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May 10, 2002
Contract No. NRC–02–97–009
Account No. 20.01402.561

U.S. Nuclear Regulatory Commission
Attn: Mr. David J. Brooks
Office of Nuclear Material Safety and Safeguards
Two White Flint North, Mail Stop 7 C6
11545 Rockville Pike
Rockville, MD 20852

Subject: Transmittal of the deliverable ""Revised Analytical Compositions of Pore Water Collected from Yucca Mountain, Nevada, and Vicinity" (1402.561.230)

Dear Mr. Brooks:

This letter transmits the deliverable "Revised Analytical Compositions of Pore Water Collected from Yucca Mountain, Nevada, and Vicinity" (IM 01402.561.230). This deliverable was established in the Period 6 Program Manager's Periodic Report.

Site-specific groundwater compositions are routinely used by the U.S. Department of Energy (DOE) in numerical simulations and experiments designed to evaluate the long-term performance of Yucca Mountain as a potential high level waste repository. Center for Nuclear Waste Regulatory Analyses (CNWRA) reviews of DOE-reported groundwater compositions have revealed that the reliability of groundwater analyses from the unsaturated zone is, however, invariably compromised by the sampling, extraction, and analytical processes. Dr. Lauren Browning and other CNWRA staff have developed a method to restore internal thermodynamic consistency to the reported pore water compositions, and have used the revised groundwater data to glean insights into the ambient chemical system at Yucca Mountain.

In this report, we present pore water compositions from a variety of different locations at Yucca Mountain, revised following the methods of Browning, et al. (2000). This information directly supports a variety of ongoing issue resolution activities that are affected by the composition of water that will seep into the drifts at Yucca Mountain. Performance affecting processes that depend on the pore water composition include drip shield corrosion, container corrosion, waste form dissolution, and near field flow and transport, among others.

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If you have any questions about this deliverable, please contact me at 210.522.5540 or Dr. Lauren Browning at 210.522.6642.

Sincerely,

English C. Pearcy

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REVISED ANALYTICAL COMPOSITIONS OF PORE WATER COLLECTED FROM YUCCA MOUNTAIN, NEVADA, AND VICINITY

Prepared for

U.S. Nuclear Regulatory Commission
Contract NRC–02–97–009

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May 2002

ABSTRACT

Browning, et al. (2000) evaluated analytical pore water compositions from Yucca Mountain, Nevada, for internal thermodynamic consistency. The data were found to include significant ionic charge imbalances, unequilibrated aqueous speciation relationships, and erratic variability with depth in some species concentrations. Browning, et al. (2000) restored internal thermodynamic consistency to the data by introducing measured CO_2 gas pressure as a constraint, imposing equilibrium aqueous speciation, and adjusting pH to achieve charge balance. The revised analytical data were used to evaluate and interpret vertical and lateral variations in water chemistry, differences between unsaturated zone pore and perched water compositions, and water-rock equilibria. Page limitations inherent to the publication format, however, prevented Browning, et al. (2000) from providing the individual revised groundwater compositions used to support their work. This report presents revised analytical pore water compositions from the UE–25 UZ#16, USW UZ–14, USW SD7, USW SD9, USW SD12 boreholes at Yucca Mountain, after the approach outlined in Browning, et al. (2000).

REFERENCE

Browning, L., W.M. Murphy, B.W. Leslie, and W.L. Dam. "Thermodynamic Interpretations of Chemical Analyses of Unsaturated Zone Water from Yucca Mountain, Nevada." Scientific Basis for Nuclear Waste Management XXIII. R.W. Smith and D.W. Shoesmith, eds. Symposium Proceedings 608. Warrendale, Pennsylvania: Materials Research Society. pp. 237–242. 2000.

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ACKNOWLEDGMENTS

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QUALITY OF DATA, ANALYSES, AND CODE DEVELOPMENT

DATA: CNWRA-generated original data contained in this report meet quality assurance requirements described in the CNWRA Quality Assurance Manual. Sources for other data should be consulted for determining the level of quality for those data.

ANALYSES AND CODES: The EQ3 Version 7.2B code was used to conduct these analyses. EQ3 Version 7.2B is controlled in accordance with TOP–018.

1 INTRODUCTION

The current U.S. Department of Energy (DOE) safety strategy for the proposed high-level waste repository at Yucca Mountain, Nevada, relies on several key attributes, including long-lived waste packages and drip shields. The environment in the emplacement drifts may have a significant effect on the long-term performance of the engineered barriers. Environmental characteristics identified as important to long-term engineered barrier performance include temperature, chemistry of deliquescent salts, groundwater composition, concentration of trace elements in the host rock and groundwater, and evaporative concentration of dissolved salts (Brossia, et al., 2001).

The chemical compositions of ambient groundwater in Yucca Mountain are expected to evolve significantly before contacting drip shields and waste packages (Brossia, et al., 2001). Several different factors will control the composition of water as it percolates through the overlying rock into the emplacement drifts, including temperature, types of materials that interact chemically with the water along the flow pathway, flow velocity versus reaction rate, gas phase chemistry, and relative mass of condensate versus seepage waters. Predictions of the quantity and chemistry of water contacting the drip shields and waste packages during the 10,000-year compliance period for the proposed Yucca Mountain repository are difficult and must be accomplished by considering both analytical data and numerical models for a realistic set of conditions. Groundwater compositions collected from Yucca Mountain under both ambient and thermally perturbed conditions generally provide the cornerstone of efforts to calibrate or validate geochemical models to site-specific data to improve confidence in long-term performance models at Yucca Mountain. Groundwater chemistry affects performance through controls on container function, waste form alteration processes, solubility and speciation of radionuclides, and radionuclide transport. Performance models for these processes depend on accurate understanding of groundwater chemistry.

2 AMBIENT PORE WATER COMPOSITION

The chemical compositions of a large number of saturated zone, perched, and unsaturated zone groundwater samples have been reported from Yucca Mountain and vicinity (Kerrisk, 1987; Perfect, et al., 1995; Yang, et al., 1996, 1998). Browning, et al. (2000) evaluated the three types of groundwater data for internal thermodynamic consistency. To evaluate suggestions that the reliability of analytical pore water data may have been compromised during the extraction process (Yang, et al., 1988, 1996, 1998), the study focused on the analytical data for unsaturated zone matrix pore waters. Because of the low moisture content of the rocks, the unsaturated zone pore water samples had to be extracted from borehole core samples using potentially disruptive high-pressure uniaxial compression and vacuum distillation techniques. Browning, et al. (2000) found that the Yucca Mountain groundwaters analyzed using these methods contained significant ionic charge imbalances, unequilibrated aqueous speciation relationships, and erratic variations in some species concentrations with depth. The geochemical code EQ3NR (Wolery, 1992) was used to restore thermodynamic consistency to the analytical data by introducing measured CO_2 gas pressure as a constraint, imposing equilibrium aqueous speciation, and adjusting pH to achieve charge balance. Where analytical K^+ concentrations were not reported, K^+ concentrations were fixed at 14 mg/L [3.58 E-4 M], based on average UZ4-TP analyses from depths of 91 to 96 m [298.5–315 ft] (Yang, et al., 1988).

Site-specific groundwater compositions are routinely used in numerical simulations and experiments designed to predict the long-term performance of Yucca Mountain as a potential high-level waste disposal facility. Synthetic pore water compositions have been used in several DOE experiments—for example, to evaluate the potential for waste package and drip shield degradation in an aqueous environment (CRWMS M&O, 2000, 2001a; Rosenberg, et al., 2001). Analytical unsaturated zone groundwater compositions are instrumental to the initialization and validation of numerical simulations that predict seepage compositions for performance assessment calculations (CRWMS M&O, 2001b). The applicability of these studies to Yucca Mountain depends in part on the accuracy with which the unsaturated zone groundwater compositions have been represented. Although at least three different approaches have been used to generate sets of revised analytical pore water compositions (Apps, 1997; Browning, et al., 2000; CRWMS M&O, 2001b), few individual water compositions are available in the literature.

Here, we present the revised analytical groundwater compositions used by Browning, et al., (2000) to evaluate and interpret vertical and lateral variations in water chemistry, differences between unsaturated zone pore and perched water compositions, and water-rock equilibria at Yucca Mountain. Appendix A contains the full Browning, et al., (2000) paper. Appendix B contains the individual revised pore water compositions in tabular format. Sample identification nomenclature is taken from Yang, et al. (1996, 1998). Temperatures were estimated from the reported bore hole sampling depths and data in Sass and Lachenbruch (1982) to represent the geothermal gradient. Total carbonate, represented as mg/L HCO_3^-, was summed from the predominant dissolved carbon species. Where data for individual species concentrations are not indicated, the calculated concentrations were <1E-12 molal.

3 CONCLUSIONS

Collecting pore water compositions from the unsaturated zone at Yucca Mountain is technically challenging (Yang, et al., 1988), and the reported analytical pore water compositions typically contain charge imbalances, unequilibrated H^+-HCO_3^--CO_3^{2-} relationships, and erratic variability in species concentrations with depth (Browning, et al., 2000). Browning, et al. (2000) developed a method to restore internal thermodynamic consistency to the reported pore water compositions and were able to use the revised groundwater data to glean some insights into the ambient chemical system at Yucca Mountain. These analyses emphasized, for example, that significant vertical and lateral variations in solution composition, even within individual lithologic units, reflect complex changes in mineral composition that could, if ignored, affect the reliability of process-level and performance assessment models. Evaluation of the revised pore water data did not lead, however, to the identification of systematic trends that could fully account for inaccuracies in the raw analytical data. This evaluation suggests that sampling, extraction, compression, and chemical analysis procedures change solution compositions in ways that are incompletely understood.

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APPENDIX A

THERMODYNAMIC INTERPRETATIONS OF CHEMICAL ANALYSES OF UNSATURATED ZONE WATER FROM YUCCA MOUNTAIN, NEVADA

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ABSTRACT

Analytical pore water compositions from Yucca Mountain were evaluated for internal thermodynamic consistency. Significant ionic charge imbalances, unequilibrated aqueous speciation relationships, and erratic variability with depth in some species concentrations were found. Thermodynamic consistency was restored by introducing measured CO_2 gas pressure as a constraint, imposing equilibrium aqueous speciation, and adjusting pH to achieve charge balance. Reinterpreted water chemistry data were used to evaluate and interpret vertical and lateral variations in water chemistry, differences between unsaturated zone pore and perched water compositions, and water-rock equilibria.

INTRODUCTION

Understanding unsaturated zone (UZ) groundwater chemistry is necessary in predicting the long-term performance of Yucca Mountain as a possible high level nuclear waste disposal facility. The composition and evolution of UZ waters may affect corrosion of engineered barriers, waste form alteration, radionuclide release, retardation of radionuclide transport, dissolution/precipitation of minerals, and changes in porosity and permeability. Predictions of waste package failure times and radionuclide release rates are particularly sensitive to the evolution of carbonate ion concentration and pH [1]. Consequently, the quantity and chemistry of groundwater contacting the engineered barriers constitute a key element of subsystem abstraction for performance assessment. Ironically, it is difficult to obtain reliable groundwater compositions from unsaturated zone environments that may otherwise be desirable for isolation of nuclear waste.

Yang et al. [2,3] measured chemical compositions of pore water and perched water from Yucca Mountain. Perched waters were sampled from boreholes using plastic bailers and pore waters were extracted from borehole core samples using high-pressure uniaxial compression techniques. Although the accuracy of the resultant pore water chemistry data was unavoidably compromised by air drilling of core samples, pore water evaporation, and compression techniques [2,3], they provide a valuable characterization of groundwater chemistry at Yucca Mountain.

This paper describes equilibrium speciation calculations performed to characterize uncertainties in analytical pore water data [2,3]. We restore thermodynamic consistency to the data given a specific set of assumptions. Revised data were used to evaluate and interpret vertical and lateral variations in UZ groundwater chemistry in terms of water-rock equilibria and to compare unsaturated zone, saturated zone, and perched water compositions.

BACKGROUND: UNSATURATED ZONE WATER CHEMISTRY ANALYSES

Yang et al. [2,3] extracted pore waters from core samples from boreholes USW UZ-14 and UE-25 UZ#16, SD-7, SD-9, and SD-12. Stratigraphic units penetrated by the boreholes are (in descending order): the Paintbrush Group (comprising the Tiva Canyon Tuff, Yucca Mountain Tuff, Pah Canyon Tuff, and Topopah Spring Tuff), the Calico Hills Formation, and the Prow Pass Tuff. Perched water compositions from boreholes USW UZ-14, and SD-7, and extracted pore water compositions, were measured using ICP spectroscopy and ion chromatography.

