	0.000770	0.000770	24.6
ReO4-	5.50e-006	5.50e-006	1.37
SO4--	0.000205	0.000205	19.7
SiO2(aq)	0.000613	0.000613	36.8
Zn++	3.12e-006	3.12e-006	0.204

Elemental composition	In fluid			Sorbed	
	total moles	moles	mg/kg	moles	mg/kg
Barium	1.139e-007	1.139e-007	0.01564		
Calcium	0.0003241	0.0003241	12.99		
Carbon	0.002098	0.002098	25.19		
Chlorine	6.273e-005	6.273e-005	2.224		
Fluorine	4.341e-005	4.341e-005	0.8245		
Hydrogen	111.0	111.0	1.119e+005		
Magnesium	0.0001409	0.0001409	3.424		
Molybdenum	1.057e-007	1.057e-007	0.01013		
Nitrogen	0.0002619	0.0002619	3.667		
Oxygen	55.52	55.52	8.880e+005		
Potassium	6.595e-005	6.595e-005	2.578		
Rhenium	5.497e-006	5.497e-006	1.023		
Silicon	0.0006132	0.0006132	17.22		
Sodium	0.001079	0.001079	24.79		
Sulfur	0.0002049	0.0002049	6.568		
Zinc	3.115e-006	3.115e-006	0.2037		

Distribution*

Washington River Protection Solutions
DJ Swanberg
WRPS Documents – TOCVND@rl.gov

Oak Ridge National Laboratory
EM Pierce

Pacific Northwest National Laboratory
KJ Cantrell
VL Freedman
JJ Neeway
NP Qafoku
GL Smith
JH Westsik, Jr
Project File
Information Release (pdf)

*All distribution will be made electronically.



Pacific Northwest
NATIONAL LABORATORY

*Proudly Operated by **Battelle** Since 1965*

902 Battelle Boulevard
P.O. Box 999
Richland, WA 99352
1-888-375-PNNL (7665)

U.S. DEPARTMENT OF
ENERGY

www.pnnl.gov