

TECHNICAL REPORT 91-18

NAGRA THERMOCHEMICAL DATA BASE II. SUPPLEMENTAL DATA 05/92

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ZUSAMMENFASSUNG

Thermodynamische Daten für wässrige Spezies, Mineralien und Gase werden von der Nagra für ihre geochemische Modellierung gebraucht. Die von der Nagra erarbeitete thermochemische Datenbasis enthält sowohl Kerndaten ("core data") als auch Ergänzungsdaten ("supplemental data"). Die Kerndaten für gut charakterisierte Komponenten wurden einzeln sorgfältig ausgewählt und sind in PEARSON & BERNER (1991) wiedergegeben. Die Ergänzungsdaten berücksichtigen die weniger häufig vorkommenden Komponenten und die für die Sicherheitsanalyse relevanten Elemente. Diese Daten wurden gruppenweise aus anderen geochemischen Datenbasen ausgewählt und wurden nicht einzeln geprüft.

In diesem Bericht wird die thermochemische Datenbasis der Nagra (Stand 5/92) tabellarisch dargestellt. Diese Datenbasis enthält neben den früher präsentierten Kerndaten die verfügbaren Werte für die Elemente Aluminium, Silizium, Eisen und Mangan, die Actinide Thorium, Uran, Neptunium, Plutonium und Americium, sowie für Elemente, die als Spaltprodukte bzw. Aktivierungsprodukte in radioaktiven Abfällen vorkommen, zum Beispiel Nickel, Zirkonium, Niobium, Molybdän, Technetium, Palladium, Zinn, Selen und Jod. Im Wasser gelöste Komplexe von vier repräsentativen organischen Anionen werden ebenfalls aufgeführt. Die Quellen dieser Ergänzungsdaten werden im Text beschrieben.

Andere Datenzusammenstellungen wurden während der Auswahl der Ergänzungsdaten studiert. Unter diesen waren die Datenbasen, die am Paul Scherrer Institut zusammen mit den geochemischen Programmen MINEQL (Version 3/91), PHREEQE (Version 4/91) gebraucht werden, sowie die HATCHES 3.0 Datenbasis. Dieser Bericht enthält auch zusätzlich Tabellen, in welchen die ausgewählten Werte mit den erwähnten Datenbasen verglichen werden.

Diese Datenbasis wurde bis anhin noch nicht für das gesamte Spektrum möglicher Anwendungen im Rahmen der Endlager getestet, und sollte deshalb lediglich als Referenz für eine Qualitätskontrolle betrachtet werden, und nicht als allgemein akzeptierten, kritisch geprüften Standard.

RÉSUMÉ

Des données thermodynamiques relatives à la chimie des spécimens aqueux, des minéraux et des gaz, sont requises par la Cédra pour l'élaboration de ses modèles géochimiques. Les données thermochimiques de la Cédra comprennent des données de base et des données complémentaires. Les données de base correspondent à des entités bien définies qui ont été sélectionnées une à une avec la plus grande attention et fournies par PEARSON & BERNER (1991). Les données complémentaires comportent des entités moins courantes et des éléments nécessaires aux évaluations de sûreté. Elles ont été sélectionnées par groupes à partir d'autres bases de données de modélisation géochimique et n'ont pas été soumises à un examen individuel détaillé.

Ce rapport contient les tableaux des données thermochimiques de base de la Cédra en date de mai 1992. Il comprend les données fondamentales décrites dans un rapport antérieur ainsi que des données complémentaires relatives aux éléments aluminium, silicium, fer et manganèse, aux actinides thorium, uranium, neptunium, plutonium et americium, à des éléments présents à titre de produits de fission, respectivement produits d'activation dans les déchets nucléaires, y compris nickel, zirconium, niobium, molybdène, technetium, palladium, étain, sélénium et iodé. Des complexes en solution de quatre anions organiques représentatifs y sont également inclus. Le rapport décrit les sources de ces données complémentaires.

D'autres compilations de données ont été examinées lors de la sélection de ces données complémentaires. Celles-ci comprenaient les bases de données utilisées à l'Institut Paul Scherrer pour les programmes géochimiques MINEQL jusqu'en mars 1991, PHREEQE jusqu'en avril 1991, ainsi que la base de données HATCHES 3.0. Le présent rapport fournit en outre des tableaux comparant des sélections de données provenant de ces trois bases avec les valeurs de la base de données de la Cédra.

Cette base de données n'a pas encore été testée pour le spectre complet d'applications dans le domaine de la gestion des déchets radioactifs, quoique des efforts dans ce sens sont en cours. C'est pourquoi cette base de données ne doit pas être considérée comme un standard éprouvé, mais plutôt comme un document de référence à ce stade des études.

SUMMARY

Chemical thermodynamic data for aqueous species, minerals, and gases are required by Nagra for geochemical modelling. The Nagra thermochemical data base contains core and supplemental data. Core data for well-characterised entities were individually carefully selected and given by PEARSON & BERNER (1991). Supplemental data are for less common entities and for elements principally of safety assessment concern. They were selected in groups from other data bases for geochemical modelling and did not receive individual scrutiny.

This report gives tables with the Nagra thermochemical data base as of 5/92. It includes the core data described in the earlier report with supplemental data for the elements aluminium, silicon, iron, and manganese, the actinides thorium, uranium, neptunium, plutonium, and americium, and elements found as fission or activation products in nuclear waste, including nickel, zirconium, niobium, molybdenum, technetium, palladium, tin, selenium and iodine. Aqueous complexes of four representative organic anions are also included. The sources of these supplemental data are described in the text.

Other compilations of data were examined during the selection on the supplemental data. These included the data bases used at the Paul Scherrer Institut with the geochemical programs MINEQL as of 3/91, PHREEQE as of 4/91, and the HATCHES 3.0 data base. This report also gives tables comparing selected data in these three data bases with values from the Nagra data base.

This data base has not yet been tested for a full range of nuclear waste management applications, although such work is in progress. It should thus be regarded as a reference fixed point for quality assurance purpose and not a critically reviewed standard.

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1 INTRODUCTION

The chemical thermodynamic data set used by Nagra for geochemical modelling includes two types of data - core data and supplemental, or auxiliary, data.

Well-characterized aqueous species, minerals, and gases of elements commonly found in significant quantities in natural waters are represented by core data. These data have been carefully selected and, to assure comparability of the results of modelling done at different times, will be fixed. The Nagra core chemical thermodynamic data are described by PEARSON & BERNER (1991).

Supplemental, or auxiliary, data are for elements that are found in natural waters, but not as major components, or that are of interest principally for the safety assessment of nuclear waste facilities. Less common aqueous species and minerals of core elements are also included among the supplemental data. Supplemental aqueous species, and minerals are less well-characterized than those in the core data. While the supplemental data set described here includes what are thought to be the best values available, it is recognized that better estimates of many values will be developed from continuing experimental work and improved critical reviews. To permit the inclusion of recent or improved data in Nagra calculations, supplemental data are subject to revision.

This data base has not yet been tested for a full range of nuclear waste management applications, although such work is in progress. It should thus be regarded as a reference fixed point for quality assurance purpose and not a critically reviewed standard.

This report describes the supplemental data in the Nagra chemical thermodynamic data base as of May, 1992. It includes the elements aluminum, silicon, iron, and manganese which are important in the chemistry of natural waters, but not included in the core data. It also contains a number of elements of importance in nuclear waste safety assessment including the actinide elements thorium, uranium, neptunium, plutonium, and americium, and certain fission activation products found in the waste, including the metals nickel, zirconium, niobium, molybdenum, technetium, palladium, tin, and the non-metals selenium and iodine. Data on aqueous complexes formed by metals in the data base with certain representative organic anions are also included.

The data are given in the tables of Appendix A. These tables include not only the supplemental data described here, but also the core data. Therefore, they represent the complete Nagra thermochemical data base as of May, 1992. A few of the core data in these tables differ from and supersede data in PEARSON & BERNER (1991). The

changes correct errors in formula weights of several master species and in the manner of writing several of the reactions from which redox potentials can be calculated from measured concentrations.

During the preparation of this data set, several existing data bases for nuclear waste studies were compared in detail. Appendix B describes how the comparison was made, and gives tables of selected values from the contents of the other data sets and of comparisons among them and with the Nagra data base.

1.1 Sources of Supplemental Data

The data for the aqueous species and minerals in the core data were selected individually (PEARSON & BERNER 1991). In contrast, the supplemental data were selected in groups from one of several existing data sets. These were:

A set of data for major water-mineral reactions selected and published by a U.S. Geological Survey group (NORDSTROM et al. 1990). These data are used in the most recent releases of the widely-used U.S. Geological Survey programs WATEQ4F (BALL & NORDSTROM 1991), and PHREEQE (1990 revision of PARKHURST et al. 1980).

The Harwell data base HATCHES 3.0 (CROSS & EWART 1991). The version in PHREEQE format was used rather than the complete data base.

The March, 1991 version of the Paul Scherrer Institut data base for MINEQL (MINEQL-PSI), developed principally by SCHWEINGRUBER (1982, 1983), WANNER (1986) and BERNER (1990).

The April, 1991 version of the Paul Scherrer Institut data base for PHREEQE (PHREEQE-PSI) developed principally by Baeyens (BAEYES & MCKINLEY 1989).

A compilation of equilibrium constants for the association of cations with various organic ligands prepared by HUMMEL (1991).

The HATCHES and the two PSI data sets are described in more detail in Appendix B, and selected data from them are listed in Tables B.3, B.4, and B.5. The organic data are discussed in Chapter 6. The sources of particular values in the supplemental data base are given in the data tables A.1 through A.4.

Other data bases widely used for geochemical modelling include those associated with the EQ3/EQ6 (WOLERY 1983; WOLERY *et al.* 1990) and SUPCRT (JOHNSON *et al.* *in press*) programs. The data accompanying a recent release of EQ3/EQ6 (version 2345 of 10/90) were examined for comparison with certain supplemental data selected, but were not considered in detail. The SUPCRT92 data set became available only as this report was in final preparation. As discussed below in Chapter 8, both these data bases should be considered in detail during the development of future Nagra supplemental data bases.

1.2 Quality of Data

The supplemental data, unlike the core data, were not examined individually, so their quality cannot be vouched for to the same degree. However, it is possible to suggest the relative quality of the supplemental data based on subjective judgments about the data sets from which they were adopted. To provide assistance to the user of Nagra data sets in forming an opinion on the information they contain, the following judgments are offered.

The Nagra core data are thought to be reliable. These include the common aqueous species and minerals of fluoride, chloride, bromide, iodide, sulphate, bisulphide, nitrate, ammonia, phosphate, As(III) and As(V), carbonate, borate, magnesium, calcium, strontium, barium, lithium, sodium, and potassium.

Of the supplemental data, those for silica, iron, manganese, uranium, and the organic complexes were taken from compilations of critically evaluated data (NORDSTROM *et al.* 1990; HUMMEL 1991), and are thought to be of first quality. Data on palladium, nickel, and selenium were taken from a data set compiled from a variety of sources (BAEYENS & MCKINLEY 1989). These data were apparently not critically evaluated with as much care and they disagree in part with values from other carefully compiled data bases such as those as EQ3/EQ6 and of the NEA (GRENTHE *et al.* 1991). Therefore, the data for these elements may be less reliable. Data for the remaining elements were taken from compilations of unknown reliability.

It is important to be cautious about using any of the supplemental data and much of the core data at temperatures too far removed from 25°C. Some of the core species and minerals are accompanied by data that permit logK values to be calculated quite precisely to temperatures approaching 100°C. The remaining core

and virtually all the supplemental species and minerals have only Δ_rH^0 values, or no data at all with which to calculate logK values at temperatures other than 25°C. Figure 2.1 of PEARSON & BERNER (1991) illustrates the errors in logK values that can result from insufficient temperature corrections.

When adapting values from other data sets for inclusion in the Nagra data base, it was sometimes necessary to change master species. For example, in the MINEQL-PSI data base from which all actinide data were adapted, the master species for carbonate is CO_3^{2-} , while in the Nagra data base, it is HCO_3^- . In making these changes, only the minimum data were carried into the Nagra data set. For example, no Δ_rH^0 value is given in the MINEQL-PSI data base for the reaction forming the aqueous species $\text{NpO}_2\text{CO}_3^0$. In the Nagra data base, a Δ_rH^0 value is available for the reaction between CO_3^{2-} and HCO_3^- , but it is not carried into the converted reaction for $\text{NpO}_2\text{CO}_3^0$ formation from HCO_3^- . The user should be aware that this could lead to differences between logK values calculated from the Nagra data base and from other data bases at temperatures different from 25°C.

1.3 Redox Reactions

As discussed in the text accompanying the core data base (PEARSON & BERNER 1991, Section 2.5), redox reactions for a given element can be treated as decoupled or coupled.

If reactions among several oxidation states of an element occur relatively slowly, or if it is common that the concentration of species in different oxidation states are analyzed separately, redox reactions of the element are treated as decoupled. Decoupled elements have several master species in the data base, one for each oxidation state. These elements and their master species are:

O₂: O_{2(aq)} and H₂O
H₂: H_{2(aq)} and H⁺
As: HAsO₄⁻², As(OH)₃, and As⁰
C: HCO₃⁻ and CH_{4(aq)}
N: NO₃⁻, N_{2(aq)}, and NH₄⁺
S: SO₄⁻², S⁰, and HS⁻

Table A.4 gives the data needed to calculate oxidation potentials (*pe* values) from measured concentrations of pairs of master species.

If it is assumed that redox reactions of an element occur relatively rapidly, or if the total concentration of an element is measured or to be calculated, coupled redox reactions are written. Only one master species is selected for redox-coupled elements, and the concentrations of other oxidation states are calculated from the total concentration, the coupled redox reactions, and the oxidation state (*pe*) of the solution (*e. g.* TRUESDELL & JONES 1974). Elements in this data base which include coupled redox reactions, and their master species, are:

Fe: Fe⁺²
Mn: Mn⁺²
Np: Np⁺⁴
Pu: Pu⁺⁴
Se: SeO₃⁻²
Sn: Sn⁺²
Tc: TcO⁺²
U: U⁺⁴

2 SILICA AND ALUMINIUM

Chemical thermodynamic data on aqueous species of these elements are important principally to support studies of water-rock reactions. The concentrations of silica in most waters are easily measurable and, except at pH values above c. 10.5, silica behaviour in solution can be modelled rather simply. In addition, under many conditions, the minerals controlling dissolved silica levels are the simple SiO_2 phases quartz, chalcedony, and amorphous silica, which also have well-known thermodynamic properties.

Aluminium, on the other hand, is present in easily measurable concentrations only in solutions with low or high pH values. Thus, the properties of aqueous aluminium species are not well defined. Aluminium concentrations in many waters appear to depend on complex alumino-silicate minerals, including clay minerals, that also have poorly defined thermodynamic properties.

The silica and aluminium data included in the supplemental data set are limited, but are from compilations of carefully selected data (NORDSTROM *et al.* 1990; EIKENBERG 1990). As improved aluminium data become available, the contents of this data set should be reviewed and replaced as appropriate, and the number of aluminium and alumino-silicate minerals increased.