Although the pore water analyses of Yang et al. [2,3] provide a valuable characterization of groundwater chemistry at Yucca Mountain, there are indications that aspects of the data are unreliable. Yang et al. [2,3] noted charge imbalances in the chemical analyses. In addition, Apps [4] concluded that measured pH values are inaccurate, based on inconsistencies of pH measurements of water from the J-13 well [5]. To correct pH, Apps [4] performed aqueous speciation calculations with EQ3 version7.2b [6] using analytical pore water chemistry from borehole USW UZ-14 to calculate pH assuming equilibrium with calcite. If these measurements and assumptions are correct, then the calculations of Apps [4] would restore charge balance without assigning an adjustable charge balancing species; however, the results showed an increase in charge imbalances from the values indicated by the analytical data. The range of analytical pH for pore waters extracted from similar depths within individual boreholes appears unreasonably wide. For example, in analyses from borehole UE-25 UZ#16, pH varies from 7.0 to 8.6 across a depth interval of less than 10 meters in the Calico Hills Formation. Erratic fluctuations in pH provide additional support for assertions that measured pH values are unreliable [4]. Similar abrupt variations are present in some reported major aqueous species concentrations. For example, analytical SiO_2 (aq) concentrations vary by a factor of more than 2.5 for samples extracted from approximately the same depth in borehole UE-25 UZ#16. Potassium occurs in primary and secondary phases at Yucca Mountain and is an important component of Yucca Mountain waters, but Yang et al. [2,3] did not always report K^+ concentrations. Finally, particulate aluminum in filtered samples resulted in unreliable Al concentrations [2]. Clearly, uncertainty in pore water analyses of Yang et al. [2,3] requires further evaluation.

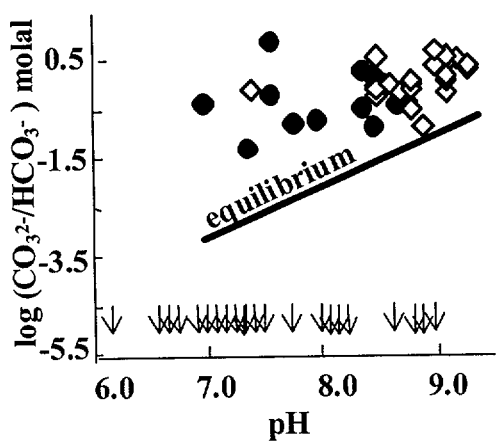

Figure 1. Analytical pore water compositions from boreholes UE-25 UZ#16 [2] (circles) and SD-7, SD-9, SD-12, NRG-6, and NRG-7a [3] (diamonds) are inconsistent with equilibrium aqueous speciation relations for the reaction $H^+ + CO_3^{2-} \Leftrightarrow HCO_3^-$. Equilibrium line calculated for 25°C. Arrows indicate all data with no reported CO_3^{2-}.

Gas samples collected from boreholes in the unsaturated zone at Yucca Mountain since 1983 [2,7] provide additional insight about the groundwater environment. After an initial stabilization period following borehole drilling, measured gas phase concentrations at any given depth remained remarkably constant with time. Measured CO_2(g) pressures are about four times atmospheric throughout most of the Topopah Spring Tuff, and are significantly higher in the Tiva Canyon and lower Topopah Spring Tuff. Biological

activity is probably responsible for the elevated near-surface $CO_2(g)$ pressures [7], and the higher $CO_2(g)$ pressures near the bottom probes may be the result of drilling-fluid contamination [2].

REEVALUATION AND REVISION OF WATER CHEMISTRY ANALYSES

We performed aqueous speciation calculations using the code EQ3 version 7.2b [6] demonstrating that analytical pH and associated CO_3^{2-}/HCO_3^- ratios are inconsistent with chemical equilibrium. Figure 1 shows that analytical values for log $[CO_3^{2-}/HCO_3]$ (molal) vs. pH do not lie on the line defined by mass action equations for the pH dependent speciation of C-bearing solutions. Moreover, many pore water analyses with high reported pH contain significant HCO_3^-, but CO_3^{2-}data are not reported. Only low pressure extractions from borehole UE25 UZ#16 were used for pH analysis, but pH values were reported for water extracted over a larger range of extraction pressures for boreholes SD-7, SD-9, SD-12, NRG-6, and NRG-7a [3]. Both techniques result in unequilibrated aqueous speciation relations. Similar problems in carbonate speciation and pH appear with perched water data of Yang et al. [2], but to a smaller degree.

Downhole gas measurements at Yucca Mountain indicate that $CO_2(g)$ pressures in the UZ are higher than atmospheric [2], suggesting that $CO_2(g)$ loss during the extraction and/or chemical processes may have contributed to the thermodynamic inconsistencies demonstrated in Figure 1. However, $CO_2(g)$ loss cannot explain either the apparent absence of CO_3^{2-} in HCO_3^--rich alkaline solutions or the lack of ionic charge balance described in [2,3], because rapid equilibration of aqueous carbonate speciation reactions is expected. A loss of $CO_2(g)$ would shift pH to higher values along the equilibrium line. One possible explanation for data lying above the equilibrium line is that $CO_2(g)$ loss occurred after the pH measurement, but before measurement of aqueous carbonate species concentrations. In this case, analytical carbonate species concentrations would reflect equilibration at a higher pH than was originally measured, increasing the CO_3^{2-}/HCO_3^- concentration.

To restore thermodynamic consistency to the pore water analyses, equilibrium aqueous speciation calculations were performed by introducing measured CO_2 gas pressure as a constraint and imposing electroneutrality by adjustment of pH. A $CO_2(g)$ concentration of 0.12 percent (1.02e-3 bar) was adopted in this study to constrain carbonate chemistry equilibria. This value is consistent with measured $CO_2(g)$ concentrations in the Topopah Spring Formation from borehole USW UZ-1 [2] and a total pressure of 0.85 bar. Where K^+ data do not exist, its concentration was fixed at 14 mg/L, based on average UZ4-TP analyses from depths of 91 to 96 m [8]. Sensitivity studies showed that pH values calculated based on charge balance were insensitive to reasonable variations in estimated K^+ concentration. Temperatures used in these calculations (20°-34°C) were estimated from the geothermal gradient [9].

The main assumptions of this approach are that $CO_2(g)$ pressures were constant throughout the sampled intervals and that the major analytical ionic concentrations (except for C-bearing species) are reliable. We judge that measured gaseous CO_2 pressures more accurately constrain carbonate chemistry equilibria in unsaturated groundwaters than analytical aqueous HCO_3^-, CO_3^{2-}, or pH values. Both aqueous carbonate species and pH are difficult to measure for pore waters from unsaturated rocks and are demonstrated to be thermodynamically inconsistent. It is reasonable to expect that equilibration was achieved between gaseous CO_2 and carbonate species in pore waters extracted from high porosity zones of unsaturated nonwelded tuffs. The apparent disequilibrium between measured $CO_2(g)$ pressures from fractures and HCO_3^- pore water concentrations noted by Yang et al. [2] may be explained by inaccuracies in analytical carbonate species concentrations.

Perched water analyses were interpreted differently because these data appear more reliable than pore water analyses - likely because standard extraction procedures yield sufficient volumes of perched water for analyses. However, charge imbalances and deviations from equilibrium in the HCO_3^--CO_3^{2-}-H^+ system were corrected by minor adjustment of HCO_3^- concentrations.

RESULTS AND DISCUSSION

Revised Pore Water Compositions

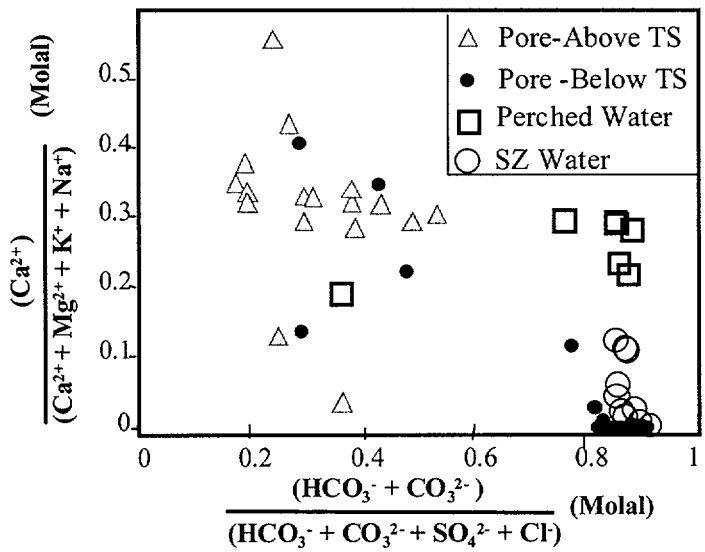

Figure 2. Comparison between revised pore water and perched water compositions from borehole USW UZ-14 [2] and saturated zone water compositions from Yucca Mountain [10]. Pore water compositions below and above the Topopah Spring (TS) have different symbols.

Revised water chemistry differs from analytical data by maintaining theoretical thermodynamic equilibrium in terms of aqueous speciation and electrical neutrality and having different total H^+ and total carbonate concentrations. Revised solution compositions from the Calico Hills Formation exhibit a slightly larger total carbonate concentration than the analytical pore water. However, the general trend in pore water composition from calcium sulfate or calcium chloride types in the Paintbrush Group to sodium bicarbonate types in the Calico Hills Formation reported by Yang et al. [2,3] is preserved (Figure 2). Figure 3 compares the pH distribution of the analytical data, the reinterpretation of [4], and this work for borehole UE-25 UZ#16. The method used by Apps [4] shifts the average pH upward to about 8.2, but does not tighten the range in reported pH. The method used by Apps [4] also does not reduce erratic variability of pH over small vertical distances. The approach introduced in this work reduces variability of pH and shifts the average pH to approximately 8.2. If natural pH varies smoothly with depth, then these results support the assumption of constant $CO_2(g)$ used in our calculations and the presence of drilling-fluid contaminants in the lower gas probes [2].

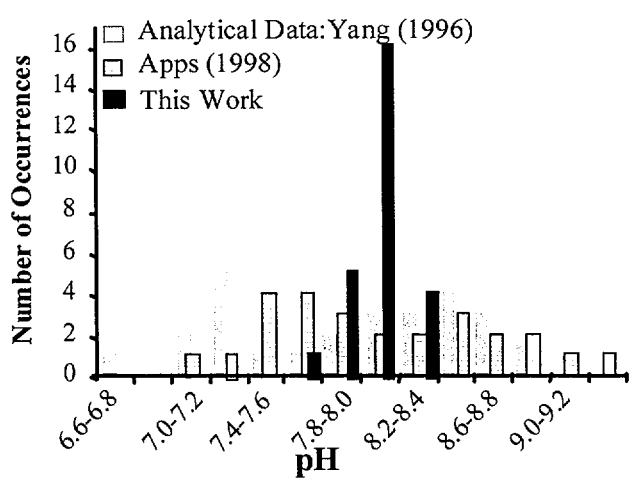

Figure 3. Distribution of pH in borehole UE-25 UZ#16.

Differences between Saturated, Perched, and Unsaturated Water Compositions

Kerrisk [10] and Murphy [11] concluded that saturated zone tuffaceous aquifer groundwaters are generally undersaturated with respect to calcite. Murphy [11] bolstered this observation using reported data for isotopic compositions of calcites and groundwaters and the absence of occurrence of calcite in rocks from groundwater producing zones in boreholes. In general, saturated zone groundwaters from the vicinity of Yucca Mountain have calculated equilibrium CO_2 fugacities (10^{-2}-10^{-3} bar) in excess of atmospheric values and in excess of values measured in the gas phase from the unsaturated zone at Yucca Mountain [10]. Measurements of pH of saturated zone groundwaters are subject to uncertainties because of the potential for degassing of CO_2 during groundwater collection, and other analytical errors, and a variety of reported pH values for these groundwaters is unsurprising. Nevertheless, interpretation of data taken from Kerrisk [10] for saturated zone waters in the vicinity of Yucca Mountain demonstrates a consistent pattern of elevated CO_2 pressure, minimal charge imbalance (when speciated at groundwater collection temperatures), and undersaturation with respect to calcite [11]. Reinterpreted perched water compositions exhibit these same characteristics.

Figure 2 compares the compositions of groundwaters from the saturated zone in the vicinity of Yucca Mountain reported by Kerrisk [10] with perched and pore water data for borehole USW UZ-14. Below the Topopah Spring Tuff, the concentrations of SO_4^{2-},Ca^{2+}, and Mg^{2+}, which are probably derived predominantly from the ground surface, are significantly diminished. The compositions of perched waters, deep pore waters, and saturated zone waters differ from near-surface pore waters by low relative proportions of Ca^{2+} and high proportions of total carbonate relative to other anions. Despite possible differences in their flow pathways and residence times, these three groundwater types have evolved to similar compositions. Pore waters are generally more concentrated than perched waters, and pore water concentrations increase with depth [2]. The Cl^- concentrations in perched waters and saturated zone waters are lower than in the adjacent pore waters, which led Yang et al. [2] to conclude that perched waters experienced less water-rock interaction and therefore must be supplied by fast fracture flow. Although perched waters may be supplied predominantly by fracture flow, Cl^- is unlikely to be affected strongly by water-rock interactions. Elevated pore water concentrations might be an artifact of the compression techniques used to extract the waters from unsaturated zone core for chemical analysis. Compression techniques were not used to collect either perched or saturated zone waters. Evaporation would cause unsaturated zone pore waters to become more concentrated, particularly in nonvolatile anions, but would have a lesser effect on adjacent perched waters replenished by fast pathway fracture flow.

Lateral and Vertical Variations in Mineral Saturation States

Thermodynamically interpreted groundwater compositions were used to infer mineralogical controls in the UZ at Yucca Mountain. Average calcite saturation states (log Q/K) are close to 0 for pore waters collected from individual boreholes - consistent with the assumption of Apps [4]. For example, log Q/K values for calcite average 0.133 in borehole UE-25 UZ#16 and –0.132 in borehole USW UZ-14. These averages, however, mask scatter in log Q/K values between +/- 0.5. Calcite is not ubiquitously present in geologic formations throughout the UZ at Yucca Mountain [12], and it is possible that pore waters undersaturated in calcite were extracted from rocks lacking calcite. Supersaturation with respect to calcite is more difficult to explain. No systematic variations occur between the saturation state of calcite and either depth or the analytical charge imbalances [2,3] which might belie our assumption

of constant $CO_2(g)$ pressures. Dissolved SiO_2 concentrations in most samples remain close to cristobalite saturation.

To explore potential relationships between vertical and lateral variations in groundwater chemistry and clinoptilolite compositions at Yucca Mountain, we estimated clinoptilolite compositions assuming equilibrium with extracted pore waters from boreholes USW UZ-14 and UE-25 UZ#16. Clinoptilolite at Yucca Mountain exhibits cation variations mainly among the major components K, Na, and Ca [13]. Unfortunately, most pore water analyses of Yang et al. [2,3] provide no information on K^+. We therefore focused on clinoptilolite-water exchange reactions among Na and Ca. Free ion concentrations of Ca^{2+} and Na^+ were used to calculate the Na to Ca ratio in clinoptilolite according to equilibrium for the reaction $Na_2Al_2Si_{10}O_{24}{:}8H_2O + Ca^{2+} \Leftrightarrow CaAl_2Si_{10}O_{24}{:}8H_2O + 2\ Na^+$.

Two approaches were used to calculate Na-Ca exchange in clinoptilolite. First, estimated thermodynamic data for endmember Ca- and Na-clinoptilolite [14] were used to calculate log K of the exchange reaction. These data were found reasonable in simulations of the natural geochemical system at Yucca Mountain [15]. Despite significant variations in the Ca^{2+}/Na^+ ratio of pore waters with depth, corresponding clinoptilolite compositions estimated in this manner remained close to the Ca-endmember composition. This result is inconsistent with observed clinoptilolite compositions [13], suggesting inaccuracies in the estimated thermodynamic data. An alternate approach, using the standard Gibbs free energy of ion exchange derived from experimental data at 25°C [16], produced estimated clinoptilolite compositions that more closely match observations.

Figure 4 shows estimated clinoptilolite compositions from boreholes UE-25 UZ#16 and USW UZ-14 superimposed on diagrams of log $(mCa^{2+}/m(Na^+)^2)$ versus depth. These boreholes are located on the eastern and western sides of Yucca Mountain, respectively. Clinoptilolite compositions were calculated assuming unit aqueous activity coefficients, ideal binary Ca-Na_2 (Gapon model) solid solution, and the standard Gibbs free energy of Ca-Na ion exchange consistent with data from [16]. Pore water compositions from both boreholes show a sharp decrease in $mCa^{2+}/m(Na^+)^2$ free ion ratios down to the base of the Calico Hills Formation. This trend indicates that Ca^{2+} is supplied to the pore waters from a near-surface environment and is progressively depleted in concentration with depth due to the precipitation of Ca-bearing minerals [2,15]. Estimated clinoptilolite compositions vary sympathetically, becoming increasingly sodic with depth in the Calico Hills Formation. Estimated Calico Hills clinoptilolite compositions from the eastern and western boreholes are consistent with "representative clinoptilolite compositions" in the Calico Hills Formation from the eastern and western sides

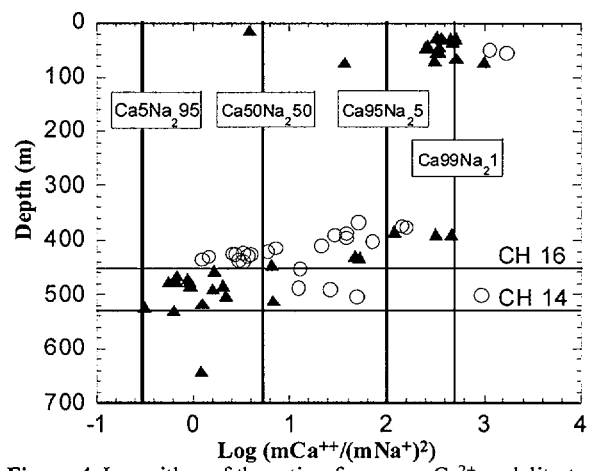

Figure 4. Logarithm of the ratio of aqueous Ca^{2+} molality to the square of aqueous Na^+ molality plotted versus depth from the ground surface for pore waters from boreholes USW UZ-14 (triangles) and UE-25 UZ#16 (circles). Vertical lines represent clinoptilolite solid solution compositions in mole percent binary Ca-Na_2 endmember components at equilibrium with solution composition ratios on the abscissa. Horizontal lines mark approximate depths of the base of the Calico Hills Formation (CH) in the two boreholes.

of Yucca Mountain [13]. However, systematic variations in pore water composition with depth imply that clinoptilolite compositions vary significantly within individual lithologic units. This argues against the applicability of "representative" clinoptilolite compositions [13]. Our calculations show a return to more Ca-rich clinoptilolite compositions below the Calico Hills Formation on the eastern side of Yucca Mountain (UE-25 UZ#16), as observed by Broxton et al. [13]. However, Broxton et al. [13] also report a general trend in western boreholes toward more calcic clinoptilolite compositions with depth beginning at the Calico Hills Formation, which is not evident in Figure 4 (USW UZ-14). Estimated clinoptilolite compositions vary both laterally and vertically in ways that are difficult to generalize in large-scale trends.

CONCLUSIONS

Reported pore water compositions at Yucca Mountain [2,3] contain charge imbalances, unequilibrated H^+-HCO_3^--CO_3^{2-} relationships, and erratic variability in species concentrations with depth. No systematic trends were identified in the inaccuracies, suggesting that extraction, compression, and/or chemical analysis procedures change solution compositions in ways that are incompletely understood. Internal thermodynamic consistency was restored to the data by fixing the CO_2 gas pressure at measured values, imposing electroneutrality by adjustment of pH, introducing a reasonable K^+ concentration, and recalculating equilibrium aqueous speciation relations at inferred in- situ temperatures. This approach reduced erratic variability in pH values with depth and shifted pH values to approximately 8.2. Revised pore water compositions provide useful information about the UZ mineralogy at Yucca Mountain. Significant vertical and lateral variations in solution composition, even within individual lithologic units, reflect complex changes in mineral composition that could, if ignored, affect the reliability of process-level and performance assessment models. Browning et al. [17] show, for example, that mineral and infiltrating fluid compositions have an important effect on the results of reactive transport simulations of gas-water-rock interactions at Yucca Mountain under both ambient steady state and thermally transient conditions. Sensitivity of repository performance to these chemical variations, both in the ambient setting and under thermally perturbed conditions, should be addressed.

ACKNOWLEDGMENTS

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APPENDIX B

Table of Revised Analytical Pore Water Compositions from the Unsaturated Zone at Yucca Mountain, Nevada								
[1]Sample Identification	References: Analytical Data	Depth (m)	[2]Temperature (C)	Total Carbonate as HCO_3. (mg/L)	pH	Eh	a H_2O	Ionic Strength
1	2	3	4	5	6	7	8	9
UZ-16/163.5-163.9	3	49.90	20.30	104.73	7.96	0.76	1.00	0.01
UZ-16/180.9-181.3	3	55.20	20.40	149.97	8.11	0.75	1.00	0.01
UZ-16/1166.19-1166.47	3	367.74	25.95	182.19	8.23	0.73	1.00	0.01
UZ-16/1227,4-1227.7	3	374.17	26.06	161.20	8.18	0.73	1.00	0.01
UZ-16/1235.1-1235.41	3	376.52	26.11	146.32	8.14	0.73	1.00	0.01
UZ-16/1269,6-1269,9	3	387.04	26.29	172.25	8.22	0.73	1.00	0.00
UZ-16/1280.4-1280.8	3	390.33	26.35	246.69	8.37	0.72	1.00	0.01
UZ-16/1296.8-1297.06	3	395.33	26.44	339.14	8.49	0.71	1.00	0.01
UZ-16/1317.9-1318.2	3	401.76	26.55	166.08	8.20	0.73	1.00	0.01
UZ-16/1343.7-1344.0	3	409.62	26.69	198.13	8.28	0.73	1.00	0.01
Z-16/1358.0-1358.4	3	413.98	26.77	155.36	8.18	0.73	1.00	0.00
Z-16/1379.6-1379.9	3	420.56	26.89	196.50	8.28	0.72	1.00	0.01
Z-16/1389.3-1389.6	3	423.52	26.94	243.92	8.37	0.72	1.00	0.01
Z-16/1395.5-1395.9	3	425.41	26.97	358.12	8.53	0.71	1.00	0.01
UZ-1397.7-1398.0	3	426.08	26.99	196.01	8.27	0.72	1.00	0.01
UZ-16/1398.5-1398.7	3	426.29	26.99	329.81	8.50	0.71	1.00	0.01
UZ-16/1408.2-1408.6	3	429.28	27.04	229.52	8.35	0.72	1.00	0.01
UZ-16/1412.9-1413.2	3	430.71	27.07	183.21	8.25	0.73	1.00	0.01
UZ-16/1428.1-1428.4	3	435.35	27.15	282.18	8.43	0.71	1.00	0.01
UZ-16/1434.2-1434.6	3	437.21	27.18	235.92	8.36	0.72	1.00	0.01
UZ-16/1442.8-1443.2	3	439.83	27.23	177.56	8.24	0.73	1.00	0.00
UZ-16/1486.9-1487.3	3	453.27	27.47	120.95	8.07	0.74	1.00	0.00
UZ-16/1601.1-1601.5	3	488.08	28.09	177.76	8.24	0.72	1.00	0.01
UZ-16/1607.7-1608.1	3	490.09	28.12	206.41	8.30	0.72	1.00	0.01
UZ-16/1643.4-1647.2	3	501.49	28.33	264.83	8.39	0.72	1.00	0.01
UZ-16/1651.6-1651.7	3	503.44	28.36	169.86	8.22	0.72	1.00	0.00
UZ-14;45.0-45.4/up1	3	13.78	19.66	269.14	8.35	0.73	1.00	0.01
UZ-14/85.2-85.6/up1	3	26.03	19.88	145.13	8.09	0.75	1.00	0.01