2.1 Silica Species and Minerals

The master species selected for silica is $\text{Si}(\text{OH})_4^0$. It is the dominant species at pH values less than c. 9 in solutions with silica concentrations of the levels found in natural waters. Thermodynamic properties of this species, based on CODATA (COX *et al.* 1989) values for quartz (SiO_2) and the solubility of that mineral, are taken from GRENTHE *et al.* (1991). These values are given in Table A.1.

The silica minerals included in the supplemental data set are quartz, chalcedony, and amorphous silica. The equations chosen for the solubilities of these minerals are those selected by NORDSTROM *et al.* (1990), which were taken from the work of Fournier. Other expressions proposed for quartz solubility are reviewed by EIKENBERG (1990). Figure 2.1 compares the solubility of quartz and amorphous silica ($\text{SiO}_2(\text{am})$) given by the equations of NORDSTROM *et al.* (1990),

with values calculated from equations (5) and (6) of EIKENBERG (1990), and concentrations given by BOWERS *et al.* (1984).

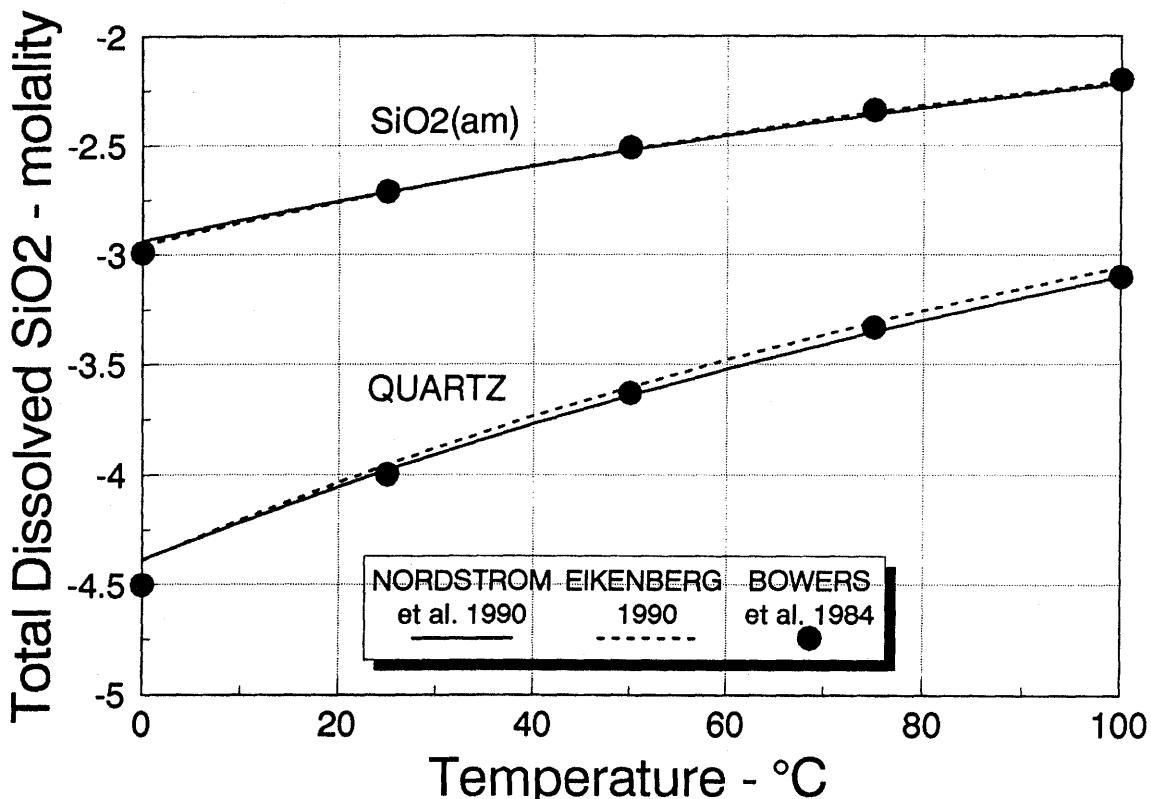


Figure 2.1: Solubility of quartz and amorphous SiO_2 from 0 to 100°C.

At pH values above c. 9, $\text{Si}(\text{OH})_4^0$ loses H^+ to form $\text{SiO}(\text{OH})_3^-$, and above pH c. 12, it loses another H^+ to form $\text{SiO}_2(\text{OH})_2^{2-}$. Also, at total dissolved silica concentrations above c. 10^{-2} mol, silica polymers may form. EIKENBERG (1990) has reviewed speciation models for dissolved silica and concludes that silica solubility at high pH values is best represented by an aqueous model that includes all three monomeric species, as well as a number of polymeric species.

Few waters have total dissolved silica concentrations approaching 10^{-2} mol (c. 600 mg SiO_2/l). Thus, only the monomeric aqueous species $\text{SiO}(\text{OH})_3^-$ and $\text{SiO}_2(\text{OH})_2^{2-}$ are included in this data base. The data for these species are those given by GRENTHE *et al.* (1991, Table IV.2) and recommended by

EIKENBERG (1990, Table 7). NORDSTROM *et al.* (1990) give 5-term expressions for the temperature dependence of logK of these species. The logK(25) and $\Delta_f H^0$ values from these expressions are -9.83 and 25.6 kJ/mol for SiO(OH)_3^- and -23.0 and 73.6 kJ/mol for $\text{SiO}_2(\text{OH})_2^{2-}$, which are in agreement with the values selected for this data base (Table A.2). These species also appear in the HATCHES data base, but their logK(25) values differ from those selected by 0.12 and -1.52, respectively (Table B.1).

Figure 2.2 shows the solubilities of quartz and amorphous silica calculated at various pH values using this data base. These figures also include analysed values for silica solubility from the compilation by EIKENBERG (1990, Appendix A). The figure illustrates that this data base will be adequate for quartz-saturated solutions at pH values up to 12, and temperatures to c. 90°C. It also shows that these data are useful only up to a silica concentration of c. 10^{-2} mol, which corresponds to amorphous silica saturation at a pH of c. 10.5 at 25°C. Although the solubility of silica minerals increases with temperature as shown in Figure 2.1, the tendency for polymers to form decreases with increasing temperature. Thus, this data base should also be useful in waters up to saturation with amorphous silica at temperatures higher than 25°C and pH values up to 10 or 10.5. If it is necessary to model solutions at higher silica concentrations or pH values, the polymeric species recommended by EIKENBERG (1990, Table 7) should be added to the data base.

2.2 Aluminium Species and Minerals

The master species selected for aluminium is Al^{+3} , which dominates only at pH values below c. 5 in natural waters. The properties of formation are those given by COX *et al.* (1989) and GRENTHE *et al.* (1991). An alternate choice for master species would be Al(OH)_4^- , which dominates at pH values above c. 8. There is no consensus about the properties of Al(OH)_4^- , however, and most data in the literature refer to reactions written with Al^{+3} .

Data for aluminium hydrolysis and association with F^- and SO_4^{2-} are taken from the compilation of NORDSTROM *et al.* (1990). Data on aluminium association with organic ligands are from HUMMEL (1991). The Al(OH)_3 solids given by NORDSTROM *et al.* (1990), crystalline and microcrystalline gibbsite and amorphous Al(OH)_3 , are also included. The stability of gibbsite in the HATCHES 3.0 data base is between the two values of NORDSTROM *et al.* (1990) (Table

B.2). NORDSTROM & MAY (1989) discuss the chemistry of aqueous aluminum at length.

2.3 Alumino-Silicate and Silicate Minerals

Alumino-silicate and silicate minerals are of great importance in determining the chemistry of water in all crystalline and in many sedimentary rock types. A number of characteristics of these minerals makes collection of their chemical thermodynamic data and their modelling very difficult. One characteristic is that many react so slowly at laboratory and normal groundwater temperatures that frequently it is not possible to attain equilibrium in reasonable experimental times. Thus, high temperature data extrapolated to lower temperatures are often used for groundwater modelling. Another characteristic is that such important alumino-silicate minerals as the clays have highly variable chemical compositions which adds uncertainty to their behaviour in solution.

Several large data sets have been compiled for use principally in examining phase relations in higher temperature assemblages resulting from metamorphic processes or the formation of hydrothermal ore deposits (BOWERS *et al*, 1984; JOHNSON *et al*, *in press*). Other data sets emphasize estimates of the properties of clay and other minerals active at lower temperatures (*e. g.* AAGAARD & HELGESON 1983; TARDY *et al*, 1987). Compilations of mineral data such as these were not reviewed and compared during the preparation of this auxiliary data set. Thus, only the limited number of alumino-silicate and silicate minerals included in the compilation of NORDSTROM *et al.* (1990) are included. The addition of alumino-silicate and silicate minerals to subsequent supplemental data sets should be given a high priority, however.

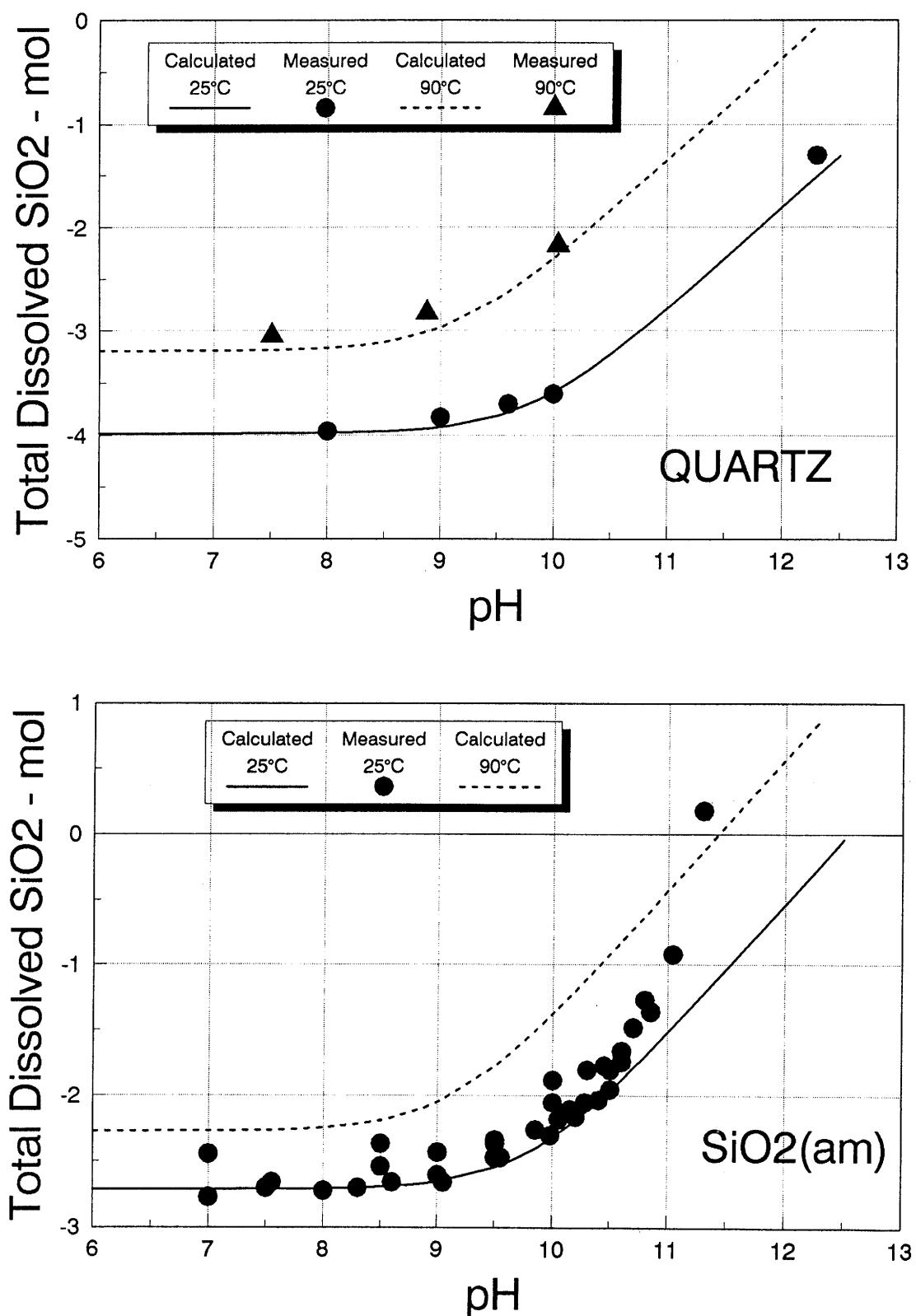


Figure 2.2: Solubilities of quartz and amorphous SiO_2 calculated from pH 6 to 12.5 and measured values reported by EIKENBERG (1990, Appendix A).

3 IRON AND MANGANESE

Iron and manganese are the most common metals in groundwaters that are influenced by redox processes. They are also significant in many commercial and environmental processes, so a great deal of chemical thermodynamic data are available for them. This supplemental data set includes the principal aqueous species of both metals, and products of their hydrolysis and of their association with the common anions F^- , Cl^- , CO_3^{2-} , and SO_4^{2-} . Ion pairs formed by these metals with representative organic anions are also included, as discussed in Chapter 6 below. The HATCHES 3.0 and MINEQL-PSI data bases include a few additional iron and manganese species, including products of their association with less common anions such as Br^- , I^- , CN^- , NH_3 , and PO_4^{3-} and its hydrolysis products (Tables B.1, B.3, and B.4).

3.1 Iron

The master species for iron is Fe^{+2} , ferrous iron, which is the stable oxidation state in aqueous solutions under reducing conditions, and is relatively soluble. The properties of formation chosen are those given by WAGMAN *et al.* (1982).

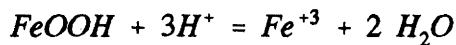
The other iron redox state of importance is Fe^{+3} , ferric iron, which is stable under oxidizing conditions. For the oxidation of Fe^{+2} to Fe^{+3} , $\log K(25) = -13.02$ and $\Delta_f H^0 = 40.5 \text{ kJ/mol}$ (NORDSTROM *et al.* 1990). Fe^{+3} forms relatively insoluble hydroxide solids and does not occur in measurable quantities in true solution, except under acid conditions. Ferric hydroxides readily form colloids. In oxidizing waters that have not been carefully filtered before analysis, these colloids can give rise to measurable iron concentrations at mid to high pH values.

Data for the ion association products of iron with inorganic ligands are taken from NORDSTROM *et al.* (1990), and virtually all are within 0.02 logK units of values in the HATCHES 3.0 and PSI data sets (Table B.1). Data on iron association with organic ligands are from HUMMEL (1991).

The solid iron phases in the auxiliary data base include ferrous carbonate (siderite) and hydrated sulphate (melanterite), and the ferric hydroxide phases goethite ($FeOOH$) and ferrihydrite ($Fe(OH)_3$). Metallic iron is also included. It is unstable in contact with water, but may be useful as a reactant when modelling corrosion and gas generation processes.