Table of Revised Analytical Pore Water Compositions from the Unsaturated Zone at Yucca Mountain, Nevada								
[1]Sample Identification	References: Analytical Data	Depth (m)	[2]Temperature (C)	Total Carbonate as HCO_{3-} (mg/L)	pH	Eh	a H_2O	Ionic Strength
UZ-14/91.0-91.3/up1	3	27.80	19.91	86.68	7.87	0.76	1.00	0.01
UZ-14/95.5-95.9/up1	3	29.17	19.94	82.70	7.84	0.76	1.00	0.01
UZ-14/96.2-96.6/up1	3	29.38	19.94	96.00	7.91	0.76	1.00	0.01
10	**11**	**12**	**13**	**14**	**15**	**16**	**17**	**18**
UZ-14/100.4-100.8/up1	3	30.66	19.96	151.29	8.11	0.75	1.00	0.01
UZ-14/114.8-115.0/up1	3	35.02	20.04	76.31	7.81	0.76	1.00	0.01
UZ-14/135.5-135.8/up1	3	41.36	20.15	161.85	8.13	0.75	1.00	0.01
UZ-14/144.8-145.2/up1	3	44.20	20.20	125.35	8.02	0.75	1.00	0.01
uz-14/147.7-148.1/up1,2	3	45.08	20.20	90.21	7.88	0.76	1.00	0.01
UZ-14/177.6-177.9/up1	3	54.19	20.38	56.05	7.67	0.77	1.00	0.01
UZ-14/178.1-178.4/up1	3	54.35	20.38	61.65	7.71	0.77	1.00	0.01
UZ-14/215.7-216.1/up2	3	65.81	20.59	55.90	7.67	0.77	1.00	0.01
UZ-14/225.9-226.2/up1	3	68.92	20.64	59.28	7.70	0.77	1.00	0.01
UZ-14/235.1-235.4/up1	3	71.72	20.69	78.00	7.82	0.76	1.00	0.01
UZ-14/240.8-241.1/up1	3	73.46	20.72	82.50	7.85	0.76	1.00	0.01
UZ-14/245.5-245.8/up1	3	74.89	20.75	60.89	7.71	0.77	1.00	0.01
UZ-14/1258.5-1258.8/up1vb	3	383.65	26.23	156.12	8.16	0.73	1.00	0.01
UZ-14/1277.4-1277.7/up1	3	389.41	26.33	138.06	8.11	0.74	1.00	0.01
UZ-14/1277.7-1278.0/up1	3	389.50	26.33	105.14	7.99	0.74	1.00	0.01
UZ-14/1409.4-1409.8/up1	3	429.65	27.05	81.99	7.89	0.75	1.00	0.01
UZ-14/1419.5-1419.8/up1	3	432.72	27.10	186.44	8.26	0.73	1.00	0.01
UZ-14/1461.9-1462.1/up1	3	445.62	27.33	285.29	8.44	0.71	1.00	0.01
UZ-14/1495.8-1496.0/up1	3	455.95	27.52	269.36	8.42	0.72	1.00	0.01
UZ-14/1524.55-1524.75/up1	3	464.73	27.67	295.03	8.46	0.71	1.00	0.01
UZ-14/1542.3-1542.8/up1,2,3	3	470.18	27.77	457.29	8.63	0.70	1.00	0.01
UZ-14/1563.6-1563.8/up1,2,3	3	476.62	27.88	347.64	8.53	0.71	1.00	0.01
UZ-14/1564.6-1564.8/up1,2,3	3	476.92	27.89	285.58	8.44	0.71	1.00	0.01
UZ-14/1564.9-1565.0/up1	3	477.01	27.89	355.16	8.53	0.71	1.00	0.01
UZ-14/1585.0-1585.2/up1	3	483.14	28.00	249.76	8.39	0.72	1.00	0.01

Table of Revised Analytical Pore Water Compositions from the Unsaturated Zone at Yucca Mountain, Nevada								
[1]Sample Identification	References: Analytical Data	Depth (m)	[2]Temperature (C)	Total Carbonate as HCO_{3-} (mg/L)	pH	Eh	a H_2O	Ionic Strength
UZ-14/1585.3-1585.6/up1,5	3	483.23	28.00	178.81	8.25	0.72	1.00	0.00
UZ-14/1605.9-1606.1/up1	3	489.51	28.11	195.17	8.29	0.72	1.00	0.00
UZ-14/1644.3-1644.5/up1	3	501.21	28.32	215.60	8.33	0.72	1.00	0.01
UZ-14/1674.8-1675.1/up1	3	510.54	28.49	111.82	8.05	.74	1.00	0.00
UZ-14/1695.4-1695.6/up1	3	516.79	28.60	238.44	8.37	0.72	1.00	0.01
UZ-14/1715.0-1715.3/up1	3	522.79	28.70	208.23	8.32	0.72	1.00	0.00
19	**20**	**21**	**22**	**23**	**24**	**25**	**26**	**27**
UZ-14/1734.5-1734.7/up1	3	528.71	28.81	409.14	8.60	0.70	1.00	0.01
UZ-14/2104.05/well bottom	3	641.33	30.81	256.49	8.41	0.71	1.00	0.01
SD7-339.7-340.2/PTn/BT	4	103.63	21.26	244.56	8.31	0.73	1.00	0.01
SD71498.4-1498.6/CHn	4	456.74	27.53	211.24	8.31	0.72	1.00	0.01
SD7-1524.6-1525.7/CHn	4	464.85	27.67	197.24	8.28	0.72	1.00	0.01
SD-7/1558.4-1558.6CHn	4	475.03	27.86	184.20	8.25	0.72	1.00	0.01
SD-7/1600.1-1600.3/CHn	4	487.74	28.08	174.44	8.23	0.72	1.00	0.00
SD-7/1617.0-1617.2/CHn	4	492.87	28.17	209.96	8.30	0.72	1.00	0.01
SD-7/1890.9/CHn/PP	4	576.35	29.65	500.74	8.69	0.69	1.00	0.01
SD-7/1952.6/CHn/PP	4	595.15	29.99	601.60	8.76	0.69	1.00	0.01
SD-7/2088.2-2088.5/PP	4	636.54	30.72	406.03	8.61	0.70	1.00	0.01
SD-7/2170.1-2170.5/PP/BT	4	661.51	31.17	387.00	8.59	0.70	1.00	0.01
SD-7/2596.1-2596.3/BF	4	791.28	33.47	274.99	8.46	0.70	1.00	0.01
SD-7/2596.5-2596.9/BF	4	791.47	33.47	309.20	8.51	0.70	1.00	0.01
SD72598.3-2598.5/BF	4	791.95	33.48	348.89	8.56	0.70	1.00	0.01
SD-9/94.2-94.4/PTn/BT	4	28.70	19.93	10.80	6.85	0.82	1.00	0.02
SD-9/114.1-114.3/PTn/YM	4	38.81	20.11	70.63	7.76	0.77	1.00	0.01
SD-9/135.1-135.3/PTn/YM	4	41.21	20.15	84.94	7.85	0.76	1.00	0.01
SD-9/154.0-154.2/PTn/BT	4	46.97	20.25	103.13	7.94	0.76	1.00	0.01
SD-9/176.2-176.4/PTn/PV	4	53.74	20.37	181.28	8.19	0.74	1.00	0.01
SD-9/251.8-252.0/PTn/BT	4	76.78	20.78	126.77	8.04	0.75	1.00	0.01
SD-9/1452.6-1452.8/Tsw	4	442.78	27.28	219.74	8.33	0.72	1.00	0.01
SD-9/1535.2-1535.4/CHn	4	467.96	27.73	250.06	8.39	0.72	1.00	0.01
SD-9/1619.9-1661.4/CHn	4	500.09	28.30	247.28	8.38	0.72	1.00	0.01

Table of Revised Analytical Pore Water Compositions from the Unsaturated Zone at Yucca Mountain, Nevada								
[1]Sample Identification	References: Analytical Data	Depth (m)	[2]Temperature (C)	Total Carbonate as HCO_{3-} (mg/L)	pH	Eh	a H_2O	Ionic Strength
SD-9/1661.1-1661.3/CHn	4	506.33	28.41	346.27	8.53	0.71	1.00	0.01
SD-9/1741.0-1741.2/CHn	4	0.69	28.84	298.15	8.47	0.71	1.00	0.01
SD-9/1741.7-1741.9/CHn	4	530.90	28.85	176.68	8.25	0.72	1.00	0.00
SD-9/1800.8/CHn/BT	4	548.88	29.17	392.42	8.58	0.70	1.00	0.01
SD-12/265.8-266.1/PTn/BT	4	81.08	20.86	106.79	7.97	0.75	1.00	0.01
SD-12/278.6-278.8/PTn/pc	4	84.95	20.93	188.91	8.21	0.74	1.00	0.01
SD-12/296.1-1296.6/TSnw	4	90.34	21.02	194.55	8.22	0.74	1.00	0.01
SD-12/1460.7-1461.0/CHn	4	445.28	27.33	206.31	8.29	0.72	1.00	0.01
SD-12/1495.5-1495.8/CHn	4	455.89	27.52	179.13	8.24	0.73	1.00	0.01
28	**29**	**30**	**31**	**32**	**33**	**34**	**35**	**36**
SD-12/1517.0-1517.4/CHn	4	462.44	27.52	355.25	8.53	0.71	1.00	0.01
SD-12/1558.9-1559.5/CHn	4	475.24	27.63	312.91	8.48	0.71	1.00	0.01
SD-12/1582.5-1582.7/CHn	4	482.38	27.99	212.24	8.32	0.72	1.00	0.00
SD-12/1600.6-1603.0/CHn	4	488.23	28.09	298.67	8.46	0.71	1.00	0.01
SD-12/1636.9/CHn/BT	4	498.93	28.28	325.13	8.50	0.71	1.00	0.01
SD-12/1901.5/CHn/PP	4	579.55	29.71	286.28	8.46	0.71	1.00	0.01
SD-12/1938.8/CHn/PP	4	590.93	29.71	360.85	8.55	0.70	1.00	0.01
SD-12/1942.4/CHn/PP	4	592.04	29.93	313.45	8.50	0.71	1.00	0.01

Al(OH)2+	Al+++	Al13O4(OH)24(7+)	AlO2-	AlOH++	Ca++	CaCl+	CaCl2(aq)	CaCO3(aq)	CaHCO3+	CaNO3+	CaOH+	CaSO4(aq)	Cl-	CO2(aq)	CO3--
Log Molal	Log Molal	Log Molal	Log Molal	Log Molal	Log Molal	Log Molal	Log Molal	Log Molal	Log Molal	Log Molal	Log Molal	Log Molal	Log Molal	Log Molal	Log Molal
1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16
-8.13			-4.75	-10.20	-3.00	-6.88	-9.92	-5.10	-4.88	-5.87	-8.00	-4.37	-3.04	-4.40	-5.10
-9.14			-5.44	-11.37	-2.89	-6.70	-9.67	-4.68	-4.62	-5.61	-7.73	-4.54	-2.97	-4.40	-4.78
					-3.17	-6.66	-9.32	-4.67	-4.82	-6.19	-7.91	-4.96	-2.64	-4.47	-4.52
-9.09			-4.96	-11.56	-3.21	-7.20	-10.39	-4.77	-4.89	-6.07	-7.97	-4.97	-3.17	-4.47	-4.63
					-3.10	-6.77	-9.63	-4.76	-4.83	-5.92	-7.92	-4.84	-2.83	-4.47	-4.71
					-3.48	-7.42	-10.56	-4.96	-5.12	-6.44	-8.21	-5.48	-3.12	-4.48	-4.57
-8.77			-4.26	-11.43	-3.34	-7.27	-10.41	-4.54	-4.84	-6.29	-7.92	-5.24	-3.10	-4.48	-4.25
					-3.16	-6.87	-9.76	-4.13	-4.55	-6.14	-7.64	-5.17	-2.85	-4.48	-3.98
-8.58			-4.40	-11.09	-3.32	-7.19	-10.25	-4.83	-4.98	-6.24	-8.06	-5.23	-3.04	-4.48	-4.60
-8.55			-4.21	-11.12	-3.41	-7.04	-9.88	-4.79	-5.00	-6.39	-8.09	-5.23	-2.80	-4.48	-4.44
-8.55			-4.40	-11.05	-4.10	-8.10	-11.31	-5.64	-5.77	-7.10	-8.86	-5.94	-3.19	-4.48	-4.65
-8.38			-4.02	-10.98	-4.00	-8.05	-11.30	-5.35	-5.58	-6.96	-8.66	-5.74	-3.23	-4.48	-4.44
-8.68			-4.13	-11.36	-4.09	-8.10	-11.31	-5.28	-5.59	-7.06	-8.68	-5.88	-3.18	-4.48	-4.25
-8.71			-3.84	-11.54	-3.95	-8.11	-11.47	-4.83	-5.30	6.99	-8.38	-5.80	-3.32	-4.48	-3.91
-8.12			-3.76	-10.70	-3.94	-7.68	-10.61	-5.32	-5.55	-6.78	-8.63	-5.47	-2.90	-4.48	-4.44
-8.34			-3.54	-11.14	-3.97	-8.22	-11.66	-4.91	-5.36	-7.01	-8.44	-5.86	-3.40	-4.48	-3.99
-8.41			-3.90	-11.07	-4.13	-8.20	-11.48	-5.35	-5.65	-7.21	-8.73	-6.07	-3.25	-4.49	-4.30
-8.75			-4.44	-11.32	-4.56	-8.52	-11.68	-5.97	-6.17	-7.40	-9.26	-6.22	-3.14	-4.49	-4.50
-8.58			-3.90	-11.33	-4.38	-8.41	-11.63	-5.44	-5.82	-7.34	-8.90	-6.19	-3.19	-4.49	-4.12
-8.18			-3.65	-10.86	-4.14	-8.16	-11.38	-5.34	-5.66	-7.17	-8.74	-6.02	-3.19	-4.49	-4.28
-8.66			-4.36	-11.23	-4.40	-8.49	-11.78	-5.82	-6.02	-7.56	-9.10	-6.38	-3.27	-4.49	-4.53
-7.06		-5.02	-3.08	-9.46	-3.82	-7.61	-10.60	-5.58	-5.61	-7.26	-8.69	-5.91	-2.97	-4.49	-4.86
-8.93			-4.59	-11.52	-3.64	-7.29	-10.15	-5.06	-5.27	-6.75	-8.35	-5.36	-2.83	-4.50	-4.51
-8.89			-4.44	-11.53	-3.24	-6.78	-9.52	-4.57	-4.83	-6.49	-7.91	-4.92	-2.70	-4.50	-4.38
-8.60			-3.96	-11.31	-2.69	-6.26	-9.02	-3.86	-4.21	-6.05	-7.28	-4.53	-2.70	-4.50	-4.18
-8.91			-4.59	-11.50	-3.40	-7.33	-10.48	-4.84	-5.04	-6.84	-8.11	-5.23	-3.12	-4.50	-4.55
-8.58			-4.44	-10.98	-3.35	-6.40	-8.59	-4.72	-4.87	-6.09	-7.99	-5.15	-2.16	-4.39	-4.26
-8.60			-4.97	-10.79	-2.93	-6.56	-9.33	-4.78	-4.69	-5.84	-7.81	-4.37	-2.77	-4.40	-4.81
					-3.02	-6.74	-9.62	-5.30	-4.99	-5.84	-8.11	-4.34	-2.88	-4.40	-5.27
					-2.90	-6.41	-9.06	-5.24	-4.90	-5.69	-8.02	-4.24	-2.65	-4.40	-5.31
					-2.96	-6.59	-9.36	-5.15	-4.88	-5.79	-8.01	-4.33	-2.78	-4.40	-5.18
					-2.93	-6.69	-9.60	-4.74	-4.66	-5.82	-7.78	-4.27	-2.91	-4.40	-4.78
					-2.94	-6.55	-9.32	-5.34	-4.97	-5.79	-8.09	-4.23	-2.76	-4.40	-5.38
					-2.80	-6.30	-8.95	-4.58	-4.53	-5.71	-7.65	-4.12	-2.63	-4.40	-4.71
					-2.82	-6.35	-9.02	-4.80	-4.65	-5.74	-7.77	-4.09	-2.66	-4.40	-4.94

Al(OH)2+	Al+++	Al13O4(OH)24(7+)	AlO2-	AlOH++	Ca++	CaCl+	CaCl2(aq)	CaCO3(aq)	CaHCO3+	CaNO3+	CaOH+	CaSO4(aq)	Cl-	CO2(aq)	CO3--
Log Molal	Log Molal	Log Molal	Log Molal	Log Molal	Log Molal	Log Molal	Log Molal	Log Molal	Log Molal	Log Molal	Log Molal	Log Molal	Log Molal	Log Molal	Log Molal
					-2.89	-6.38	-9.02	-5.16	-4.86	-5.81	-7.98	-4.15	-2.63	-4.40	-5.22
					-2.80	-6.22	-8.78	-5.50	-4.99	-5.71	-8.11	-3.98	-2.55	-4.40	-5.64
					-2.83	-6.25	-8.83	-5.43	-4.97	-5.77	-8.09	-4.03	-2.56	-4.40	-5.56
17	**18**	**19**	**20**	**21**	**22**	**23**	**24**	**25**	**26**	**27**	**28**	**29**	**30**	**31**	**32**
					-2.82	-6.30	-8.93	-5.50	-5.00	-5.93	-8.12	-3.98	-2.62	-4.41	-5.64
					-2.87	-6.31	-8.90	-5.49	-5.02	-5.92	-8.14	-4.07	-2.58	-4.41	-5.59
					-2.80	-6.29	-8.92	-5.18	-4.83	-5.88	-7.95	-4.10	-2.63	-4.41	-5.35
-7.40	-11.97	-5.46	-4.20	-9.36	-3.13	-6.54	-9.10	-5.45	-5.13	-6.15	-8.25	-4.36	-2.55	-4.41	-5.29
					-2.81	-6.33	-8.99	-5.40	-4.95	-5.98	-8.06	-4.17	-2.66	-4.41	-5.57
					-2.99	-6.44	-9.08	-4.61	-4.70	-6.03	-7.79	-4.92	-2.61	-4.48	-4.65
					-2.84	-6.30	-8.94	-4.57	-4.61	-5.86	-7.70	-4.42	-2.61	-4.48	-4.76
					-2.75	-6.04	-8.52	-4.74	-4.65	-5.83	-7.74	-4.43	-2.44	-4.48	-5.00
-9.03			-5.44	-11.22	-3.16	-6.68	-9.39	-5.32	-5.15	-6.71	-8.23	-4.34	-2.67	-4.49	-5.20
-8.61			-4.29	-11.19	-3.34	-7.33	-10.52	-4.74	-4.94	-6.78	-8.02	-5.16	-3.17	-4.49	-4.49
-9.05			-4.36	-11.80	-3.70	-7.71	-10.91	-4.75	-5.14	-7.15	-8.22	-5.31	-3.17	-4.49	-4.11
-9.62			-4.96		-4.33	-8.27	-11.40	-5.42	-5.79	-7.53	-8.87	-6.34	-3.10	-4.49	-4.15
-9.14			-4.39	-11.92	-4.62	-8.59	-11.76	-5.63	-6.05	-7.76	-9.12	-6.45	-3.13	-4.49	-4.07
-8.40			-3.29	-11.34	-4.15	-8.27	-11.57	-4.83	-5.42	-7.82	-8.50	-5.94	-3.25	-4.49	-3.69
-8.19			-3.29	-11.04	-4.60	-8.79		-5.47	-5.96	-8.24	-9.04	-6.64	-3.35	-4.50	-3.92
-8.20			-3.46	-10.98	-4.55	-8.73		-5.57	-5.98	-8.18	-9.06	-6.48	-3.35	-4.50	-4.10
-8.16			-3.24	-11.01	-4.45	-8.49	-11.72	-5.32	-5.81	-8.70	-8.89	-6.18	-3.19	-4.50	-3.90
-8.37			-3.74	-11.11	-4.70	-8.92		-5.82	-6.18	-8.08	-9.25	-6.84	-3.40	-4.50	-4.22
-7.58		-11.18	-3.22	-10.18	-4.55	-8.87		-5.95	-6.17	-7.99	-9.24	-6.72	-3.51	-4.50	-4.51
-8.09			-3.66	-10.74	-4.64	-8.74		-5.96	-6.21	-8.07	-9.29	-6.80	-3.29	-4.50	-4.43
-7.47		-9.44	-2.95	-10.15	-4.30	-8.53	-11.96	-5.55	-5.85		-8.92	-6.49	-3.40	-4.50	-4.34
-7.17		-7.51	-3.18	-9.60	-4.36	-8.71		-6.13	-6.17	-7.96	-9.24	-6.49	-3.55	-4.50	-4.92
-8.06			-3.44	-10.79	-4.51	-8.56	-11.83	-5.67	-6.01	-8.04	-9.09	-6.25	-3.23	-4.50	-4.24
-9.18			-4.66	-11.88	-5.34	-9.63		-6.59	-6.89	-9.06	-9.96	-7.25	-3.47	-4.50	-4.37
-10.52			-5.43		-4.40	-8.21	-11.21	-5.13	-5.70	-7.91	-8.77	-6.36	-2.95	-4.51	-3.77
-7.67			-2.86	-10.49	-4.34	-8.72		-5.40	-5.82	-7.98	-8.88	-6.15	-3.55	-4.53	-4.15
					-2.60	-6.14	-8.83	-4.02	-4.16	-6.70	-7.28	-4.04	-2.66	-4.41	-4.35
					-3.15	-7.07	-10.18	-4.45	-4.71	-6.24	-7.79	-5.17	-3.09	-4.49	-4.38
					-3.05	-6.95	-10.05	-4.41	-4.64	-6.19	-7.72	-5.02	-3.07	-4.49	-4.44
					-3.04	-7.02	-10.20	-4.45	-4.66	-6.31	-7.74	-5.03	-3.15	-4.49	-4.49
					-3.27	-7.15	-10.23	-4.70	-4.91	-6.73	-7.98	-5.33	-3.06	-4.50	-4.54
					-3.03	-6.61	-9.39	-4.34	-4.61	-6.23	-7.69	-5.08	-2.74	-4.50	-4.37

Al(OH)2+	Al+++	Al13O4(OH)24(7+)	AlO2-	AlOH++	Ca++	CaCl+	CaCl2(aq)	CaCO3(aq)	CaHCO3+	CaNO3+	CaOH+	CaSO4(aq)	Cl-	CO2(aq)	CO3--
Log Molal	Log Molal	Log Molal	Log Molal	Log Molal	Log Molal	Log Molal	Log Molal	Log Molal	Log Molal	Log Molal	Log Molal	Log Molal	Log Molal	Log Molal	Log Molal
													-3.29	-4.52	-3.58
													-3.21	-4.52	-3.42
													-3.37	-4.53	-3.75
													-3.29	-4.53	-3.79
					-4.89	-8.35	-11.05	-5.84	-6.34	-8.63	-9.39	-6.98	-2.63	-4.56	-4.05
													-2.89	-4.56	-3.95
33	**34**	**35**	**36**	**37**	**38**	**39**	**40**	**41**	**42**	**43**	**44**	**45**	**46**	**47**	**48**
					-4.74	-8.78		-5.48	-6.09	-8.38	-9.14	-6.65	-3.21	-4.56	-3.84
					-2.55	-5.77	-8.12	-6.93	-5.58	-5.81	-8.70	-3.53	-2.32	-4.40	-7.25
					-2.66	-5.96	-8.40	-5.20	-4.77	-5.91	-7.89	-3.75	-2.41	-4.40	-5.44
					-2.68	-5.96	-8.37	-5.05	-4.70	-5.89	-7.82	-3.81	-2.39	-4.40	-5.27
					-2.78	-6.22	-8.82	-4.93	-4.69	-6.37	-7.81	-4.04	-2.58	-4.40	-5.11
					-3.01	-6.63	-9.38	-4.67	-4.68	-7.00	-7.80	-4.19	-2.74	-4.40	-4.61
					-2.99	-6.61	-9.39	-4.92	-4.79	-6.08	-7.91	-4.36	-2.77	-4.41	-4.92
					-3.82	-8.00	-11.39	-5.09	-5.36	-7.02	-8.44	-5.19	-3.35	-4.49	-4.33
					-4.75	-8.93		-5.88	-6.23	-7.95	-9.31	-6.70	-3.36	-4.49	-4.22
					-5.05	-8.73	-11.62	-6.19	-6.55	-8.33	-9.62	-6.95	-2.85	-4.50	-4.22
					-4.83	-8.61	-11.58	-5.71	-6.20	-8.17	-9.27	-6.75	-2.93	-4.50	-3.92
					-5.36	-9.46		-6.33	-6.78	-8.95	-9.85	-7.52	-3.27	-4.51	-4.05
					-5.33	-9.51		-6.71	-6.94	-8.96	-10.01	-7.49	-3.37	-4.51	-4.51
					-4.79	-8.68	-11.78	-5.55	-6.11	-8.38	-9.18	-6.67	-3.04	-4.51	-3.80
					-2.94	-6.63	-9.48	-5.00	-4.81	-5.97	-7.92	-4.47	-2.85	-4.41	-5.07
					-2.77	-6.52	-9.42	-4.38	-4.42	-5.82	-7.53	-4.17	-2.89	-4.41	-4.57
					-2.75	-6.38	-9.16	-4.32	-4.38	-5.75	-7.50	-4.69	-2.77	-4.41	-4.55
					-3.15	-6.79	-9.63	-4.49	-4.73	-6.53	-7.81	-4.86	-2.80	-4.49	-4.39
					-3.44	-7.07	-9.90	-4.89	-5.08	-6.77	-8.16	-4.88	-2.79	-4.49	-4.51
					-3.53	-7.38	-10.42	-4.41	-4.89	-6.98	-7.97	-5.39	-3.00	-4.49	-3.92
					-4.03	-7.91	-10.99	-5.01	-5.44	-8.68	-8.52	-5.50	-3.03	-4.49	-4.02
					-4.57	-8.71		-5.83	-6.12	-8.13	-9.19	-6.27	-3.32	-4.50	-4.36
					-4.25	-8.19	-11.33	-5.23	-5.67	-8.07	-8.74	-6.31	-3.11	-4.50	-4.06
					-4.09	-8.29	-11.70	-5.00	-5.47	-8.10	-8.55	-6.21	-3.37	-4.50	-3.98
					-4.55	-8.58	-11.83	-5.53	-5.98	-8.02	-9.04	-6.73	-3.21	-4.52	-4.07
					-4.54	-8.41	-11.48	-5.35	-5.89	-8.79	-8.96	-6.32	-3.02	-4.52	-3.87
					-4.56	-8.57	-11.78	-5.47	-5.96	-8.26	-9.03	-6.34	-3.17	-4.52	-3.99