NORDSTROM *et al.* (1990) give two logK(25) values for siderite and ferrihydrite to indicate the range of stability of these minerals with varying crystallinity. Values for these minerals in the HATCHES 3.0 data base are between the value pairs in the auxiliary data base (Table B.2).

The value of logK(25) for the dissolution of goethite (FeOOH),



given by NORDSTORM *et al.* (1990) is -1.0. This is considerably different from the value 0.5 that is used in the HATCHES 3.0 and PSI data bases, and in other widely used data bases such as EQ3/EQ6-2345.1090 and the original PHREEQE (PARKHURST *et al.* 1980). The logK(25) value in this data base for the reaction



is -12.02, based on NORDSTROM *et al.* (1990). If the user prefers the more widely-used value for goethite stability, the logK(25) value in this data base should be changed to -13.52.

3.2 Manganese

The master species for manganese is Mn⁺², the manganous ion. This species is stable in aqueous solutions under most oxidizing conditions. Its properties of formation are those given by WAGMAN *et al.* (1982). In the presence of dissolved oxygen, relatively insoluble Mn⁺³ and Mn⁺⁴ oxide and hydroxide solids form, lowering the dissolved manganese concentration. Mn⁺³ and Mn⁺⁴ do not occur in measurable quantities in aqueous solutions, however.

Data for the ion association constants of Mn⁺² with inorganic ligands are taken from NORDSTROM *et al.* (1990) and, with a few exceptions, agree well with the data in the HATCHES 3.0 and PSI data bases (Table B.1). Data on Mn⁺² organic association are from HUMMEL (1991).

Data for manganese solids are also taken from NORDSTROM *et al.* (1990). These include Mn⁺² carbonate (rhodochrosite) and hydroxide (pyrochroite) and the Mn⁺³ and Mn⁺⁴ hydroxide and oxides MnOOH (manganite), Mn₃O₄ (hausmanite), and MnO₂ (pyrolusite).

There are two values for rhodochrosite, the more stable designated crystalline, and the less stable synthetic, following NORDSTROM *et al.* (1990). MINEQL-PSI includes both values while the data in HATCHES 3.0 and PHREEQE-PSI correspond to the less stable member of the pair. Values for pyrochroite are identical in the HATCHES 3.0, and both PSI data bases. Pyrolusite is 0.2 logK units less stable in the HATCHES 3.0 and MINEQL-PSI data bases, and in the HATCHES 3.0 data set, hausmanite is 0.3 and manganite is 14. logK units less stable than the values in the PSI and this auxiliary data base (Table B.2).

4 ACTINIDE ELEMENTS

Data for five of the actinide elements – thorium, uranium, neptunium, plutonium, and americium – are included in the supplemental data base. The data adopted for these elements are from the MINEQL-PSI data base. For all elements but uranium, these are derived from data used previously in calculations for the Nagra programme (*e. g.* SCHWEINGRUBER 1983). The data for uranium were taken from an early review draft of the NEA uranium data base (GRENTHÉ *et al.* 1991). All data for organic ligands are from HUMMEL (1991).

The MINEQL-PSI data base is redox decoupled – that is, each redox state of an element is represented by its own master species. The supplemental data for these elements are redox coupled, so that only one master species is given for them. The reaction data given here result from combining the association reactions in the MINEQL-PSI data base with reactions among the redox species selected for this data base, and given in Table A.2.

By virtue of the similarity of their electronic structure, these elements should have comparable chemical behaviour and thermodynamic properties. An actinide data set developed using correlation procedures similar to those used by HUMMEL (1991) for organic ligands could be made consistent and complete with respect to both the identity and the thermodynamic properties of aqueous species and solids of the various elements. For example, consistency and completeness checks based on elemental similarities were used to select the actinide data employed for assessing the performance of a potential Canadian repository (LEMIRE & GARISTO 1989). Such checks were not made on the contents of this data set, but are highly recommended as part of the preparation of future revisions.

4.1 Thorium

Thorium occurs only in the (IV) state in aqueous solutions, so Th^{+4} is the master species. Inorganic aqueous species and minerals of Th^{+4} are as given in the MINEQL-PSI data base. Data for solution complexes with organic ligands are those of HUMMEL (1991). The HATCHES 3.0 data base also includes data on thorium. With the exception of a few aqueous complexes and minerals, there is good agreement between the HATCHES and the MINEQL-PSI data sets (Tables B.1 and B.2). Data for a number of solids are included in the MINEQL-PSI data set, and even more in HATCHES. All the MINEQL-PSI minerals are included in

the supplemental data, but for groundwater systems, probably only the oxides and hydrated oxides will be important.

4.2 Uranium

Uranium IV (U^{+4}) and VI (UO_2^{+2}) are the most important redox states of uranium under natural conditions, although uranium III (U^{+3}) and V (UO_2^+) have limited fields of stability in aqueous solutions. U^{+4} is the master species in this data base, and many minerals and aqueous species of it and of UO_2^{+2} are included. U^{+3} and UO_2^+ and a limited number of their aqueous species and minerals are also included. Data for the reactions among the various redox states of uranium were taken from GRENTHÉ *et al.* (1991).

Data for uranium inorganic aqueous species and minerals are from the MINEQL-PSI data set, and data for organic aqueous species are from HUMMEL (1991). The MINEQL data were taken from a draft of the NEA uranium data set (GRENTHÉ *et al.* 1991). The final version of this data set (GRENTHÉ *et al.* 1992) was published during the last revision of this report, and the Nagra data have not been checked against the final NEA values.

Many uranium data are also given in the HATCHES 3.0 data base. As Tables B.1 and B.2 indicate, the agreement with the data chosen here is generally not good. The PHREEQE-PSI data base also includes a few uranium species, the values for which are in general agreement with the HATCHES 3.0 values. The PHREEQE-PSI data appear to be taken from the original PHREEQE data set (PARKHURST *et al.* 1980), and to include most species of importance in natural groundwaters.

A very large number of uranium solids are given in the MINEQL-PSI data base, most of which are also included in the supplemental data. For modelling groundwaters, probably only the oxide and hydrated oxide minerals will be important under reducing conditions. Oxidized uranium minerals form only under relatively high dissolved uranium concentrations.

4.3 Neptunium

Neptunium III (Np^{+3}), IV (Np^{+4}), V (NpO_2^+), and VI (NpO_2^{+2}) oxidation states are found in aqueous solutions. This data set uses Np^{+4} as the master species, and

includes aqueous species and minerals representing all four redox states. Data for the reactions among the various redox states were taken from an International Atomic Energy Agency critical review of the chemical thermodynamics of actinide elements and compounds (FUGER & OETTING 1976).

Data for neptunium inorganic species and minerals were taken from the MINEQL-PSI data base, and data for organic aqueous species, from HUMMEL (1991). The HATCHES 3.0 data base also contains data on a number of neptunium aqueous species and minerals. As Tables B.1 and B.2 show, the agreement between the two data sets ranges from fair to excellent.

Only a few neptunium solids are given in the MINEQL-PSI and this supplemental data base. The most important minerals for modelling will probably be the oxide or hydrated oxide of the dominant redox state of the element.

4.4 Plutonium

Like neptunium, plutonium occurs in aqueous solution in the III (Pu^{+3}), IV (Pu^{+4}), V (PuO_2^+), and VI (PuO_2^{+2}) redox states. Pu^{+4} is the master species in this data set, and data on the reactions among the redox states are taken from FUGER & OETTING (1976).

Data on aqueous species and minerals of plutonium were taken from the MINEQL-PSI data base and from HUMMEL (1991). The HATCHES 3.0 data base also contains plutonium data, most of which are in good to excellent agreement with the MINEQL-PSI data (Tables B.1 and B.2).

As for neptunium, only a few plutonium solids are given in the MINEQL-PSI and this supplemental data set. The oxide or hydrated oxides of the dominant redox state of the element will probably be the most important solids for modelling.

4.5 Americium

In aqueous solution, the americium III redox state dominates. Therefore, Am^{+3} is chosen as the master species, with thermodynamic properties given by FUGER & OETTING (1976). Data on inorganic species and minerals were taken from the MINEQL-PSI, and data on organic complexes from HUMMEL (1991). The

HATCHES 3.0 data base also includes americium data, which agree only moderately well with those from MINEQL-PSI (Tables B.1 and B.2).

Only the hydrated oxide $\text{Am}(\text{OH})_3$ solid is included in the MINEQL-PSI and this supplemental data set. The HATCHES 3.0 data base includes a number of additional solids, but the hydrated oxide should be sufficient for most modelling.

5 OTHER METALS

5.1 Nickel

The master species for nickel is Ni^{+2} , which is the stable oxidation state of the element in all natural waters. The properties of formation are those given by WAGMAN *et al.* (1982).

BAEYENS & MCKINLEY (1989) assembled data for aqueous species and minerals of nickel, which are included in the PHREEQE-PSI data base. All of these data for aqueous species are included in the supplemental data set. Nickel complexes with several organic ligands are also included, with data from HUMMEL (1991). There is generally excellent agreement between the data for inorganic aqueous species of nickel in the supplemental and PHREEQE-PSI data bases, and in the MINEQL-PSI and HATCHES 3.0 data sets (Table B.1).

Not all minerals in the PHREEQE-PSI data base are included here. Solids likely to be found under natural conditions have been selected. As Table B.2 shows, there is reasonable agreement among the data for nickel solids in the several data bases, except for some of those which include reduced sulphur species.

5.2 Zirconium

Only the HATCHES 3.0 data set includes information on inorganic zirconium aqueous species and minerals. These data, together with zirconium complexes with several organic ligands from HUMMEL (1991), are included in the supplemental data set.

5.3 Niobium

The data for niobium aqueous species and minerals are based on properties of formation given by WAGMAN *et al.* (1982). The master species is NbO_3^- , in which niobium is present as Nb(V). According to data given by BROOKINS (1988, p. 110), Nb^{+3} is stable in aqueous solutions only under strongly acidic reducing conditions.

WAGMAN *et al.* (1982) include data for a number of niobium solids. Only the oxides of Nb(IV) and Nb(V) are included here.

None of the other data bases examined include any niobium species or minerals.

5.4 Molybdenum

The master species for molybdenum is MoO_4^{-2} , in which molybdenum is present as Mo(VI). The properties of formation of this species are taken from WAGMAN *et al.* (1982).

The only aqueous species is a hydration product HMnO_4^- , which is given in the MINEQL-PSI data set. None of the other data bases include any molybdenum data.

Three molybdenum solid phases are included in the supplemental data set - elemental Mo, and the oxides MoO_2 and MoO_3 . The properties of the solids are those given by WAGMAN *et al.* (1982).

5.5 Technetium

The HATCHES 3.0 data base includes data on many aqueous species and minerals of this element. These, in turn, appear to have been taken from the most recent EQ3/EQ6 data base, version 3245.1090. The HATCHES data for inorganic aqueous species and minerals are included in this supplemental data set, as are the data of HUMMEL (1991) for organic ligands.

Species containing technetium in five oxidation states are included: III (Tc^{+3}), IV (TcO^{+2}), V (TcO_4^{-3}), VI (TcO_4^{-2}), and VII (TcO_4^{-1}). Technetium IV (TcO^{+2}) is the master species for this element. MINEQL-PSI also includes a few data for technetium which are in good to excellent agreement with those in HATCHES.

5.6 Palladium

The master species for palladium is Pd^{+2} . Its properties of formation are those given by WAGMAN *et al.* (1982).

BAEYENS & MCKINLEY (1989) assembled data for the aqueous species and minerals of palladium, which are included in the PHREEQE-PSI data base. The data for all but one of these aqueous species are included in this supplemental data set. The $\text{Pd}(\text{NO}_2)_4^{+2}$ species is not included because, as given in the PHREEQE-PSI data set, it dominates the solution chemistry of Pd^{+2} , which is unlikely. Palladium complexes with several organic ligands are also included, using data of HUMMEL (1991). The MINEQL-PSI data base also includes palladium species which are identical with those in PHREEQE-PSI data set.

Only solids likely to be formed under natural conditions have been selected from the PHREEQE-PSI data base for inclusion in the supplemental data set. These include elemental palladium and palladium oxide, hydroxide, and sulphides.

5.7 Tin

Tin is found in one of two oxidation states, Sn(II) or Sn(IV) in natural waters. Sn^{+2} has been chosen as the master species with data from WAGMAN *et al.* (1982).

Both the MINEQL-PSI and HATCHES 3.0 data bases include aqueous species and solids of tin. Aqueous species data from the HATCHES data base have been included in the supplemental data set together with complex data on tin complexes with organic ligands from HUMMEL (1991). Only SnOH^+ is common to both the MINEQL-PSI and HATCHES data bases, and the agreement between its properties is poor (Table B.1).

Only solids likely to be formed from natural waters have been selected for inclusion in the supplemental data set. These include oxides, hydroxides, and sulphides.

Tin is an important metal commercially, and is often found in ore deposits of hydrothermal origin. Chemical thermodynamic data on tin aqueous species and minerals have been developed for modelling the formation of tin deposits. Such data are included in the data base for EQ3/6 2345.1090 and should be examined as part of the next revision of the tin data included here.

6 ORGANIC ANIONS

Many organic substances yield anions that form aqueous complexes with metallic cations. Such substances may be naturally present in groundwater, or may be in the waste itself. There is an enormous number of organic compounds which are capable of forming complexes in aqueous solutions, and many organic ligands are included in some data bases. For examples, HATCHES 3.0 has 17, and MINEQL-PSI, 34 organic ligands.

This data base has adopted the approach and data of HUMMEL (1991). Rather than trying to assemble data on a large number of organic ligands, Hummel has chosen four compounds that are typical of large classes of complexing ligands, and has developed complete, consistent data for their complexes.

These ligands are two carboxylic acids, oxalic (OX^{-2}) and citric (CIT^{-3}), and two polyaminopolycarboxylic acids, nitrilotriacetic (NTA^{-3}) and ethylenedinitriolo-tetraacetic (EDTA^{-4}).

Hummel gives constants for the association of these ligands with the univalent ions H^+ , Na^+ , K^+ , NpO_2^+ , and PuO_2^+ , the divalent ions Mg^{+2} , Ca^{+2} , Sr^{+2} , Mn^{+2} , Fe^{+2} , Ni^{+2} , Pd^{+2} , Sn^{+2} , TcO_2^{+2} , UO_2^{+2} , NpO_2^{+2} , and PuO_2^{+2} , the trivalent ions Fe^{+3} , Al^{+3} , Am^{+3} , and Pu^{+3} , and the quadrivalent ions Zr^{+4} , Th^{+4} , U^{+4} , Np^{+4} , and Pu^{+4} . Hummel's data have been included directly in the supplemental data set, except that all reactions including elements with several redox states (*e. g.* iron, technetium, uranium, neptunium, and plutonium) have been written in terms of the master species of the element in this data base.

The HATCHES 3.0 data set also includes a number of the organic complexes given in this supplemental data base. As Table B.1 shows, many of the HATCHES values differ from those in this compilation. As discussed by HUMMEL (1991), these differences arise from the use of different procedures in adjusting measured data to zero ionic strength, or from the selection of data from different sources.