H+	H2SiO4--	H4(H2SiO4)4----	H2SO4 (aq)	H6(H2SiO4)4--	HAlO2 (aq)	HCl(aq)	HCO3-	HNO3 (aq)	HSiO3-	HSO4-	K+	KCl(aq)	KHSO4 (aq)	KOH(aq)	KSO4-
Log Molal	Log Molal	Log Molal	Log Molal	Log Molal	Log Molal	Log Molal	Log Molal	Log Molal	Log Molal	Log Molal	Log Molal	Log Molal	Log Molal	Log Molal	Log Molal
1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16
-7.92	-9.80			-9.16	-6.18	-11.70	-2.79		-4.93	-9.32	-3.45	-8.10		-9.99	-5.90
-8.08	-9.46			-8.73	-7.04	-11.78	-2.63		-4.74	-9.76	-3.45	-8.03		-9.84	-6.18
-8.19	-9.38			-9.16		-11.57	-2.54		-4.70	-9.94					
-8.15	-9.45			-9.11	-6.75		-2.60		-4.71	-9.90	-3.45	-8.17		-9.76	-6.31
-8.10	-9.60			-9.47		-11.68	-2.64		-4.83	-9.82	-3.45	-7.84		-9.81	-6.28
-8.19	-9.43			-9.21			-2.56		-4.72	-10.18	-3.45	-8.11		-9.72	-6.55
-8.33	-9.02			-8.51	-6.24		-2.41		-4.47	-10.22	-3.45	-8.11		-9.58	-6.45
-8.45	-8.94			-9.00			-2.28		-4.53	-10.41	-3.45	-7.87		-9.46	-6.53
-8.17	-9.09			-7.78	-6.21	-11.95	-2.58		-4.37	-10.06	-3.45	-8.04		-9.74	-6.46
-8.24	-9.26			-8.93	-6.10	-11.79	-2.50		-4.61	-10.03	-3.45	-7.80		-9.67	-6.36
-8.15	-9.59			-9.59	-6.19		-2.61		-4.82	-9.99	-3.45	-8.18		-9.76	-6.41
-8.25	-9.24			-8.83	-5.92		-2.50		-4.58	-9.98	-3.45	-8.22		-9.66	-6.30
-8.34	-9.08			-8.75	-6.13		-2.41		-4.52	-10.10	-3.45	-8.18		-9.57	-6.33
-8.49	-8.60			-7.85	-6.00		-2.25		-4.21	-10.31	-3.45	-8.33		-9.42	-6.38
-8.24	-9.16			-8.51	-5.67	-11.88	-2.51		-4.51	-9.73	-3.45	-7.90		-9.67	-6.06
-8.46	-8.52			-7.33	-5.67		-2.28		-4.10	-10.31	-3.45	-8.41		-9.45	-6.42
-8.32	-9.09			-8.64	-5.88		-2.44		-4.50	-10.24	-3.45	-8.24		-9.59	-6.49
-8.22	-9.24			-8.65	-6.31		-2.53		-4.55	-9.86	-3.45	-8.13		-9.69	-6.22
-8.40	-8.84			-8.19	-5.97		-2.35		-4.34	-10.18	-3.45	-8.19		-9.51	-6.35
-8.33	-8.86			-7.81	-5.64		-2.43		-4.28	-10.18	-3.45	-8.18		-9.59	-6.42
-8.21	-9.31			-8.84	-6.23		-2.55		-4.60	-10.18	-3.45	-8.26		-9.70	-6.54
-8.04	-9.11			-7.04	-4.79	-11.75	-2.72		-4.23	-10.12	-3.45	-7.96		-9.87	-6.65
-8.21	-9.57			-9.96	-6.48	-11.77	-2.55		-4.87	-9.90	-3.45	-7.81		-9.70	-6.27
-8.26	-9.47			-9.93	-6.39	-11.71	-2.49		-4.83	-9.89	-3.45	-7.69		-9.65	-6.21
-8.35	-8.96			-8.49	-6.01	-11.81	-2.40		-4.42	-10.11	-3.45	-7.71		-9.57	-6.35
-8.19	-9.50			-9.52	-6.47		-2.57		-4.76	-10.00	-3.45	-8.10		-9.72	-6.39
-8.30	-9.08			-8.82	-6.27	-11.23	-2.38		-4.65	-10.08	-3.45	-7.25		-9.61	-6.28
-8.05	-9.45			-8.63	-6.53	-11.57	-2.64		-4.73	-9.51	-3.45	-7.84		-9.86	-5.95
-7.83	-9.95			-9.26		-11.45	-2.87		-5.00	-9.18	-3.45	-7.94		-10.08	-5.85
-7.81	-9.98			-9.28		-11.20	-2.89		-5.02	-9.16	-3.45	-7.72		-10.11	-5.86
-7.88	-9.86			-9.19		-11.40	-2.82		-4.96	-9.27	-3.45	-7.84		-10.04	-5.89
-8.07	-9.40			-8.55		-11.72	-2.63		-4.70	-9.43	-3.45	-7.97		-9.84	-5.86
-7.78	-9.99			-9.10		-11.28	-2.93		-4.99	-9.08	-3.45	-7.83		-10.14	-5.81
-8.09	-9.34			-8.48		-11.48	-2.60		-4.67	-9.41	-3.45	-7.71		-9.82	-5.82
-7.99	-9.61			-8.91		-11.40	-2.71		-4.83	-9.26	-3.45	-7.73		-9.93	-5.78

H+	H2SiO4--	H4(H2SiO4)4----	H2SO4 (aq)	H6(H2SiO4)4--	HAlO2 (aq)	HCl(aq)	HCO3-	HNO3 (aq)	HSiO3-	HSO4-	K+	KCl(aq)	KHSO4 (aq)	KOH(aq)	KSO4-
Log Molal	Log Molal	Log Molal	Log Molal	Log Molal	Log Molal	Log Molal	Log Molal	Log Molal	Log Molal	Log Molal	Log Molal	Log Molal	Log Molal	Log Molal	Log Molal
-7.84	-9.92			-9.29		-11.22	-2.85		-5.00	-9.11	-3.45	-7.70		-10.07	-5.77
-7.63	-10.34			-9.70		-10.93	-3.07		-5.20	-8.80	-3.45	-7.62		-10.29	-5.68
-7.67	-10.18			-9.30		-10.99	-3.02		-5.08	-8.87	-3.45	-7.63		-10.24	-5.71
17	**18**	**19**	**20**	**21**	**22**	**23**	**24**	**25**	**26**	**27**	**28**	**29**	**30**	**31**	**32**
-7.63	-10.24			-9.30		-11.00	-3.07		-5.10	-8.79	-3.45	-7.69		-10.28	-5.67
-7.66	-10.22			-9.36		-10.99	-3.04		-5.10	-8.87	-3.45	-7.65		-10.26	-5.72
-7.78	-10.14			-9.77		-11.15	-2.92		-5.14	-9.08	-3.45	-7.69		-10.13	-5.81
-7.81	-10.10			-9.77	-5.55	-11.11	-2.89		-5.12	-9.05	-3.45	-7.62		-10.10	-5.75
-7.68	-10.50			-10.53		-11.08	-3.03		-5.38	-9.05	-3.45	-7.72		-10.24	-5.88
-8.13	-9.72			-10.14		-11.48	-2.61		-4.98	-10.03	-3.45	-7.61		-9.78	-6.47
-8.07	-9.73			-9.84		-11.43	-2.67		-4.93	-9.61	-3.45	-7.62		-9.84	-6.11
-7.95	-10.03			-10.32		-11.13	-2.79		-5.11	-9.58	-3.45	-7.45		-9.97	-6.20
-7.85	-10.05			-9.82	-6.96	-11.27	-2.89		-5.02	-8.99	-3.45	-7.68		-10.06	-5.71
-8.22	-9.33			-9.05	-6.17		-2.53		-4.65	-10.03	-3.45	-8.16		-9.69	-6.38
-8.40	-8.90			-8.46	-6.43		-2.35		-4.40	-9.97	-3.45	-8.17		-9.51	-6.15
-8.38	-9.03			-8.83	-7.01		-2.37		-4.51	-10.36	-3.45	-8.10		-9.53	-6.55
-8.42	-8.96			-8.82	-6.49		-2.33		-4.48	-10.20	-3.45	-8.13		-9.49	-6.36
-8.59	-8.17	-11.31		-6.82	-5.58		-2.15		-3.89	-10.31	-3.45	-8.26		-9.32	-6.30
-8.49	-8.70			-8.21	-5.47		-2.26		-4.29	-10.48	-3.45	-8.34		-9.42	-6.57
-8.41	-8.58			-7.21	-5.55		-2.34		-4.08	-10.31	-3.45	-8.34		-9.50	-6.48
-8.49	-8.80			-8.70	-5.43		-2.25		-4.41	-10.16	-3.45	-8.19		-9.42	-6.25
-8.36	-8.97			-8.42	-5.77		-2.40		-4.41	-10.47	-3.45	-8.39		-9.55	-6.69
-8.22	-9.26			-8.68	-5.12		-2.54		-4.54	-10.37	-3.45	-8.49		-9.69	-6.73
-8.26	-9.23			-8.80	-5.59		-2.51		-4.55	-10.40	-3.45	-8.27		-9.65	-6.73
-8.30	-9.09			-8.54	-4.93		-2.46		-4.47	-10.45	-3.45	-8.39		-9.61	-6.74
-8.03	-9.73			-9.33	-4.89		-2.75		-4.80	-10.15	-3.45	-8.52		-9.88	-6.71
-8.34	-9.12			-8.95	-5.47		-2.42		-4.54	-10.04	-3.45	-8.21		-9.57	-6.29
-8.29	-9.27			-9.15	-6.63		-2.48		-4.62	-10.18	-3.45	-8.45		-9.62	-6.47
-8.56	-8.70			-8.69	-7.70		-2.19		-4.36	-10.46	-3.45	-7.95		-9.36	-6.49
-8.38	-8.23	-10.68		-5.67	-4.98		-2.39		-3.67	-10.12	-3.45	-8.52		-9.53	-6.35
-8.27	-9.03			-8.32		-11.69	-2.43		-4.52	-9.69	-3.45	-7.73		-9.65	-5.94
-8.28	-9.19			-8.84			-2.48		-4.56	-10.27	-3.45	-8.08		-9.64	-6.57
-8.25	-9.22			-8.76			-2.51		-4.56	-10.19	-3.75	-8.36		-9.97	-6.82
-8.22	-9.27			-8.80			-2.54		-4.58	-10.18	-3.45	-8.14		-9.69	-6.54
-8.20	-9.33			-8.91		-12.00	-2.56		-4.61	-10.24	-3.45	-8.04		-9.71	-6.62
-8.27	-9.20			-8.86		-11.75	-2.48		-4.56	-10.27	-3.45	-7.73		-9.64	-6.59