7 NON-METALS

7.1 Selenium

The master species chosen to represent selenium is selenite, SeO_3^{-2} , which dominates at moderate redox conditions at pH values above c. 7.3. The data base also includes the more oxidized selenate species, SeO_4^{-2} , and selenide, Se^{-2} , species, which prevail under strongly reducing conditions. BROOKINS (1988, Figure 4) shows the distribution of dissolved selenium species under various conditions of pH and redox potential.

The thermodynamic data chosen for all aqueous species except HSeO_3^- and H_2SeO_3 are the $\Delta_f G^\circ$ and $\Delta_f H^\circ$ values given by WAGMAN *et al.* (1982). The logK values for reactions calculated from these data are virtually identical with values given in the HATCHES 3.0 and EQ3/EQ6 version 3245.1090 data bases.

The NEA data set (GRENTHÉ *et al.* 1991) includes constants for the hydrolysis reactions of SeO_3^{-2} which differ from those corresponding to the WAGMAN *et al.* (1982) data. The GRENTHÉ *et al.* (1991) values were chosen for logK(25) and $\Delta_r H^\circ$ of HSeO_3^- . The values included in the MINEQL-PSI and PHREEQE-PSI data sets also adopt the GRENTHÉ *et al.* (1991) data for the hydrolysis of SeO_3^{-2} and are the same as those chosen here. The selenium data set included in the compilation by BAEYENS & MCKINLEY (1989), adopted the WAGMAN *et al.* (1982) data for all aqueous species.

COWAN (1988) has made an extensive review of selenium thermodynamic data. Data from this report were chosen by WERES *et al.* (1989) in their extensive field study of the behaviour of selenium in the Kesterson Reservoir, California. COWAN (1988) was not examined by BAEYENS & MCKINLEY (1989), nor during the preparation of the present report. Some of the values selected by GRENTHÉ *et al.* (1991) differ from Cowan's data, however.

A number of selenium solids are included in the EQ3/EQ6 data base, and in the compilation of BAEYENS & MCKINLEY (1989). The vast majority of these solids are either relatively soluble selenium chemical salts or rare minerals found as accessories in sulfide ore deposits and their oxidation zones. The only selenium solid exerting significant control on the selenium concentration of natural waters is

elemental selenium (WERES *et al.* 1989), so only that solid is included in this data base. Other solids could be added using the data of BAEYENS & MCKINLEY (1989) or EQ3/EQ6.

7.2 Iodine

Only three aqueous species of iodine are included in the supplemental data set, iodine (-I) as I^- and I_3^- and iodine (O) as I_2 . I^- is the master species with data of formation taken from COX *et al.* (1989). The constants for the other species are from the PHREEQE-PSI data base.

The HATCHES 3.0 data base includes a much larger number of iodine species, which could easily be included in the supplemental data set, if required.

8 FUTURE SUPPLEMENTAL DATA NEEDS

There are three broad areas in which further work would improve Nagra's ability to model geochemical processes. The first would be to extend the existing modelling capability to include such important but presently unmodelled processes as solid solution and sorption. The second would be to expand and refine the present thermochemical data base to include additional elements, aqueous species, and solids, as well as to delete species and solids that are unlikely to be important in any system being modelled. As the capability to model additional processes improves, it will also be necessary to include the data required for the additional processes. Finally, in order to assure that the results of geochemical modelling are of continuing high quality, it will be important to maintain familiarity with new thermochemical data and compilations, and to update the Nagra data set in response to this new information.

Several more specific recommendations are possible within the scope of these three broad areas. These include specific data needs, suggestions of sources of additional data, and approaches to reducing the data base size to improve the ease and speed of geochemical modelling.

The present data base includes few alumino-silicate minerals, even though the chemistry of many waters of importance to Nagra, in the crystalline and in clayey units such as the Opalinus and Valanginian marl, are probably controlled by reactions with such minerals. Information on alumino-silicate minerals can be found in data bases assembled for studying hydrothermal reactions, ore deposition and metamorphism, such as the most recent product of Helgeson and his students, SUPCRT92 (JOHNSON, *et al. in press*). Such data are also present in great profusion in the EQ3/EQ6 data base. There are also data sets developed for reactions occurring at normal groundwater temperatures (*e. g.* TARDY *et al.* 1987; GRIMAUD, *et al.* 1990) which are likely to be of particular interest.

The SUPCRT92 and EQ3/EQ6 data bases also include information on metals such as copper which are absent from the supplemental data base, and tin which, while present, may not be complete. The metals in SUPCRT92 are important in ore deposition, while EQ3/EQ6 is intended also for use in nuclear waste performance assessment and site characterization, and so also includes elements of particular interest for that purpose.

Extensive data bases such as HATCHES 3.0, EQ3/EQ6, and to a lesser extent the present Nagra supplemental data base, often contain very large numbers of aqueous species and solids for given combinations of elements. Such large data sets make calculation unwieldy by increasing the computer size requirements and time needed for modelling. Many of these species and minerals are probably unimportant under the conditions that are to be modelled using this data set, and modelling could be made more efficient if they were deleted from the data set. For example, LEMIRE & GARISTO (1989) have used a relatively small set of aqueous species and minerals in their modelling of the Canadian conceptual repository. This is particularly important if many repetitive geochemical calculations are to be done, as required in support of risk analyses, for example.

There are several specific groups of data that should be examined for early inclusion as supplemental data. All sulphide species are not included in this data set, but missing species should be in order that such processes as sulphide mineral oxidation or the precipitation of solid sulphide phases can be modelled. Inclusion of the sulphides will involve decisions about which stability values to adopt for the S⁻² ion, the inclusion of aqueous polysulphide species, and the addition of sulphide mineral data consistent with the choice of aqueous sulphide values. Aqueous sulphides are discussed by GRENTHE *et al.* (1991) and NORDSTROM & PUIGDOMENECH (1986), and aqueous species and extensive mineral data appear in SUPCRT92 (JOHNSON *et al. in press*) and in the EQ3/EQ6 data base.

The present Nagra data base is intended for use at pH values are below c. 10 to 11, but if environments including cement are considered, higher pH values are possible. BERNER (1990) describes the modelling of pore water evolution in cement. If this data base is to be used for such modelling, Berner's approach should be examined and his data included.

9 REFERENCES

- AAGAARD, P. & HELGESON, H.C. 1983: Activity/composition relations among silicates and aqueous solutions: II. Chemical and thermodynamic consequences of ideal mixing of atoms on homological sites in montmorillonites, illites, and mixed-layer clays: *Clays and Clay Minerals*, v. 31, p. 207-217.
- BAES, C.F., JR. & MESMER, R.E. 1976: *The Hydrolysis of Cations*. New York, John Wiley & Sons, 489 p.
- BAEYENS, B. & MCKINLEY, I.G. 1989: A PHREEQE Data Base for Pd, Ni, and Se. Baden, Switzerland, Nagra, Technical Report 88-28, 59 p.
- BALL, J.W. & NORDSTROM, D.K. 1991: User's Manual for WATEQ4F, with revised thermodynamic data base and test cases for calculating speciation of major, trace, and redox elements in natural waters. U. S. Geological Survey Open-File Report 91-183, 189 p.
- BERNER, U. 1990: A Thermodynamic Description of the Evolution of Pore Water Chemistry and Uranium Speciation During the Degradation of Cement: Baden, Switzerland, Nagra, Technical Report 90-12, 68 p.
- BOWERS, T.S., JACKSON, K.J. & HELGESON, H.C. 1984: Equilibrium Activity Diagrams for Co-Existing Minerals and Aqueous Solutions at Pressures and Temperatures to 5kb and 600°C. Berlin, Springer-Verlag, 397 p.
- BROOKINS, D.G. 1988: Eh-pH Diagrams for Geochemistry. Berlin, Springer-Verlag, 174 p.
- BUSENBERG, E. & PLUMMER, L.N. 1986: The solubility of BaCO₃(CR) (witherite) in CO₂-H₂O solutions between 0 and 90°C, evaluation of the association constants of BaHCO⁺₃(aq) and BaCO⁰₃(aq) between 5 and 80°C, and a preliminary evaluation of the thermodynamic properties of Ba²⁺(aq). *Geochimica et Cosmochimica Acta*, v. 50, p. 2225-2233.

BUSENBERG, E., PLUMMER, L.N. & PARKER, V.B. 1984: The solubility of strontianite (SrCO_3) in $\text{CO}_2\text{-H}_2\text{O}$ solutions between 2 and 91°C, the association constants of SrHCO_3^+ (aq) and SrCO_3^0 (aq) between 5 and 80°C and an evaluation of the thermodynamic properties of Sr^{2+} (aq) and SrCO_3 (cr) at 25°C and 1 atm total pressure. *Geochimica et Cosmochimica Acta*, v. 48, p. 2021-2035.

COWAN, C.E. 1988: Review of Selenium Thermodynamic Data. Palo Alto, California, Electric Power Research Institute, Report EA-5655, 62 p.

COX, J.D., WAGMAN, D.D., & MEDVEDEV, V.A., eds. 1989: CODATA Key Values for Thermodynamics. New York, Hemisphere Publishing, 271 p.

CROSS, J.E. & EWART, F.T. 1991: HATCHES - a thermodynamic database and management system: *Radiochimica Acta*, v. 52/53: Pt. 2, p. 421-422.

EIKENBERG, J. 1990: On the Problem of Silica Solubility at High pH. Baden, Switzerland, Nagra, Technical Report 90-36, 54 p.

FUGER, J. & OETTING, F.L. 1976: The Chemical Thermodynamics of Actinide Elements and Compounds Part 2: The Actinide Aqueous Ions: Vienna, International Atomic Energy Agency, 65 p.

GARVIN, D., PARKER, V.B. & WHITE, H.J., Jr., eds. 1987: CODATA Thermo-dynamic Tables: Selections for Some Compounds of Calcium and Related Mixtures: A Prototype Set of Tables. Washington, Hemisphere Publishing, 356 p.

GRENTHE, I., LEMIRE, R.J., MULLER, A.B., NGUYEN-TRUNG, C. & WANNER, H. 1991: Chemical Thermodynamics of Uranium. Gif-Sur-Yvette, Nuclear Energy Agency - Organisation for Economic Cooperation and Development, NEA-TDB, 655 p. (*Version of June, 1991*)

GRENTHE, I., FUGER, J., KONINGS, R.J.M., LEMIRE, R.J., MULLER, A.B., NGUYEN-TRUNG, C., WANNER, H. 1992: Chemical Thermodynamics 1: Chemical Thermodynamics of Uranium. Amsterdam, North-Holland, Nuclear Energy Agency, 715 p.

- GRIMAUD, D., BEAUCAIRE, C. & MICHARD, G. 1990: Modelling of the evolution of ground waters in a granite system at low temperature: the Stripa ground waters, Sweden: Applied Geochemistry, v. 5, p. 515-525.
- HUMMEL, W. *in press*: A new method to estimate the influence of organics on the solubility and speciation of radionuclides ("The backdoor approach"): Radiochimica Acta.
- HUMMEL, W. 1991: Thermodynamic Data Base for Organic Ligands: Würenlingen and Villigen, Switzerland, Paul Scherrer Institute, Internal Report TM-41-91-43, 52 p.
- JOHNSON, J.W., OELKERS, E.H. & HELGESON, H.C. *in press*: SUPCRT92: A software package for calculating the standard molal thermodynamic properties of minerals, gases, aqueous species, and reactions from 1 to 5000 bars and 0° to 1000°: Computers and Geosciences.
- LEMIRE, R.J. & GARISTO, F. 1989: The solubility of U, Np, Pu, Th and Tc in a geological disposal vault for used nuclear fuel: Pinawa, Manitoba, Atomic Energy of Canada Limited, AECL 10009, 123 p.
- NORDSTROM, D.K. & MAY, H.M. 1989: Aqueous Equilibrium Data for Mono-nuclear Aluminum Species: *in Sposito, G., ed., The Environmental Chemistry of Aluminum:* Boca Raton, FL, CRC Press, p. 29-53.
- NORDSTROM, D.K., PLUMMER, L.N., LANGMUIR, D., BUSENBERG, E., MAY, H.M., JONES, B.F. & PARKHURST, D.L. 1990: Revised Chemical Equilibrium Data for Major Water-Mineral Reactions and Their Limitations: *in Melchior, D. C., and Bassett, R. L., eds. Chemical Modeling of Aqueous Systems II.* Washington, D.C., American Chemical Society, ACS Symposium Series 416, p. 398-413.
- NORDSTROM, D.K. & PUIGDOMENECH, I. 1986: Redox chemistry of deep groundwaters in Sweden. Stockholm, Svensk Kärnbränslehantering AB [Swedish Nuclear Fuel and Waste Management Co.], SKB Technical Report 86-03, 30 p.

PARKHURST, D.L. 1990: Ion-Association Models and Mean Activity Coefficients of Various Salts: *in* Melchior, D. C., and Bassett, R.L. *eds.*, Chemical Modeling of Aqueous Systems II. American Chemical Society, ACS Symposium Series 41, p. 30-43.

PARKHURST, D.L., THORSTENSON, D.C. & PLUMMER, L.N. 1980: PHREEQE - A computer program for geochemical calculations. U. S. Geological Survey, Water-Resources Investigations 80-96, 210 p., revised and reprinted August 1990.

PEARSON, F.J., JR. & AVIS, J.D. 1989: PMATCH; A Program to Manage Thermochemical Data: Contract Report to Riso National Laboratory, Roskilde, Denmark, for the Commission of the European Communities. Directorate General for Science, Research and Development, 62 p.

PEARSON, F.J., JR. & BERNER, U. 1991: Nagra Thermochemical Data Base I. Core Data. Wettingen, Switzerland, Nagra, Technical Report 91-17, 70 p.

PLUMMER, L.N. & BUSENBERG, E. 1982: The solubilities of calcite, argonite and vaterite in CO₂-H₂O solutions between 0 and 90°C, and an evaluation of the aqueous model for the system CaCO₃-CO₂-H₂O. Geochimica et Cosmochimica Acta, v. 46, p. 1011-1040.

SCHWEINGRUBER, M. 1982: User's Guide for Extended MINEQL (EIR Version) - Standard Subroutine/Data Library Package. Würenlingen, Switzerland, EIR TM-45-82-38.

SCHWEINGRUBER, M. 1983: Actinide Solubility in Deep Groundwaters - Estimates for Upper Limits Based on Chemical Equilibrium Calculations. Baden, Switzerland, Nagra, Technical Report 83-24, 63 p.

TARDY, Y., DUPLAY, J. & FRITZ, B. 1987: Stability fields of smectites and illites as a function of temperature and chemical composition: Stockholm, Sweden, Svensk Karnbranslehantering AB (Swedish Nuclear Fuel and Waste Management Co.), SKB Technical Report 87-20, 34 p.

TRUESDELL, A.H. & JONES, B.F. 1974: WATEQ, A computer program for calculating chemical equilibria of natural waters. U. S. Geological Survey Journal of Research, v. 2, p. 233-248.

- WAGMAN, D.D., EVANS, W.H., PARKER, V.B., SCHUMM, R.H., HALOW, I., BAILEY, S.M., CHURNEY, K.L. & NUTTALL, R.L. 1982: The NBS tables of chemical thermodynamic properties: Selected values for inorganic and C₁ and C₂ organic substances in SI units. Journal of Physical and Chemical Reference Data, v. 11, Supplement No. 2, 392 p.
- WANNER, H. 1986: Modelling Interaction of Deep Groundwaters with Bentonite and Radionuclide Speciation. Würenlingen, Switzerland, Eidgenössisches Institut für Reaktorforschung, EIR-Bericht 589, 103 p.
- WERES, O., JAOUNI, A.R. & TSAO, L. 1989: The distribution, speciation and geochemical cycling of selenium in a sedimentary environment, Kesterson Reservoir, California, U.S.A.: Applied Geochemistry, v. 4, p. 543-563.
- WHITFIELD, M. 1979: Activity Coefficients in Natural Waters: *in* Pytkowicz, R. M., *ed.*. Activity Coefficients in Electrolyte Solutions, Volume II. Boca Raton, Florida, CRC Press, p. 153-299.
- WOLERY, T.J. 1983: EQ3NR A Computer Program for Geochemical Aqueous Speciation-Solubility Calculations: User's Guide and Documentation. Livermore, CA, Lawrence Livermore National Laboratory, UCRL 53414, 191 p.
- WOLERY, T.J., JACKSON, K.J., BOURCIER, W.L., BRUTON, C.J., VIANI, B.E., KNAUSS, K.G., and DELANY, J.M. 1990: Current Status of the EQ3/6 Software Package for Geochemical Modeling: *in* Melchior, D.C., and Bassett, R.L., *eds.*, Chemical Modeling of Aqueous Systems II. Washington, D.C., American Chemical Society, ACS Symposium Series 416, p. 104-116.

**APPENDIX A: Nagra Chemical Thermodynamic Data Base
05/92**

The Nagra chemical thermodynamic data are given in four tables:

- | | |
|-----|---------------------------|
| A.1 | Master Species |
| A.2 | Aqueous Product Species |
| A.3 | Minerals and Gases |
| A.4 | Reactions to Calculate Pe |

In the table for the master species, there is one line of data and at least one line of text for each species. The line of data contains:

Master species name

Formula Weight

Charge

OPV: Operational Valence (see PEARSON & BERNER 1991, Section 2.4)

DH a: Debye-Hückel parameter a_i or a_i^0

DH b: Debye-Hückel parameter b_i or zero

$\Delta_f G^0$: Gibbs energy of formation (kJ mol⁻¹)

$\Delta_f H^0$: Enthalpy of formation (kJ mol⁻¹)

$\Delta_f S^0$: Entropy of formation (J K⁻¹ mol⁻¹)

CpA, CpB, CpC: Coefficients a, b, and c of the Maier-Kelley heat capacity equation (see PEARSON & BERNER 1991, Section 2.2)

The first line of text gives the sources for the data. The citations are as they appear in the reference section of this report. The second line, if present, gives values from other data bases for comparison with the values chosen.

Tables A2 through A4 contain the reaction data for aqueous product species, minerals and gases, and reactions with which Pe values can be calculated from measured concentrations of oxidized and reduced species. There are three lines of data and at least one line of text for each entity.

The first line begins with the name of the product species, mineral, gas, or redox couple, and continues with the association reaction for the entity. The second line includes thermodynamic and other properties of the entity and its association reaction. Many of the properties given in this line are the same as for the master species, but the following additional properties also appear:

$\Delta_f C_p^0$: Heat capacity of formation at 25 °C

$\Delta_r C_p^0$: Heat capacity of reaction at 25 °C

$\Delta_r H^0$: Enthalpy of reaction at 25 °C

$\log K(25)$: logK of reaction at 25 °C.

The third line of data contains one or more of the five parameters A through E of the following equation for logK as a function of temperature:

$$\log K(T) = A + BT + \frac{C}{T} + D\log(T) + \frac{E}{T^2}$$

Following the numerical data, there are one or more lines of text. The first line or two gives the sources of the data chosen for the reaction. For some entities, there is an additional first line of text that gives values for properties of the entity from sources of data other than the source chosen. Comparing these values with the numerical data for the entity indicates the level of consistency of the Nagra data set with other thermodynamic data sets.

As an example, consider the product species CO_3^{2-} . The first line of text shows that the values chosen for the data set were the coefficients of the logK equation given by PLUMMER AND BUSENBERG (1982), which are the same values given by NORDSTROM *et al.* (1990). The second line of text provides the information that the $\Delta_f G^0$ and $\Delta_f H^0$ values given by COX *et al.* (1989) are -527.90 and -675.23 kJ mol⁻¹, respectively. For comparison, the values of these properties in the core data set given in the second line of data are -527.919 and -675.314 kJ mol⁻¹, respectively.

Table A.1

Nagra Data Base, 05/92 Master Species

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	Formula Weight	Charge	OPV	DH a	DH b	$\Delta_f G^0$	$\Delta_f H^0$	$\Delta_f S^0$	CpA	CpB	CpC
H+	1.008 dfG0, dfH0 = 0.0 by convention	1.0	0.00	9.00	0.00	0.000	0.000	0.000	0.000	0.000000E+00	0.000000E+00
E-	0.001 dfG0, dfH0 = 0.0 by convention	-1.0	-1.00	0.00	0.00	0.000	0.000	0.000	0.000	0.000000E+00	0.000000E+00
H2O	18.015 dfG0, dfH0, dfCp0: COX et al.(1989)	0.0	0.00	0.00		-237.140	-285.830	-163.307	31.826	0.000000E+00	0.000000E+00
AL+3	26.982 dfG0, dfH0: COX et al.(1989) EQ3/6 3245.1090: dfG0 = -482.74 jk/mol, dfH0 = -527.68 jk/mol	3.0	0.00	6.65	0.19	-491.500	-538.400	-157.303			
AM+3	243.000 dfG0, dfH0: FUGER & OETTING (1976); EQ3/6 3245.1090	3.0	3.00	9.00	0.00	-599.100	-616.700	-59.031			
AS(OH)3	125.944 dfG0, dfH0: WAGMAN et al. (1982)	0.0	3.00	0.00		-639.800	-742.200	-343.451			
B(OH)3	61.832 dfG0, dfH0: WAGMAN et al. (1982); COX et al.(1989)	0.0	0.00	0.00		-969.300	-1072.800	-347.141			
BA+2	137.330 dfG0, dfH0: BUSENBERG & PLUMMER (1986)	2.0	0.00	4.55	0.09	-555.360	-532.500	76.673			
BR-	79.904 dfG0, dfH0: COX et al.(1989); dfCp0: WAGMAN et al. (1982)	-1.0	0.00	3.00	0.00	-103.850	-121.410	-58.897	-194.100		
CA+2	40.080 dfG0, dfH0: COX et al.(1989).	2.0	0.00	4.86	0.15	-552.807	-543.000	32.893	-278.470		
CH4(AQ)	16.043 dfG0, dfH0: WAGMAN et al. (1982); CH4(g); WHITFIELD (1979) solubility data	0.0	-4.00	0.00		-34.416	-88.607	-181.758	177.310	-2.385011E-03	
CIT-3	189.101 dfG0, dfH0 = 0.0 by default	-3.0	0.00	0.00	0.00	0.000	0.000	0.000			
CL-	35.453 dfG0, dfH0: COX et al.(1989); dfCp0: WAGMAN et al. (1982)	-1.0	0.00	3.71	0.01	-131.220	-167.080	-120.275	-167.800		

Table A.1

Nagra Data Base, 05/92 Master Species

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	Formula Weight	Charge	OPV	DH a	DH b	$\Delta_f G^0$	$\Delta_f H^0$	$\Delta_f S^0$	CpA	CpB	CpC
EDTA-4	288.213	-4.0	0.00	0.00	0.00	0.000	0.000	0.000			
						dfG0, dfH0 = 0.0 by default					
F-	18.998	-1.0	0.00	3.46	0.08	-281.520	-335.350	-180.547	-136.800		
						dfG0, dfH0: COX et al.(1989); dfCp0: WAGMAN et al. (1982)					
FE+2	55.847	2.0	2.00	5.08	0.16	-78.900	-89.100	-34.211			
						dfG0, dfH0: WAGMAN et al. (1982)					
						EQ3/6 3245.1090: dfG0 = -91.50 kj/mol, dfH0 = -92.26 kj/mol					
H2(AQ)	2.016	0.0	2.00	0.00		17.726	-4.039	-73.000	218.769	-2.501489E-01	
						dfG0, dfH0, dfCp0: COX et al.(1989): H2(g); WHITFIELD (1979) solubility					
HASO4-2	139.927	-2.0	5.00	4.00	0.00	-714.600	-906.340	-643.099			
						dfG0, dfH0: WAGMAN et al. (1982); GRENTHE et al. (1991)					
HCO3-	61.017	-1.0	4.00	5.40	0.00	-586.875	-690.215	-346.604	749.276	-1.572479E+00	3.888421E+07
						dfG0, dfH0, dfCp0: COX et al.(1989): CO2(g); PLUMMER & BUSENBERG (1982) logK(h) logK(1).					
HPO4-2	95.979	-2.0	0.00	4.00	0.00	-1095.990	-1299.000	-680.899			
						dfG0, dfH0: COX et al.(1989)					
HS-	33.068	-1.0	-2.00	3.50	0.00	12.240	-16.300	-95.724			
						dfG0, dfH0: COX et al.(1989)					
I-	126.905	-1.0	0.00	3.00	0.00	-51.720	-56.780	-16.971			
						dfG0, dfH0: COX et al.(1989)					
K+	39.098	1.0	0.00	3.71	0.01	-282.510	-252.140	101.861			
						dfG0, dfH0: COX et al.(1989)					
Li+	6.941	1.0	0.00	4.76	0.20	-292.920	-278.470	48.466			
						dfG0, dfH0: COX et al.(1989)					
MG+2	24.305	2.0	0.00	5.46	0.22	-455.400	-467.000	-38.907			
						dfG0, dfH0: COX et al.(1989)					
MN+2	54.938	2.0	2.00	7.04	0.22	-228.100	-220.750	24.652			
						dfG0, dfH0: WAGMAN et al. (1982); EQ3/6 3245.1090					

Table A.1

Nagra Data Base, 05/92 Master Species

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Table A.1

Nagra Data Base, 05/92 Master Species

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Table A.2

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Table A.2

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Table A.2

Nagra Data Base, 05/92 Product Aqueous Species

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Charge log(K(T)):	OPV A	DH a B	DH b C	$\Delta_f G^0$ $\Delta_f H^0$	$\Delta_f S^0$ $\Delta_f Cp^0$	CpA E	CpB	CpC	$\Delta_r Cp^0$	$\Delta_r H^0$	logK(25)
ALOH2+		1.000	AL+3	2.000 H2O	-2.000 H+						
	1.0	0.00	4.00	0.00 -908.080	-997.494 -299.895				-225.492	112.566	-10.109
				8.850000E+01 0.000000E+00	-9.391600E+03 -2.712100E+01	0.000000E+00					
						logK coef: NORDSTROM et al. (1990)					
						NORDSTROM & MAY(1989): GF = -904.3, HF = -990., CPAF = -194.					
ALOH30		1.000	AL+3	3.000 H2O	-3.000 H+						
	0.0	0.00	0.00	-1106.226 -1228.987	-411.744				-611.908	166.903	-16.940
				2.263740E+02 0.000000E+00	-1.824780E+04 -7.359700E+01	0.000000E+00					
						logK coef: NORDSTROM et al. (1990)					
						NORDSTROM & MAY(1989): GF = -1104., HF = -1222., CPAF = -505.					
ALOH4-		1.000	AL+3	4.000 H2O	-4.000 H+						
	-1.0	0.00	0.00	0.00 -1310.689 -1504.747	-650.872				-123.592	176.973	-22.665
				5.157800E+01 0.000000E+00	-1.116890E+04 -1.486500E+01	0.000000E+00					
						logK coef: NORDSTROM et al. (1990)					
						NORDSTROM & MAY(1989): GF = -1307., HF = -1478., CPAF = 58.5					
ALOHEDTA-2		1.000	AL+3	1.000 EDTA-4	1.000 H2O	-1.000 H+					
	-2.0	0.00	0.00	0.00 -801.701						12.800	
				1.280000E+01							
						logK(25): HUMMEL(1991)					
ALOHNTA-		1.000	AL+3	1.000 NTA-3	1.000 H2O	-1.000 H+					
	-1.0	0.00	0.00	0.00 -776.016						8.300	
				8.300000E+00							
						logK(25): HUMMEL(1991)					
ALOX+		1.000	AL+3	1.000 OX-2							
	1.0	0.00	0.00	0.00 -534.880						7.600	
				7.600000E+00							
						logK(25): HUMMEL(1991)					
ALOX2-		1.000	AL+3	2.000 OX-2							
	-1.0	0.00	0.00	0.00 -566.274						13.100	
				1.310000E+01							
						logK(25): HUMMEL(1991)					

Table A.2

Nagra Data Base, 05/92 Product Aqueous Species

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Charge logK(T):	OPV A	DH a B	DH b C	$\Delta_f G^0$ $\Delta_f H^0$	$\Delta_f S^0$ $\Delta_f Cp^0$	CpA E	CpB F	CpC G	$\Delta_f Cp^0$ $\Delta_f H^0$	logK(25)
AMCO33-3		1.000	AM+3	3.000	HCO3-	-3.000	H+			
	-3.0	15.00	0.00	0.00	-2263.909					-16.787
				-1.678654E+01						
				LogK(25): MINEQL-PSI Mar-91						
AMEDTA-		1.000	AM+3	1.000	EDTA-4					
	-1.0	3.00	0.00	0.00	-714.970					20.300
				2.030000E+01						
				LogK(25): HUMMEL(1991)						
AMEDTA2-5		1.000	AM+3	2.000	EDTA-4					
	-5.0	3.00	0.00	0.00	-737.231					24.200
				2.420000E+01						
				LogK(25): HUMMEL(1991)						
AMF+2		1.000	AM+3	1.000	F-					
	2.0	3.00	0.00	0.00	-906.306					4.500
				4.500074E+00						
				LogK(25): MINEQL-PSI Mar-91						
AMF2+		1.000	AM+3	2.000	F-					
	1.0	3.00	0.00	0.00	-1207.803					8.000
				7.999956E+00						
				LogK(25): MINEQL-PSI Mar-91						
AMF3		1.000	AM+3	3.000	F-					
	0.0	3.00	0.00		-1507.589					11.200
				1.120008E+01						
				LogK(25): MINEQL-PSI Mar-91						
AMH2PO4+		1.000	AM+3	1.000	HPO4-2	1.000	H+			
	2.0	3.00	0.00	0.00	-1751.363					9.859
				9.858782E+00						
				LogK(25): MINEQL-PSI Mar-91						
AMH4PO42		1.000	AM+3	2.000	HPO4-2	2.000	H+			
	1.0	3.00	0.00	0.00	-2894.493					18.118
				1.811750E+01						
				LogK(25): MINEQL-PSI Mar-91						