H+	H2SiO4--	H4(H2SiO4)4----	H2SO4 (aq)	H6(H2SiO4)4--	HAlO2 (aq)	HCl(aq)	HCO3-	HNO3 (aq)	HSiO3-	HSO4-	K+	KCl(aq)	KHSO4 (aq)	KOH(aq)	KSO4-
Log Molal	Log Molal	Log Molal	Log Molal	Log Molal	Log Molal	Log Molal	Log Molal	Log Molal	Log Molal	Log Molal	Log Molal	Log Molal	Log Molal	Log Molal	Log Molal
-8.65	-8.40			-8.06			-2.11		-4.15	-10.78	-3.45	-8.29		-9.27	-6.74
-8.72	-8.25			-7.92			-2.03		-4.07	-10.83	-3.45	-8.21		-9.20	-6.72
-8.57	-8.66			-8.56			-2.19		-4.30	-10.28	-3.45	-8.35		-9.34	-6.32
-8.55	-8.69			-8.57			-2.21		-4.30	-10.40	-3.45	-8.27		-9.36	-6.46
-8.42	-8.88			-8.54		-11.81	-2.36		-4.33	-10.41	-3.45	-7.58		-9.49	-6.63
-8.48	-8.86			-8.78			-2.31		-4.36	-10.46	-3.45	-7.84		-9.44	-6.62
33	**34**	**35**	**36**	**37**	**38**	**39**	**40**	**41**	**42**	**43**	**44**	**45**	**46**	**47**	**48**
-8.53	-8.51			-7.69			-2.26		-4.06	-10.34	-3.45	-8.16		-9.39	-6.45
-6.80	-11.96			-11.37		-9.89	-3.88		-6.04	-7.74	-3.45	-7.42		-11.12	-5.45
-7.72	-10.23			-9.87		-10.89	-2.97		-5.20	-8.79	-3.45	-7.50		-10.20	-5.57
-7.80	-10.08			-9.77		-10.95	-2.88		-5.14	-8.91	-3.45	-7.48		-10.12	-5.62
-7.90	-9.95			-9.76		-11.23	-2.80		-5.08	-9.16	-3.45	-7.65		-10.02	-5.77
-8.15	-9.43			-9.17		-11.64	-2.55		-4.81	-9.33	-3.45	-7.82		-9.77	-5.69
-8.00	-9.77			-9.58		-11.52	-2.70		-4.98	-9.39	-3.45	-7.83		-9.91	-5.90
-8.29	-9.16			-8.83			-2.46		-4.55	-9.63	-3.45	-8.35		-9.62	-5.91
-8.36	-9.10			-8.95			-2.40		-4.55	-10.28	-3.75	-8.65		-9.85	-6.80
-8.35	-9.10			-8.93		-11.94	-2.41		-4.53	-10.21	-3.99	-8.38		-10.10	-6.99
-8.49	-8.86			-8.89			-2.26		-4.45	-10.35	-3.45	-7.92		-9.42	-6.45
-8.44	-8.96			-8.89			-2.32		-4.47	-10.55	-3.45	-8.25		-9.47	-6.70
-8.22	-9.41			-9.29			-2.55		-4.68	-10.36	-3.45	-8.34		-9.68	-6.73
-8.54	-8.66			-8.44			-2.21		-4.30	-10.36	-3.81	-8.40		-9.74	-6.77
-7.93	-9.87			-9.51		-11.52	-2.78		-5.00	-9.50	-4.12	-8.57		-10.65	-6.74
-8.17	-9.31			-8.80		-11.80	-2.53		-4.70	-9.57	-3.45	-7.95		-9.75	-5.91
-8.19	-9.29			-8.75		-11.70	-2.52		-4.68	-10.13	-3.45	-7.83		-9.73	-6.45
-8.26	-9.20			-8.80		-11.81	-2.49		-4.56	-9.93	-3.45	-7.80		-9.65	-6.25
-8.20	-9.19			-8.41		-11.74	-2.55		-4.49	-9.60	-3.45	-7.79		-9.71	-5.98
-8.49	-8.79			-8.61			-2.25		-4.40	-10.29	-3.45	-8.00		-9.42	-6.38
-8.44	-8.76			-8.20			-2.31		-4.32	-9.85	-3.45	-8.04		-9.47	-5.99
-8.29	-9.13			-8.63			-2.47		-4.50	-9.97	-3.45	-8.30		-9.62	-6.26
-8.43	-8.87			-8.49			-2.32		-4.39	-10.45	-3.45	-8.10		-9.48	-6.61
-8.47	-8.80			-8.45			-2.29		-4.36	-10.54	-3.45	-8.36		-9.44	-6.66
-8.42	-8.75			-7.95			-2.34		-4.23	-10.56	-3.45	-8.18		-9.49	-6.73
-8.51	-8.76			-8.64			-2.24		-4.36	-10.22	-3.45	-8.00		-9.40	-6.31
-8.46	-8.84			-8.59			-2.30		-4.37	-10.18	-3.45	-8.15		-9.45	-6.32

Mg++	MgCl+	MgCO3(aq)	MgHCO3+	MgSO4(aq)	Na+	NaAlO2(aq)	NaCl(aq)	NaCO3-	NaHCO3(aq)	NaHSiO3(aq)	NaOH(aq)	NaSO4-	NO3-	O2(aq)	OH-	SiO2(aq)
Log Molal	Log Molal	Log Molal	Log Molal	Log Molal	Log Molal	Log Molal	Log Molal	Log Molal	Log Molal	Log Molal	Log Molal	Log Molal	Log Molal	Log Molal	Log Molal	Log Molal
1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17
-3.30	-6.60	-5.72	-5.19	-4.40	-3.03	-8.62	-6.94	-7.72	-5.70	-6.34	-10.06	-5.54	-3.43	-3.63	-6.16	-2.89
-3.37	-6.61	-5.48	-5.11	-4.76	-3.06	-9.35	-6.90	-7.44	-5.58	-6.19	-9.93	-5.85	-3.28	-3.63	-6.00	-2.87
-3.28	-6.20	-5.12	-4.93	-4.75	-2.44		-5.93	-6.61	-4.92	-5.59	-9.02	-5.37	-3.56	-3.68	-5.70	-3.03
-3.62	-7.05	-5.53	-5.31	-5.06	-2.68	-8.45	-6.70	-6.94	-5.20	-5.83	-9.30	-5.60	-3.43	-3.68	-5.74	-2.99
-3.52	-6.62	-5.52	-5.25	-4.94	-2.65		-6.33	-7.00	-5.22	-5.91	-9.31	-5.54	-3.38	-3.68	-5.78	-3.06
-4.03	-7.40	-5.86	-5.68	-5.71	-2.53		-6.49	-6.73	-5.02	-5.68	-9.10	-5.70	-3.54	-3.68	-5.70	-3.03
-3.85	-7.23	-5.40	-5.36	-5.44	-2.40	-7.47	-6.35	-6.30	-4.74	-5.30	-8.82	-5.46	-3.51	-3.68	-5.55	-2.94
-3.14	-6.28	-4.46	-4.54	-4.83	-2.37		-6.08	-6.02	-4.60	-5.35	-8.68	-5.52	-3.52	-3.68	-5.41	-3.13
-3.70	-7.01	-5.57	-5.37	-5.29	-2.59	-7.78	-6.47	-6.81	-5.09	-5.38	-9.17	-5.66	-3.49	-3.68	-5.71	-2.67
-4.04	-7.11	-5.77	-5.64	-5.54	-2.37	-7.38	-6.02	-6.45	-4.81	-5.42	-8.87	-5.34	-3.54	-3.68	-5.63	-3.00
-4.94	-8.38	-6.83	-6.62	-6.46	-2.48	-7.67	-6.50	-6.75	-5.01	-5.73	-9.07	-5.50	-3.59	-3.68	-5.73	-3.11
-4.64	-8.13	-6.35	-6.23	-6.06	-2.39	-7.21	-6.45	-6.46	-4.82	-5.40	-8.88	-5.30	-3.54	-3.68	-5.62	-2.97
-4.47	-7.92	-6.00	-5.98	-5.93	-2.31	-7.24	-6.33	-6.20	-4.65	-5.26	-8.71	-5.25	-3.53	-3.68	-5.53	-3.00
-4.96	-8.57	-6.19	-6.32	-6.49	-2.18	-6.83	-6.35	-5.75	-4.37	-4.84	-8.42	-5.17	-3.59	-3.68	-5.36	-2.86
-4.73	-7.90	-6.46	-6.34	-5.93	-2.27	-6.84	-6.02	-6.36	-4.71	-5.22	-8.77	-4.95	-3.40	-3.68	-5.62	-2.89
-4.83	-8.52	-6.12	-6.22	-6.40	-2.20	-6.56	-6.46	-5.84	-4.43	-4.75	-8.48	-5.24	-3.59	-3.68	-5.39	-2.71
-4.94	-8.45	-6.51	-6.47	-6.56	-2.35	-7.05	-6.44	-6.29	-4.72	-5.28	-8.77	-5.46	-3.65	-3.68	-5.55	-2.96
-5.42	-8.82	-7.19	-7.04	-6.76	-2.36	-7.60	-6.33	-6.49	-4.82	-5.34	-8.87	-5.19	-3.41	-3.68	-5.64	-2.91
-5.43	-8.89	-6.84	-6.88	-6.92	-2.24	-6.95	-6.27	-6.01	-4.52	-5.02	-8.57	-5.20	-3.51	-3.68	-5.45	-2.89
-4.64	-8.10	-6.20	-6.16	-6.20	-2.31	-6.76	-6.34	-6.23	-4.67	-5.04	-8.72	-5.35	-3.59	-3.69	-5.53	-2.76
-4.51	-8.03	-6.28	-6.13	-6.17	-2.46	-7.61	-6.57	-6.61	-4.93	-5.49	-8.98	-5.62	-3.74	-3.69	-5.65	-2.95
-4.50	-7.73	-6.61	-6.30	-6.26	-2.46	-6.34	-6.27	-6.95	-5.11	-5.13	-9.14	-5.73	-4.02	-3.69	-5.81	-2.42
-4.94	-8.03	-6.72	-6.58	-6.33	-2.36	-7.75	-6.03	-6.52	-4.85	-5.68	-8.86	-5.25	-3.68	-3.69	-5.62	-3.23
-4.95	-7.92	-6.63	-6.54	-6.29	-2.33	-7.57	-5.88	-6.37	-4.77	-5.62	-8.77	-5.16	-3.79	-3.69	-5.56	-3.26
-3.35	-6.35	-4.87	-4.86	-4.84	-2.83	-7.61	-6.40	-6.70	-5.19	-5.73	-9.18	-5.80	-3.89	-3.69	-5.46	-2.95
-4.94	-8.31	-6.74	-6.59	-6.44	-2.54	-7.93	-6.49	-6.73	-5.05	-5.75	-9.04	-5.55	-4.02	-3.69	-5.63	-3.11
-3.64	-6.11	-5.32	-5.16	-5.17	-1.97	-7.28	-5.02	-5.87	-4.25	-5.03	-8.64	-4.85	-3.25	-3.63	-5.78	-3.02
-3.30	-6.35	-5.47	-5.06	-4.48	-2.73	-8.54	-6.37	-7.14	-5.25	-5.84	-9.63	-5.29	-3.45	-3.63	-6.04	-2.83
-3.42	-6.57	-6.02	-5.40	-4.48	-2.79		-6.54	-7.65	-5.54	-6.17	-9.92	-5.25	-3.38	-3.63	-6.26	-2.88
-3.31	-6.23	-5.96	-5.31	-4.38	-2.78		-6.31	-7.69	-5.56	-6.19	-9.94	-5.25	-3.33	-3.63	-6.28	-2.87
-3.32	-6.37	-5.84	-5.25	-4.42	-2.84		-6.49	-7.61	-5.54	-6.18	-9.92	-5.33	-3.38	-3.63	-6.22	-2.88
-3.29	-6.47	-5.42	-5.03	-4.37	-2.75		-6.53	-7.13	-5.26	-5.84	-9.64	-5.21	-3.43	-3.63	-6.02	-2.82
-3.41	-6.45	-6.13	-5.44	-4.43	-2.81		-6.44	-7.78	-5.62	-6.18	-9.99	-5.22	-3.40	-3.63	-6.31	-2.81
-3.28	-6.20	-5.37	-5.01	-4.33	-2.62		-6.13	-6.94	-5.11	-5.68	-9.48	-5.04	-3.43	-3.63	-5.98	-2.82
-3.36	-6.31	-5.66	-5.19	-4.36	-2.68		-6.22	-7.23	-5.28	-5.91	-9.65	-5.07	-3.45	-3.63	-6.09	-2.87

Mg++	MgCl+	MgCO3(aq)	MgHCO3+	MgSO4(aq)	Na+	NaAlO2(aq)	NaCl(aq)	NaCO3-	NaHCO3(aq)	NaHSiO3(aq)	NaOH(aq)	NaSO4-	NO3-	O2(aq)	OH-	SiO2(aq)
Log Molal	Log Molal	Log Molal	Log Molal	Log Molal	Log Molal	Log Molal	Log Molal	Log Molal	Log Molal	Log Molal	Log Molal	Log Molal	Log Molal	Log Molal	Log Molal	Log Molal
-3.37	-6.29	-5.96	-5.34	-4.36	-2.65		-6.16	-7.48	-5.39	-6.04	-9.76	-5.03	-3.45	-3.63	-6.23	-2.89
-3.39	-6.23	-6.40	-5.58	-4.29	-2.68		-6.11	-7.94	5.64	-6.28	-10.00	-4.96	-3.43	-3.63	-6.44	-2.89
-3.41	-6.26	-6.34	-5.56	-4.34	-2.67		-6.11	-7.85	-5.59	-6.15	-9.95	-4.99	-3.47	-3.63	-6.40	-2.81
18	**19**	**20**	**21**	**22**	**23**	**24**	**25**	**26**	**27**	**28**	**29**	**30**	**31**	**32**	**33**	34
-3.41	-6.32	-6.42	-5.60	-4.30	-2.77		-6.26	-8.03	-5.73	-6.26	-10.08	-5.05	-3.65	-3.64	-6.43	-2.79
-3.42	-6.29	-6.37	-5.58	-4.35	-2.68		-6.14	-7.88	-5.61	-6.18	-9.96	-5.00	-3.59	-3.64	-6.40	-2.82
-3.41	-6.32	-6.11	-5.44	-4.43	-2.90		-6.40	-7.86	-5.71	-6.44	-10.06	-5.32	-3.62	-3.64	-6.28	-2.98
-4.44	-7.27	-7.08	-6.44	-5.40	-2.35	-7.40	-5.78	-7.25	-5.13	-5.87	-9.48	-4.71	-3.56	-3.64	-6.25	-3.00
-3.34	-6.28	-6.25	-5.48	-4.43	-3.41		-6.94	-8.58	-6.33	-7.18	-10.67	-5.89	-3.72	-3.64	-6.39	-3.12
-3.84	-6.72	-5.80	-5.56	-5.45	-2.54		-5.99	-6.84	-5.08	-5.95	-9.17	-5.62	-3.59	-3.68	-5.75	-3.24
-3.77	-6.66	-5.85	-5.54	-5.03	-2.67		-6.14	-7.09	-5.28	-6.05	-9.36	-5.40	-3.56	-3.68	-5.80	-3.14
-3.70	-6.43	-6.03	-5.61	-5.06	-2.71		-6.00	-7.37	-5.44	-6.27	-9.52	-5.52	-3.62	-3.68	-5.92	-3.20
-4.60	-7.56	-7.11	-6.60	-5.45	-2.42	-8.68	-5.95	-7.27	-5.25	-5.89	-9.30	-4.74	-4.09	-3.68	-6.00	-3.03
-4.64	-8.07	-6.39	-6.25	-6.14	-2.53	-7.62	-6.54	-6.65	-4.99	-5.61	-9.04	-5.53	-4.02	-3.68	-5.64	-3.01
-5.44	-8.88	-6.84	-6.89	-6.72	-2.26	-7.42	-6.27	-6.02	-4.55	-5.11	-8.58	-5.02	-4.00	-3.69	-5.44	-2.96
					-2.28	-8.04	-6.22	-6.08	-4.58	-5.23	-8.61	-5.44	-3.76	-3.69	-5.46	-3.04
-5.43	-8.84	-6.80	-6.86	-6.93	-2.23	-7.43	-6.21	-5.95	-4.50	-5.16	-8.52	-5.21	-3.70	-3.69	-5.42	-3.06
-4.76	-8.31	-5.79	-6.03	-6.21	-2.05	-6.16	-6.16	-5.42	-4.15	-4.41	-8.17	-4.97	-4.19	-3.69	-5.23	-2.66
-5.13	-8.76	-6.36	-6.50	-6.84	-2.18	-6.27	-6.37	-5.76	-4.38	-4.92	-8.40	-5.37	-4.19	-3.69	-5.34	-2.94
-5.13	-8.74	-6.51	-6.57	-6.73	-2.25	-6.52	-6.44	-6.00	-4.54	-4.78	-8.55	-5.35	-4.19	-3.69	-5.42	-2.65
-4.75	-8.22	-5.97	-6.11	-6.14	-2.14	-6.19	-6.18	-5.71	-4.34	-5.01	-8.35	-5.01	-4.79	-3.69	-5.33	-3.07
-4.94	-8.61	-6.42	-6.43	-6.75	-2.34	-6.87	-6.58	-6.19	4.67	-5.19	-8.68	-5.65	-3.95	-3.69	-5.47	-2.92
-4.71	-8.47	-6.46	-6.33	-6.54	-2.43	-6.45	-6.77	-6.57	-4.91	-5.42	-8.92	-5.78	-4.01	-3.69	-5.62	-2.92
-4.93	-8.48	-6.61	-6.52	-6.77	-2.42	-6.87	-6.55	-6.48	-4.86	-5.41	-8.86	-5.76	-4.01	-3.69	-5.58	-2.96
-4.57	-8.24	-6.17	-6.12	-6.43	-2.32	-6.06	-6.56	-6.31	-4.73	-5.24	-8.72	-5.68		-3.69	-5.53	-2.92
-4.62	-8.41	-6.75	-6.43	-6.42	-2.60	-6.56	-6.97	-7.14	-5.28	-5.83	-9.26	-5.93	-4.19	-3.69	-5.80	-2.98
-4.39	-7.88	-5.90	-5.90	-5.79	-2.30	-6.53	-6.37	-6.20	-4.67	-5.29	-8.65	-5.21	-4.09	-3.69	-5.47	-3.05
					-2.42	-7.86	-6.72	-6.42	-4.84	-5.48	-8.81	-5.51	-4.30	-3.70	-5.52	-3.07
-4.97	-8.22	-6.06	-6.28	-6.60	-2.10	-8.34	-5.91	-5.55	-4.25	-4.93	-8.22	-5.21	-4.04	-3.70	-5.23	-3.10
-4.58	-8.41	-6.01	-6.07	-6.04	-2.21	-5.86	-6.60	-6.04	-4.57	-4.36	-8.45	-5.18	-4.19	-3.71	-5.36	-2.25
-3.26	-6.22	-5.00	-4.82	-4.42	-3.06		-6.61	-7.05	-5.40	-6.00	-9.72	-5.61	-4.62	-3.64	-5.77	-2.87
-4.64	-7.99	-6.29	-6.21	-6.33	-2.54		-6.47	-6.56	-4.95	-5.54	-8.98	-5.72	-3.66	-3.69	-5.57	-2.99
-4.46	-7.80	-6.17	-6.06	-6.10	-2.60		-6.51	-6.68	-5.05	-5.60	-9.07	-5.74	-3.70	-3.69	-5.60	-2.95
-4.46	-7.87	-6.22	-6.08	-6.12	-2.73		-6.72	-6.87	-5.21	-5.75	-9.22	-5.89	-3.84	-3.69	-5.62	-2.95
-4.63	-7.95	-6.42	-6.27	-6.36	-2.59		-6.48	-6.77	-5.09	-5.64	-9.09	-5.83	-4.04	-3.69	-5.63	-2.97
-4.81	-7.83	-6.48	-6.40	-6.53	-2.47		-6.05	-6.50	-4.90	-5.48	-8.90	-5.67	-3.75	-3.69	-5.55	-3.00

Mg++	MgCl+	MgCO3(aq)	MgHCO3+	MgSO4(aq)	Na+	NaAlO2(aq)	NaCl(aq)	NaCO3-	NaHCO3(aq)	NaHSiO3(aq)	NaOH(aq)	NaSO4-	NO3-	O2(aq)	OH-	SiO2(aq)
Log Molal	Log Molal	Log Molal	Log Molal	Log Molal	Log Molal	Log Molal	Log Molal	Log Molal	Log Molal	Log Molal	Log Molal	Log Molal	Log Molal	Log Molal	Log Molal	Log Molal
-5.16	-8.75	-6.07	-6.39	-7.04	-2.05		-6.20	-5.33	-4.13	-4.68	-8.06	-5.41	-4.11	-3.70	-5.12	-2.99
-5.01	-8.52	-5.78	-6.17	-6.87	-1.97		-6.04	-5.10	-3.98	-4.53	-7.90	-5.30	-3.97	-3.70	-5.03	-3.00
					-2.13		-6.35	-5.57	-4.30	-4.91	-8.18	-5.07	-4.19	-3.71	-5.16	-3.08
					-2.15		-6.29	-5.63	-4.34	-4.93	-8.21	-5.24	-4.21	-3.71	-5.17	-3.07
-5.13	-8.04	-6.45	-6.58	-6.84	-2.17		-5.63	-5.92	-4.52	-4.99	-8.28	-5.42	-4.29	-3.73	-5.23	-2.99
					-2.19		-5.91	-5.84	-4.50	-5.05	-8.26	-5.45	-4.45	-3.73	-5.18	-3.08
35	**36**	**37**	**38**	**39**	**40**	**41**	**42**	**43**	**44**	**45**	**46**	**47**	**48**	**49**	**50**	51
					-2.18		-6.22	-5.73	-4.43	-4.74	-8.20	-5.26	-4.19	-3.73	-5.13	-2.83
-3.07	-5.71	-7.76	-6.10	-3.77	-2.73		-5.95	-9.63	-6.52	-7.18	-10.90	-4.78	-3.76	-3.63	-7.27	-2.91
-3.20	-5.91	-6.05	-5.30	-4.01	-2.63		-5.93	-7.70	-5.50	-6.23	-9.87	-4.80	-3.76	-3.63	-6.35	-2.99
-3.27	-5.97	-5.95	-5.30	-4.13	-2.55		-5.83	-7.45	-5.33	-6.09	-9.70	-4.77	-3.72	-3.63	-6.27	-3.00
-3.32	-6.19	-5.80	-5.24	-4.31	-2.81		-6.27	-7.53	-5.50	-6.29	-9.86	-5.18	-4.12	-3.63	-6.17	-3.04
-3.47	-6.50	-5.45	-5.14	-4.38	-2.39		-6.01	-6.61	-4.83	-5.60	-9.19	-4.68	-4.52	-3.63	-5.92	-3.02
-3.52	-6.57	-5.78	-5.33	-4.62	-2.64		-6.28	-7.16	-5.23	-6.01	-9.57	-5.14	-3.64	-3.64	-6.06	-3.04
					-2.32		-6.51	-6.30	-4.71	-5.31	-8.75	-4.85	-3.77	-3.69	-5.56	-3.00
-5.42	-9.04	-6.91	-6.91	-7.04	-2.32		-6.51	-6.17	-4.65	-5.30	-8.67	-5.44	-3.77	-3.69	-5.48	-3.06
					-2.23		-5.92	-6.10	-4.58	-5.22	-8.57	-5.29	-3.84	-3.69	-5.47	-3.05
					-2.15		-5.93	-5.74	-4.37	-5.06	-8.35	-5.21	-3.88	-3.69	-5.32	-3.11
					-2.27		-6.38	-5.97	-4.54	-5.20	-8.51	-5.59	-4.15	-3.70	-5.37	-3.08
					-2.49		-6.69	-6.63	-4.98	-5.62	-8.95	-5.84	-4.21	-3.70	-5.59	-3.07
					-2.11		-6.00	-5.59	-4.28	-4.88	-8.24	-5.13	-4.13	-3.70	-5.24	-3.03
-3.54	-6.65	-5.92	-5.41	-4.80	-2.91		-6.62	-7.57	-5.57	-6.29	-9.90	-5.59	-3.59	-3.64	-6.13	-2.99
-3.33	-6.50	-5.26	-4.98	-4.46	-2.93		-6.69	-7.12	-5.36	-6.03	-9.70	-5.45	-3.59	-3.64	-5.88	-2.93
-3.51	-6.56	-5.40	-5.14	-5.17	-3.04		-6.68	-7.20	-5.46	-6.12	-9.78	-6.10	-3.54	-3.64	-5.87	-2.93
					-2.41		-6.06	-6.46	-4.84	-5.42	-8.88	-5.28	-3.93	-3.69	-5.59	-2.98
-5.13	-8.20	-6.94	-6.78	-6.24	-2.33		-5.97	-6.49	-4.82	-5.27	-8.85	-4.93	-3.89	-3.69	-5.64	-2.85
					-2.19		-6.04	-5.77	-4.39	-5.04	-8.42	-5.19	-3.99	-3.69	-5.35	-3.05
-5.45	-8.77	-6.78	-6.86	-6.59	-2.18		-6.06	-5.86	-4.43	-4.95	-8.45	-4.79	-5.19	-3.69	-5.39	-2.92
-5.43	-9.00	-7.04	-6.98	-6.80	-2.38		-6.53	-6.37	-4.78	-5.32	-8.79	-5.25	-4.14	-3.69	-5.54	-2.94
					-2.25		-6.20	-5.97	-4.52	-5.09	-8.53	-5.48	-4.38	-3.69	-5.39	-2.98
					-2.25		-6.46	-5.89	-4.49	-5.07	-8.48	-5.53	-4.56	-3.69	-5.35	-2.99
					-2.28		-6.32	-6.01	-4.58	-4.97	-8.51	-5.63	-4.04	-3.70	-5.35	-2.84
					-2.15		-6.01	-5.70	-4.36	-4.98	-8.29	-5.07	-4.79	-3.70	-5.25	-3.07
					-2.22		-6.23	-5.88	-4.48	-5.06	-8.41	-5.16	-4.25	-3.70	-5.30	-3.02