Table A.2

Nagra Data Base, 05/92 Product Aqueous Species

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Nagra Data Base, 05/92 Product Aqueous Species

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Charge logK(T):	OPV A	DH a B	DH b C	$\Delta_f G^0$ $\Delta_f H^0$	$\Delta_f S^0$ $\Delta_f Cp^0$	$\Delta_f Cp^0$ E	CpA CpB	CpC	$\Delta_r Cp^0$ $\Delta_r H^0$	logK(25)
FE3(OH)4+5		3.000	FE+2	4.000 H2O	-4.000 H+	-3.000 E-				
	5.0	9.00	9.00	0.00 -926.349	-1229.285	-1016.053			0.000	181.334
				-1.359099E+01	0.000000E+00	-9.471929E+03	0.000000E+00	-0.000000E+00		-45.360
FECIT		1.000	FE+2	-1.000 E-	1.000 CIT-3					
	0.0	3.00	0.00	-76.845						-0.360
				-3.600000E-01						
FECIT-		1.000	FE+2	1.000 CIT-3						
	-1.0	2.00	0.00	0.00 -113.718						6.100
				6.100000E+00						
FECIT2-3		1.000	FE+2	-1.000 E-	2.000 CIT-3					
	-3.0	3.00	0.00	0.00 -108.067						5.110
				5.110000E+00						
FECL+		1.000	FE+2	1.000 CL-						
	1.0	2.00	4.00	0.00 -210.919						0.140
				1.400000E-01						
FECL2+		1.000	FE+2	-1.000 E-	1.000 CL-					
	2.0	3.00	4.00	0.00 -144.251	-192.249	-160.985			0.000	63.931
				-3.394829E-01	0.000000E+00	-3.339434E+03	0.000000E+00	-0.000000E+00		-11.540
FECL2+		1.000	FE+2	-1.000 E-	2.000 CL-					
	1.0	3.00	4.00	0.00 -279.181	-382.759	-347.402			0.000	40.501
				-3.794386E+00	0.000000E+00	-2.115557E+03	0.000000E+00	-0.000000E+00		-10.890
FECL30		1.000	FE+2	-1.000 E-	3.000 CL-					
	0.0	3.00	0.00	-404.693	-549.839	-486.822			0.000	40.501
				-4.794386E+00	0.000000E+00	-2.115557E+03	0.000000E+00	-0.000000E+00		-11.890

logK(25), drHO: NORDSTROM et al. (1990)
 logK(25): HUMMEL(1991), plus Fe+3 redox
 logK(25): HUMMEL(1991)

logK(25), drHO: NORDSTROM et al. (1990)
 logK(25): HUMMEL(1991), plus Fe+3 redox
 logK(25), drHO: NORDSTROM et al. (1990)

logK(25), drHO: NORDSTROM et al. (1990)
 logK(25), drHO: NORDSTROM et al. (1990)

logK(25), drHO: NORDSTROM et al. (1990)
 logK(25), drHO: NORDSTROM et al. (1990)

logK(25), drHO: NORDSTROM et al. (1990)

1 INTRODUCTION

The chemical thermodynamic data set used by Nagra for geochemical modelling includes two types of data - core data and supplemental, or auxiliary, data.

Well-characterized aqueous species, minerals, and gases of elements commonly found in significant quantities in natural waters are represented by core data. These data have been carefully selected and, to assure comparability of the results of modelling done at different times, will be fixed. The Nagra core chemical thermodynamic data are described by PEARSON & BERNER (1991).

Supplemental, or auxiliary, data are for elements that are found in natural waters, but not as major components, or that are of interest principally for the safety assessment of nuclear waste facilities. Less common aqueous species and minerals of core elements are also included among the supplemental data. Supplemental aqueous species, and minerals are less well-characterized than those in the core data. While the supplemental data set described here includes what are thought to be the best values available, it is recognized that better estimates of many values will be developed from continuing experimental work and improved critical reviews. To permit the inclusion of recent or improved data in Nagra calculations, supplemental data are subject to revision.

This data base has not yet been tested for a full range of nuclear waste management applications, although such work is in progress. It should thus be regarded as a reference fixed point for quality assurance purpose and not a critically reviewed standard.

This report describes the supplemental data in the Nagra chemical thermodynamic data base as of May, 1992. It includes the elements aluminum, silicon, iron, and manganese which are important in the chemistry of natural waters, but not included in the core data. It also contains a number of elements of importance in nuclear waste safety assessment including the actinide elements thorium, uranium, neptunium, plutonium, and americium, and certain fission activation products found in the waste, including the metals nickel, zirconium, niobium, molybdenum, technetium, palladium, tin, and the non-metals selenium and iodine. Data on aqueous complexes formed by metals in the data base with certain representative organic anions are also included.

The data are given in the tables of Appendix A. These tables include not only the supplemental data described here, but also the core data. Therefore, they represent the complete Nagra thermochemical data base as of May, 1992. A few of the core data in these tables differ from and supersede data in PEARSON & BERNER (1991). The

Table A.2

Nagra Data Base, 05/92 Product Aqueous Species

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Table A.2

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and virtually all the supplemental species and minerals have only Δ_rH^0 values, or no data at all with which to calculate logK values at temperatures other than 25°C. Figure 2.1 of PEARSON & BERNER (1991) illustrates the errors in logK values that can result from insufficient temperature corrections.

When adapting values from other data sets for inclusion in the Nagra data base, it was sometimes necessary to change master species. For example, in the MINEQL-PSI data base from which all actinide data were adapted, the master species for carbonate is CO_3^{2-} , while in the Nagra data base, it is HCO_3^- . In making these changes, only the minimum data were carried into the Nagra data set. For example, no Δ_rH^0 value is given in the MINEQL-PSI data base for the reaction forming the aqueous species $\text{NpO}_2\text{CO}_3^0$. In the Nagra data base, a Δ_rH^0 value is available for the reaction between CO_3^{2-} and HCO_3^- , but it is not carried into the converted reaction for $\text{NpO}_2\text{CO}_3^0$ formation from HCO_3^- . The user should be aware that this could lead to differences between logK values calculated from the Nagra data base and from other data bases at temperatures different from 25°C.

1.3 Redox Reactions

As discussed in the text accompanying the core data base (PEARSON & BERNER 1991, Section 2.5), redox reactions for a given element can be treated as decoupled or coupled.

If reactions among several oxidation states of an element occur relatively slowly, or if it is common that the concentration of species in different oxidation states are analyzed separately, redox reactions of the element are treated as decoupled. Decoupled elements have several master species in the data base, one for each oxidation state. These elements and their master species are:

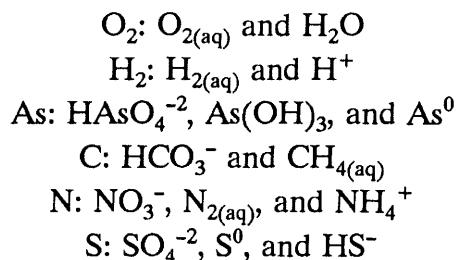


Table A.4 gives the data needed to calculate oxidation potentials (*pe* values) from measured concentrations of pairs of master species.

If it is assumed that redox reactions of an element occur relatively rapidly, or if the total concentration of an element is measured or to be calculated, coupled redox reactions are written. Only one master species is selected for redox-coupled elements, and the concentrations of other oxidation states are calculated from the total concentration, the coupled redox reactions, and the oxidation state (*pe*) of the solution (*e. g.* TRUESDELL & JONES 1974). Elements in this data base which include coupled redox reactions, and their master species, are:

Fe: Fe⁺²
Mn: Mn⁺²
Np: Np⁺⁴
Pu: Pu⁺⁴
Se: SeO₃⁻²
Sn: Sn⁺²
Tc: TcO⁺²
U: U⁺⁴

Table A.2

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Table A.2

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Charge logK(T):	OPV A	DH a B	DH b C	$\Delta_f G^0$ $\Delta_f H^0$	$\Delta_f S^0$ $\Delta_f Cp^0$	CpA E	CpB	CpC	$\Delta_f Cp^0$ $\Delta_f H^0$	logK(25)
MGEDTA-2		1.000	MG+2	1.000	EDTA-4					
	-2.0	0.00	0.00	0.00	-515.333					10.500
				1.050000E+01						
				logK(25): HUMMEL(1991)						
MGF+		1.000	MG+2	1.000	F-					
	1.0	0.00	4.00	0.00	-747.308 -788.961	-139.704			0.000	13.389
				4.165659E+00	0.000000E+00	-6.993582E+02	0.000000E+00	-0.000000E+00		1.820
				logK(25), drHO: NORDSTROM et al. (1990)						
MGH2CIT+		1.000	MG+2	2.000	H+	1.000	CIT-3			
	1.0	0.00	0.00	0.00	-525.607					12.300
				1.230000E+01						
				logK(25): HUMMEL(1991)						
MGHCIT		1.000	MG+2	1.000	H+	1.000	CIT-3			
	0.0	0.00	0.00		-506.771					9.000
				9.000000E+00						
				logK(25): HUMMEL(1991)						
MGHCO3+		1.000	MG+2	1.000	HCO3-					
	1.0	4.00	4.00	0.00	-1048.372 -1153.927	-354.032			173.960	3.288
				-5.921500E+01	0.000000E+00	2.537455E+03	2.092298E+01	0.000000E+00		1.068
				logK coef: NORDSTROM et al. (1990)						
MGHEDTA-		1.000	MG+2	1.000	H+	1.000	EDTA-4			
	-1.0	0.00	0.00	0.00	-539.877					14.800
				1.480000E+01						
				logK(25): HUMMEL(1991)						
MGNTA-		1.000	MG+2	1.000	NTA-3					
	-1.0	0.00	0.00	0.00	-492.501					6.500
				6.500000E+00						
				logK(25): HUMMEL(1991)						
MGOH+		1.000	MG+2	1.000	H2O	-1.000	H+			
	1.0	0.00	0.00	0.00	-627.242					-11.440
				-1.144000E+01						
				logK(25), drHO: NORDSTROM et al. (1990)						

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Charge logK(T):	OPV A	DH a B	DH b C	$\Delta_f G^0$ $\Delta_f H^0$	$\Delta_f S^0$ $\Delta_f Cp^0$	CpA E	CpB	CpC	$\Delta_f Cp^0$	$\Delta_f H^0$	logK(25)
MGOX		1.000	MG+2	1.000	OX-2						
	0.0	0.00	0.00	-474.921							3.420
				3.420000E+00							
				logK(25): HUMMEL(1991)							
MGOX2-2		1.000	MG+2	2.000	OX-2						
	-2.0	0.00	0.00	0.00	-484.396						5.080
				5.080000E+00							
				logK(25): HUMMEL(1991)							
MGSO40		1.000	MG+2	1.000	SO4-2						
	0.0	6.00	0.00	-1212.928	-1357.303	-484.236			0.000	19.037	2.370
				5.705234E+00	0.000000E+00	-9.943999E+02	0.000000E+00	-0.000000E+00			
				logK(25), drHO: NORDSTROM et al. (1990)							
MNCIT-		1.000	MN+2	1.000	CIT-3						
	-1.0	2.00	0.00	0.00	-257.210						5.100
				5.100000E+00							
				logK(25): HUMMEL(1991)							
MNCL+		1.000	MN+2	1.000	CL-						
	1.0	2.00	4.00	0.00	-362.802						0.610
				6.100000E-01							
				logK(25), drHO: NORDSTROM et al. (1990)							
MNCL20		1.000	MN+2	2.000	CL-						
	0.0	2.00	0.00	-491.967							0.250
				2.500000E-01							
				logK(25), drHO: NORDSTROM et al. (1990)							
MNCL3-		1.000	MN+2	3.000	CL-						
	-1.0	2.00	4.00	0.00	-619.991						-0.310
				-3.100000E-01							
				logK(25), drHO: NORDSTROM et al. (1990)							
MNCO30		1.000	MN+2	1.000	HCO3-	-1.000	H+				
	0.0	6.00	0.00	-783.987							-5.429
				-5.429000E+00							
				logK(25), drHO: NORDSTROM et al. (1990)							

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Charge logK(T):	OPV A	DH a B	DH b C	$\Delta_f G^0$ $\Delta_f H^0$	$\Delta_f S^0$ $\Delta_f Cp^0$	CpA E	CpB F	CpC G	$\Delta_f Cp^0$ $\Delta_f H^0$	logK(25)
NI4(OH)4		4.000	NI+2	4.000 H2O	-4.000 H+					
	4.0	0.00	0.00	0.00 -972.623						-27.740
				-2.774000E+01						
				LogK(25), drHO: PHREEQE-PSI Apr-91						
NICIT-		1.000	NI+2	1.000 CIT-3						
	-1.0	0.00	0.00	0.00 -82.701						6.500
				6.500000E+00						
				LogK(25): HUMMEL(1991)						
NICIT2-4		1.000	NI+2	2.000 CIT-3						
	-4.0	0.00	0.00	0.00 -95.259						8.700
				8.700000E+00						
				LogK(25): HUMMEL(1991)						
NICL+		1.000	NI+2	1.000 CL-						
	1.0	0.00	0.00	0.00 -179.103						0.400
				4.000000E-01						
				LogK(25), drHO: PHREEQE-PSI Apr-91						
NICL2		1.000	NI+2	2.000 CL-						
	0.0	0.00	0.00	-313.520						0.960
				9.600000E-01						
				LogK(25), drHO: PHREEQE-PSI Apr-91						
NICO3		1.000	NI+2	1.000 HCO3-	-1.000 H+					
	0.0	4.00	0.00	-606.510						-4.549
				-4.549000E+00						
				LogK(25), drHO: PHREEQE-PSI Apr-91						
NICO32		1.000	NI+2	2.000 HCO3-	-2.000 H+					
	-2.0	8.00	0.00	0.00 -1159.143						-10.548
				-1.054800E+01						
				LogK(25), drHO: PHREEQE-PSI Apr-91						
NIEDTA-2		1.000	NI+2	1.000 EDTA-4						
	-2.0	0.00	0.00	0.00 -160.329						20.100
				2.010000E+01						
				LogK(25): HUMMEL(1991)						

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Charge logK(T):	OPV A	DH a B	DH b C	$\Delta_f G^0$ $\Delta_f H^0$	$\Delta_f S^0$ $\Delta_f Cp^0$	CpA E	CpB	CpC	$\Delta_r Cp^0$ $\Delta_r H^0$	logK(25)
NINH32		1.000	NI+2	2.000 NH4+	-2.000 H+					
	2.0	-6.00	0.00	0.00 -128.085	-247.969	-402.093		0.000	72.551	-13.370
				-6.594615E-01	0.000000E+00	-3.789647E+03	0.000000E+00	-0.000000E+00		
				LogK(25), drHO: PHREEQE-PSI Apr-91						
NINH36		1.000	NI+2	6.000 NH4+	-6.000 H+					
	2.0	-18.00	0.00	0.00 -256.240	-634.695	-1269.345		0.000	218.865	-46.560
				-8.215809E+00	0.000000E+00	-1.143232E+04	0.000000E+00	-0.000000E+00		
				LogK(25), drHO: PHREEQE-PSI Apr-91						
NINO3+		1.000	NI+2	1.000 NO3-						
	1.0	5.00	0.00	0.00 -158.673						0.400
				4.000000E-01						
				LogK(25), drHO: PHREEQE-PSI Apr-91						
NINO32		1.000	NI+2	2.000 NO3-						
	0.0	5.00	0.00	-263.755						-0.600
				-6.000000E-01						
				LogK(25), drHO: PHREEQE-PSI Apr-91						
NINTA-		1.000	NI+2	1.000 NTA-3						
	-1.0	0.00	0.00	0.00 -118.433						12.760
				1.276000E+01						
				logK(25): HUMMEL(1991)						
NINTA2-4		1.000	NI+2	2.000 NTA-3						
	-4.0	0.00	0.00	0.00 -142.349						16.950
				1.695000E+01						
				logK(25): HUMMEL(1991)						
NIOH+		1.000	NI+2	1.000 H2O	-1.000 H+					
	1.0	0.00	0.00	0.00 -227.316	-287.907	-203.221		0.000	51.923	-9.710
				-6.132421E-01	0.000000E+00	-2.712198E+03	0.000000E+00	-0.000000E+00		
				LogK(25), drHO: PHREEQE-PSI Apr-91						
NIOH2		1.000	NI+2	2.000 H2O	-2.000 H+					
	0.0	0.00	0.00	-405.722						-20.000
				-2.000000E+01						
				LogK(25), drHO: PHREEQE-PSI Apr-91						

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Charge logK(T):	OPV A	DH a B	$\Delta_f G^0$	$\Delta_f H^0$	$\Delta_f S^0$	$\Delta_f Cp^0$	CpA E	CpB	CpC	$\Delta_r Cp^0$	$\Delta_r H^0$	logK(25)
NPO2OX2-3 -3.0	1.000 5.00	NP+4 0.00	2.000 -957.008	H2O	-4.000 -3.534000E+00	H+	-1.000 LogK(25): HUMMEL(1991), plus NpO2+ redox	E-	2.000 OX-2			-3.534
NPO2SO4 0.0	1.000 12.00	NP+4 0.00	-2.000 -1558.636	E-	-4.000 -2.847699E+01	H+	2.000 LogK(25), drHO: MINEQL-PSI Mar-91	H2O	1.000 SO4-2			-28.477
NPO2S042 -2.0	1.000 18.00	NP+4 0.00	-2.000 -2310.627	E-	-4.000 -2.707700E+01	H+	2.000 LogK(25), drHO: MINEQL-PSI Mar-91	H2O	2.000 SO4-2			-27.077
NPOH+2 2.0	1.000 3.00	NP+4 0.00	1.000 -714.285	E-	-1.000 -4.512163E+00	H+	1.000 LogK(25), drHO: MINEQL-PSI Mar-91	H2O				-4.512
NPOH+3 3.0	1.000 4.00	NP+4 0.00	-1.000 -731.478	H+	1.000 -1.500025E+00	H2O LogK(25), drHO: MINEQL-PSI Mar-91						-1.500
NPOH2+ 1.0	1.000 3.00	NP+4 0.00	1.000 -905.761	E-	-2.000 -1.251229E+01	H+	2.000 LogK(25), drHO: MINEQL-PSI Mar-91	H2O				-12.512
NPOH2+2 2.0	1.000 4.00	NP+4 0.00	-2.000 -954.348	H+	2.000 -4.000066E+00	H2O LogK(25), drHO: MINEQL-PSI Mar-91						-4.000
NPOH3 0.0	1.000 3.00	NP+4 0.00	1.000 -1085.822	E-	-3.000 -2.251228E+01	H+	3.000 LogK(25), drHO: MINEQL-PSI Mar-91	H2O				-22.512

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Charge logK(T):	OPV A	DH a B	DH b C	$\Delta_f G^0$ $\Delta_f H^0$	$\Delta_f S^0$ $\Delta_f Cp^0$	CpA E	CpB CpC	$\Delta_f Cp^0$ $\Delta_f H^0$	logK(25)
NPOH3+		1.000	NP+4	-3.000	H+	3.000	H2O		
	1.0	4.00	0.00	0.00	-1168.657				-8.000
				-7.999956E+00					
					LogK(25), drHO: MINEQL-PSI Mar-91				
NPOH3CO3		1.000	NP+4	1.000	HCO3-	-4.000	H+	3.000	H2O
	-1.0	8.00	0.00	0.00	-1736.531				-11.329
				-1.132885E+01					
					LogK(25), drHO: MINEQL-PSI Mar-91				
NPOH4-		1.000	NP+4	1.000	E-	-4.000	H+	4.000	H2O
	-1.0	3.00	0.00	0.00	-1265.883				-32.512
				-3.251227E+01					
					LogK(25), drHO: MINEQL-PSI Mar-91				
NPOH4		1.000	NP+4	-4.000	H+	4.000	H2O		
	0.0	4.00	0.00		-1377.257				-13.000
				-1.300004E+01					
					LogK(25), drHO: MINEQL-PSI Mar-91				
NPOH5-		1.000	NP+4	-5.000	H+	5.000	H2O		
	-1.0	4.00	0.00	0.00	-1574.442				-20.000
				-1.999998E+01					
					LogK(25), drHO: MINEQL-PSI Mar-91				
NPOX+2		1.000	NP+4	1.000	OX-2				
	2.0	4.00	0.00	0.00	-570.253				11.800
				1.180000E+01					
					logK(25): HUMMEL(1991)				
NPSO4+2		1.000	NP+4	1.000	SO4-2				
	2.0	10.00	0.00	0.00	-1269.161				3.900
				3.900029E+00					
					LogK(25), drHO: MINEQL-PSI Mar-91				
NPSO42		1.000	NP+4	2.000	SO4-2				
	0.0	16.00	0.00		-2023.435				5.700
				5.699989E+00					
					LogK(25), drHO: MINEQL-PSI Mar-91				

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Charge log(K(T):	OPV A	DH a B	DH b C	$\Delta_f G^0$ $\Delta_f H^0$	$\Delta_f S^0$ $\Delta_f Cp^0$	CpA E	CpB	CpC	$\Delta_r Cp^0$ $\Delta_r H^0$	logK(25)
SNOH6-2		1.000	SN+2	6.000 H2O	-6.000 H+	-2.000 E-				
	-2.0	4.00	0.00	0.00 -1299.123						-26.510
				-2.651000E+01						
				LogK(25), drHO: HATCHES 3.0						
SNOX2-2		1.000	SN+2	2.000 OX-2						
	-2.0	2.00	0.00	0.00 -101.232						12.900
				1.290000E+01						
				logK(25): HUMMEL(1991)						
SO3-2		1.000	SO4-2	2.000 H+	2.000 E-	-1.000 H2O				
	-2.0	4.00	4.50	0.00 -487.470 -635.500	-496.495 0.000	0.000 0.000000E+00	0.000000E+00	434.826	-11.990	-3.397
				-1.576198E+02 0.000000E+00	7.398158E+03 5.229849E+01	-0.000000E+00				
				dfG0: GRENTHE et al. (1991); dfHO: WAGMAN et al. (1982)						
SR(HOX)2		1.000	SR+2	2.000 H+	2.000 OX-2					
	0.0	0.00	0.00	-625.475						10.800
				1.080000E+01						
				logK(25): HUMMEL(1991)						
SR CIT-		1.000	SR+2	1.000 CIT-3						
	-1.0	0.00	0.00	0.00 -588.374						4.300
				4.300000E+00						
				logK(25): HUMMEL(1991)						
SRCO3O		1.000	SR+2	-1.000 H+	1.000 HCO3-					
	0.0	4.00	0.00	-1107.760 -1204.387	-324.088					
				-1.089061E+02 -1.970249E-02	5.151790E+03 3.892561E+01	-5.637139E+05				
				logK coef: BUSENBERG et al. (1984) = NORDSTROM et al. (1990)						
				BUSENBERG et al. (1984): dfG0 = -1107.82, dfHO = -1204.30						
SREDTA-2		1.000	SR+2	1.000 EDTA-4						
	-2.0	0.00	0.00	0.00 -623.192						10.400
				1.040000E+01						
				logK(25): HUMMEL(1991)						
SRHCO3+		1.000	SR+2	1.000 HCO3-						
	1.0	4.00	4.00	0.00 -1157.467 -1215.814	-195.699					
				-3.248000E+00 1.486700E-02	0.000000E+00 0.000000E+00	0.000000E+00				
				logK coef: BUSENBERG et al. (1984) = NORDSTROM et al. (1990)						
				BUSENBERG et al. (1984): dfG0 = -1157.52, dfHO = -1215.56						

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UL2OH2EDTA-2	2.000	U+4	6.000	H2O	-10.000	H+	-4.000	E-	1.000	EDTA-4		-9.376
	-2.0	12.00	0.00	0.00	-2429.043							
					-9.376000E+00							
						logK(25): HUMMEL(1991), plus UO2+2 redox						
UL2OH3	2.000	U+4	-4.000	E-	-12.000	H+	7.000	H2O	1.000	HCO3-		-29.285
	-1.0	16.00	0.00	0.00	-3139.418							
					-2.928517E+01							
						LogK(25), drHO: MINEQL-PSI Mar-91						
UL3C36-6	3.000	U+4	-6.000	E-	-18.000	H+	6.000	H2O	6.000	HCO3-		-35.107
	-6.0	42.00	0.00	0.00	-6333.280							
					-3.510745E+01							
						LogK(25), drHO: MINEQL-PSI Mar-91						
UL3OH4+2	3.000	U+4	-6.000	E-	-16.000	H+	10.000	H2O				-39.044
	2.0	18.00	0.00	0.00	-3738.118							
					-3.904444E+01							
						LogK(25), drHO: MINEQL-PSI Mar-91						
UL3OH5+	3.000	U+4	-6.000	E-	-17.000	H+	11.000	H2O				-42.694
	1.0	18.00	0.00	0.00	-3954.424							
					-4.269447E+01							
						LogK(25), drHO: MINEQL-PSI Mar-91						
UL3OH5C+	3.000	U+4	-6.000	E-	-16.000	H+	10.000	H2O	1.000	HCO3-		-36.683
	1.0	22.00	0.00	0.00	-4338.470							
					-3.668333E+01							
						LogK(25), drHO: MINEQL-PSI Mar-91						
UL3OH7-	3.000	U+4	-6.000	E-	-19.000	H+	13.000	H2O				-58.144
	-1.0	18.00	0.00	0.00	-4340.517							
					-5.814444E+01							
						LogK(25), drHO: MINEQL-PSI Mar-91						
UL4OH7+	4.000	U+4	-8.000	E-	-23.000	H+	15.000	H2O				-58.053
	1.0	24.00	0.00	0.00	-5345.181							
					-5.805264E+01							
						LogK(25), drHO: MINEQL-PSI Mar-91						

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Charge logK(T):	OPV A	DH a B	DH b B	$\Delta_f G^0$	$\Delta_f H^0$	$\Delta_f S^0$	$\Delta_f Cp^0$	CpA	CpB	CpC	$\Delta_r Cp^0$	$\Delta_r H^0$	logK(25)
ULCIT- -1.0	1.000 6.00	U+4 0.00	2.000 0.00	H2O -1002.211 -3.380000E-01 logK(25): HUMMEL(1991), plus U02+2 redox		-4.000 H+		-2.000 E-	1.000 CIT-3				-0.338
ULCIT)2-2 -2.0	2.000 12.00	U+4 0.00	4.000 0.00	H2O -2025.997 3.104000E+00 logK(25): HUMMEL(1991), plus U02+2 redox		-8.000 H+		-4.000 E-	2.000 CIT-3				3.104
ULCL+ 1.0	1.000 6.00	U+4 0.00	-2.000 0.00	E- -1084.171 -8.968087E+00 LogK(25), drHO: MINEQL-PSI Mar-91		-4.000 H+		2.000 H2O	1.000 CL-				-8.968
ULCL2 0.0	1.000 6.00	U+4 0.00	-2.000 -1208.712 -1.013822E+01 LogK(25), drHO: MINEQL-PSI Mar-91	E- -1535.380 -9.747007E+00 LogK(25), drHO: MINEQL-PSI Mar-91		-4.000 H+		2.000 H2O	2.000 CL-				-10.138
ULCO30 0.0	1.000 10.00	U+4 0.00	-2.000 -1535.380 -9.747007E+00 LogK(25), drHO: MINEQL-PSI Mar-91	E- -2105.366 -1.270589E+01 LogK(25), drHO: MINEQL-PSI Mar-91		-5.000 H+		2.000 H2O	1.000 HCO3-				-9.747
ULCO32-2 -2.0	1.000 14.00	U+4 0.00	-2.000 0.00	E- -2659.713 -1.840465E+01 LogK(25), drHO: MINEQL-PSI Mar-91		-6.000 H+		2.000 H2O	2.000 HCO3-				-12.706
ULCO33-4 -4.0	1.000 18.00	U+4 0.00	-2.000 0.00	E- -1027.326 4.062000E+00 LogK(25): HUMMEL(1991), plus U02+2 redox		-7.000 H+		2.000 H2O	3.000 HCO3-				-18.405
ULEDTA-2 -2.0	1.000 6.00	U+4 0.00	2.000 0.00	H2O -1027.326 4.062000E+00 LogK(25): HUMMEL(1991), plus U02+2 redox		-4.000 H+		-2.000 E-	1.000 EDTA-4				4.062

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logK(25)	OPV	Nagra Data Base, 05/92 Minerals and Gases							Page 7 of 24			
		$\Delta_f G^0$		$\Delta_f H^0$		$\Delta_f S^0$		$\Delta_f Cp^0$	CpA	CpB	CpC	$\Delta_r Cp^0$
		logK(T):	A	B	C	D	E					$\Delta_r H^0$
NI2SiO4		2.000	NI+2	1.000	Si(OH)4	-4.000	H+					
		0.00		-1288.715	-1523.970	-789.048					0.000	40.990
		-1.212873E+01	0.000000E+00	-2.141095E+03	0.000000E+00	-0.000000E+00						-19.310
		logK(25), drHO: PHREEQE-PSI Apr-91										
NI2SiO4S		2.000	NI+2	1.000	Si(OH)4	-4.000	H+					
		0.00		-1280.724	-1522.350	-810.417					0.000	42.610
		-1.324492E+01	0.000000E+00	-2.225715E+03	0.000000E+00	-0.000000E+00						-20.710
		logK(25), drHO: PHREEQE-PSI Apr-91										
NI3S2		3.000	NI+2	2.000	HS-	-2.000	H+	2.000	E-			
		-6.00		-310.333	-229.100	272.457					0.000	-34.500
		2.864675E+01	0.000000E+00	1.802093E+03	0.000000E+00	-0.000000E+00						34.691
		logK(25), drHO: PHREEQE-PSI Apr-91										
NI3S4		3.000	NI+2	4.000	HS-	-4.000	H+	-2.000	E-			
		-6.00		-671.822	-325.200	1162.574					0.000	-98.000
		8.514183E+01	0.000000E+00	5.118988E+03	0.000000E+00	-0.000000E+00						102.311
		logK(25), drHO: PHREEQE-PSI Apr-91										
NiCO3S		1.000	NI+2	1.000	HC03-	-1.000	H+					
		4.00		-613.302	-720.215	-358.587					0.000	24.000
		8.456943E-01	0.000000E+00	-1.253630E+03	0.000000E+00	-0.000000E+00						-3.359
		logK(25), drHO: PHREEQE-PSI Apr-91										
NiF2S		1.000	NI+2	2.000	F-							
		0.00		-610.638	-709.000	-329.909					0.000	15.700
		3.100571E+00	0.000000E+00	-8.200827E+02	0.000000E+00	-0.000000E+00						0.350
		logK(25), drHO: PHREEQE-PSI Apr-91										
NiFe2O4		1.000	NI+2	2.000	FE+2	4.000	H2O	-8.000	H+	-2.000	E-	
		6.00		-972.960	-1305.120	-1114.070						0.000
		-1.902623E+01	0.000000E+00	-3.677313E+03	0.000000E+00	-0.000000E+00						70.400
		logK(25), drHO: PHREEQE-PSI Apr-91										-31.360
NiO		1.000	NI+2	1.000	H2O	-2.000	H+					
		0.00		-211.677	-315.900	-349.567					0.000	23.930
		-8.257569E+00	0.000000E+00	-1.249973E+03	0.000000E+00	-0.000000E+00						-12.450
		logK(25), drHO: PHREEQE-PSI Apr-91										

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	OPV	$\Delta_f G^0$	$\Delta_f H^0$	$\Delta_f S^0$	$\Delta_f Cp^0$	CpA	CpB	CpC	$\Delta_r Cp^0$	$\Delta_r H^0$
logK(25)		A	B	C	D	E				
NIS		1.000 NI+2 -2.00 9.192969E+00	1.000 HS- -85.993 0.000000E+00	-1.000 H+ -70.460 52.097					0.000	-0.160 9.221
					0.000000E+00	-0.000000E+00				
NIS2		1.000 NI+2 -2.00 3.208984E+01	2.000 HS- -248.586 -130.900	-2.000 H+ 394.720		-2.000 E-			0.000	-44.300 39.851
					0.000000E+00	-0.000000E+00				
NISI03		1.000 NI+2 0.00 2.060000E+00	1.000 Si(OH)4 -1127.953	-1.000 H2O		-2.000 H+				2.060
NISO47AQ		1.000 NI+2 6.00 1.508429E+00	1.000 SO4-2 -2461.110 -2967.070	7.000 H2O -1696.998					0.000	-2.920 2.020
					0.000000E+00	-0.000000E+00				
NP(OH)3CR		1.000 NP+4 3.00 -1.951223E+01	1.000 E- -1102.946	-3.000 H+		3.000 H2O				-19.512
NP(OH)4CR		1.000 NP+4 4.00 -7.999431E-01	-4.000 H+ -1446.894	4.000 H2O						-0.800
NPO2		1.000 NP+4 4.00 2.699939E+00	-4.000 H+ -992.591	2.000 H2O						2.700
NPO2OH2C		1.000 NP+4 6.00 -3.707699E+01	-2.000 E- -1239.828	-6.000 H+		4.000 H2O				-37.077

LogK(25), drHO: MINEQL-PSI Mar-91

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	OPV	$\Delta_f G^0$	$\Delta_f H^0$	$\Delta_f S^0$	$\Delta_f Cp^0$	CpA	CpB	CpC	$\Delta_r Cp^0$	$\Delta_r H^0$
logK(25)		A	B	C	D	E				
logK(T):										
RHODO_CR	1.000 MN+2	1.000 HCO3-	-1.000 H+							
	6.00 -9.570888E+01	-819.548 -3.252849E-02	-890.081 4.839264E+03	-236.570 3.892561E+01				-290.506	20.884	0.801
	logK(25), drHO: NORDSTROM et al. (1990)									
RHODO_SY	1.000 MN+2	1.000 HCO3-	-1.000 H+							
	6.00 -9.749710E+01	-815.324 -3.252849E-02	-896.064 5.151790E+03	-270.804 3.892561E+01				-290.506	14.901	0.061
	logK(25), drHO: NORDSTROM et al. (1990)									
SE	1.000 SEO3-2	6.000 H+	4.000 E-	-3.000 H2O						
	0.00 -1.168555E+00	0.000 0.000 0.000 1.819278E+04	0.000 0.000 0.000 0.000000E+00	0.000 0.000 0.000 0.000000E+00				0.000	-348.290	59.850
	dfG0, dfH0 = 0.0 by convention									
SIDR_CR	1.000 FE+2	1.000 HCO3-	-1.000 H+							
	6.00 -9.517921E+01	-668.978 -3.252849E-02	-754.038 4.609790E+03	-285.293 3.892561E+01				-290.506	25.277	0.561
	logK(25), drHO: NORDSTROM et al. (1990)									
SIDR_PPT	1.000 FE+2	1.000 HCO3-	-1.000 H+							
	6.00 -9.743710E+01	-666.466 -3.252849E-02	-764.414 5.151790E+03	-328.519 3.892561E+01				-290.506	14.901	0.121
	logK(25), drHO: NORDSTROM et al. (1990)									
SIO2_AM	1.000 SI(OH)4	-2.000 H2O								
	0.00 2.600000E-01	-848.934 0.000000E+00	-899.295 7.310000E+02	-168.911 0.000000E+00				0.000	-13.995	2.712
	logK coef: NORDSTROM et al. (1990)									
SN(SO4)2	1.000 SN+2	-2.000 E-	2.000 SO4-2							
	16.00 -1.956316E+01	-1394.535 0.000000E+00	-1818.180 -4.910049E+02	-1420.911 0.000000E+00				0.000	9.400	-21.210
	LogK(25), drHO: HATCHES 3.0									
SN(W)	1.000 SN+2	2.000 E-								
	0.00 -4.770000E+00	-0.373								
	LogK(25), drHO: HATCHES 3.0									

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	OPV	$\Delta_f G^0$	$\Delta_f H^0$	$\Delta_f S^0$	$\Delta_f Cp^0$	CpA	CpB	CpC	$\Delta_r Cp^0$	$\Delta_r H^0$
logK(25)		A	B	C	D	E				
logK(T):										
TCO3		1.000	TCO+2	-4.000	H+	2.000	H2O	-2.000	E-	
	6.00			-460.151						-20.100
				-2.010000E+01						
				LogK(25), drHO: HATCHES 3.0						
TCOH(S)		2.000	E-	1.000	TCO+2					
	2.00			-234.964	-67.395	562.030		0.000	-67.395	23.540
				1.173269E+01	0.000000E+00	3.520349E+03	0.000000E+00	-0.000000E+00		
				LogK(25), drHO: HATCHES 3.0						
TCOH2(S)		1.000	TCO+2	1.000	H2O	2.000	E-			
	2.00			-461.202	-319.527	475.179		0.000	-33.697	21.630
				1.572635E+01	0.000000E+00	1.760174E+03	0.000000E+00	-0.000000E+00		
				LogK(25), drHO: HATCHES 3.0						
TCOH3(S)		1.000	TCO+2	-1.000	H+	2.000	H2O	1.000	E-	
	3.00			-658.558						14.660
				1.466000E+01						
				LogK(25), drHO: HATCHES 3.0						
TCS2		-9.000	H2O	1.000	TCO+2	2.000	SO4-2	18.000	H+	16.000 E-
	0.00			-215.147	673.510	2980.570		0.000	-80.280	133.290
				1.192253E+02	0.000000E+00	4.193391E+03	0.000000E+00	-0.000000E+00		
				LogK(25), drHO: HATCHES 3.0						
TCS3		1.000	TCO+2	26.000	H+	-13.000	H2O	22.000	E-	3.000 SO4-2
	0.00			1103.539	867.350	-792.183		0.000	-120.420	-61.900
				-8.299705E+01	0.000000E+00	6.290086E+03	0.000000E+00	-0.000000E+00		
				LogK(25), drHO: HATCHES 3.0						
TH(OH)4CR		1.000	TH+4	-4.000	H+	4.000	H2O			
	0.00			-1574.791	-1880.940	-1026.829	0.000	0.000	0.000000E+00	0.000000E+00
				-8.302344E+00	0.000000E+00	-1.639121E+03	0.000000E+00	-0.000000E+00	0.000	31.380
				LogK(25), drHO: MINEQL-PSI Mar-91						-13.800
THF4_AQ		1.000	TH+4	4.000	F-	2.500	H2O			
	0.00			-2612.862	-2854.891	-811.769	0.000	0.000	0.000000E+00	0.000000E+00
				2.785890E+01	0.000000E+00	1.562649E+03	0.000000E+00	-0.000000E+00	0.000	-29.916
				LogK(25), drHO: MINEQL-PSI Mar-91						33.100

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logK(25) logK(T):	OPV		$\Delta_f G^0$	$\Delta_f H^0$	$\Delta_f S^0$	$\Delta_f Cp^0$	CpA	CpB	CpC	$\Delta_r Cp^0$	$\Delta_r H^0$
	A	B	C	D	E						
U5012CL	5.000 24.00 1.034344E+02	U+4 -5517.971 0.000000E+00	-5.000 -5854.417 -3.649227E+04	E- -1128.445 0.000000E+00	-24.000 0.000 0.000000E+00	H+ 0.000 -0.000000E+00	12.000 0.000 0.000000E+00	H2O 0.000 0.000000E+00	1.000 0.000000E+00 0.000000E+00	CL- 0.000000E+00 0.000000E+00	0.000 698.623 -18.961
UCL2F2	1.000 4.00 2.641967E+01	U+4 -1376.060 0.000000E+00	2.000 -1465.979 -6.794725E+03	CL- -301.590 0.000000E+00	2.000 0.000 -0.000000E+00	F- 0.000 -0.000000E+00	0.000 0.000000E+00 0.000000E+00	0.000 0.000000E+00 0.000000E+00	0.000 130.081 3.630		
UCL3CR	1.000 3.00 1.807230E+01	U+4 -800.268 0.000000E+00	1.000 -866.033 -1.182627E+04	E- -220.577 0.000000E+00	3.000 0.000 -0.000000E+00	CL- 0.000 -0.000000E+00	0.000 0.000000E+00 0.000000E+00	0.000 0.000000E+00 0.000000E+00	0.000 226.407 -21.593		
UCL3F	1.000 4.00 2.215471E+01	U+4 -1146.648 0.000000E+00	3.000 -1242.941 -9.655507E+03	CL- -322.968 0.000000E+00	1.000 0.000 -0.000000E+00	F- 0.000 -0.000000E+00	0.000 0.000000E+00 0.000000E+00	0.000 0.000000E+00 0.000000E+00	0.000 184.849 -10.230		
UCL4CR	1.000 4.00 2.026522E+01	U+4 -929.623 0.000000E+00	4.000 -1018.731 -1.257751E+04	CL- -298.870 0.000000E+00	1.000 0.000 -0.000000E+00		0.000 0.000000E+00 0.000000E+00	0.000 0.000000E+00 0.000000E+00	0.000 240.789 -21.920		
UCL5CR	1.000 5.00 2.310865E+01	U+4 -949.800 0.000000E+00	-1.000 -1058.538 -1.922556E+04	E- -364.709 0.000000E+00	5.000 0.000 -0.000000E+00	CL- 0.000 -0.000000E+00	0.000 0.000000E+00 0.000000E+00	0.000 0.000000E+00 0.000000E+00	0.000 368.062 -41.374		
UCL6	1.000 6.00 2.382520E+01	U+4 -951.371 0.000000E+00	-2.000 -1091.879 -2.621136E+04	E- -471.266 0.000000E+00	6.000 0.000 -0.000000E+00	CL- 0.000 -0.000000E+00	0.000 0.000000E+00 0.000000E+00	0.000 0.000000E+00 0.000000E+00	0.000 501.801 -64.088		
UCLF3	1.000 4.00 3.068586E+01	U+4 -1606.442 0.000000E+00	1.000 -1689.980 -3.883640E+03	CL- -280.188 0.000000E+00	3.000 0.000 -0.000000E+00	F- 0.000 -0.000000E+00	0.000 0.000000E+00 0.000000E+00	0.000 0.000000E+00 0.000000E+00	0.000 74.350 17.660		

LogK(25), drHO: MINEQL-PSI Mar-91

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logK(25) logK(T):	OPV	$\Delta_f G^0$	$\Delta_f H^0$	$\Delta_f S^0$	$\Delta_f Cp^0$	CpA	CpB	CpC	$\Delta_f Cp^0$	$\Delta_f H^0$
	A	B	C	D	E					
ULCL2_1	1.000 6.00 2.178890E+01 LogK(25), drHO: MINEQL-PSI Mar-91	U+4 -1404.984 0.000000E+00	-2.000 -1559.745 -1.165379E+04	E- -519.071 0.000	-4.000 0.000 0.000000E+00	H+ 0.000 -0.000000E+00	3.000 0.000 0.000000E+00	H2O 0.000000E+00 0.000000E+00	2.000 0.000000E+00 0.000000E+00	CL- 0.000000E+00 -17.298
ULCL2_3	1.000 6.00 1.877589E+01 LogK(25), drHO: MINEQL-PSI Mar-91	U+4 -1894.618 0.000000E+00	-2.000 -2163.957 -9.953453E+03	E- -903.367 0.000	-4.000 0.000 0.000000E+00	H+ 0.000 -0.000000E+00	5.000 0.000 0.000000E+00	H2O 0.000000E+00 0.000000E+00	2.000 0.000000E+00 0.000000E+00	CL- 0.000000E+00 -14.608
ULCL2CR	1.000 6.00 2.325056E+01 LogK(25), drHO: MINEQL-PSI Mar-91	U+4 -1145.811 0.000000E+00	-2.000 -1243.539 -1.324047E+04	E- -327.781 0.000	-4.000 0.000 0.000000E+00	H+ 0.000 -0.000000E+00	2.000 0.000 0.000000E+00	H2O 0.000000E+00 0.000000E+00	2.000 0.000000E+00 0.000000E+00	CL- 0.000000E+00 -21.158
ULCLOH_-	1.000 6.00 1.969829E+01 LogK(25), drHO: MINEQL-PSI Mar-91	U+4 -1782.177 0.000000E+00	-2.000 -2010.391 -9.247555E+03	E- -765.434 0.000	-5.000 0.000 0.000000E+00	H+ 0.000 -0.000000E+00	5.000 0.000 0.000000E+00	H2O 0.000000E+00 0.000000E+00	1.000 0.000000E+00 0.000000E+00	CL- 0.000000E+00 -11.318
ULCO3CR	1.000 10.00 2.370817E+01 LogK(25), drHO: MINEQL-PSI Mar-91	U+4 -1562.892 0.000000E+00	-2.000 -1689.628 -8.537583E+03	E- -425.075 0.000	-5.000 0.000 0.000000E+00	H+ 0.000 -0.000000E+00	2.000 0.000 0.000000E+00	H2O 0.000000E+00 0.000000E+00	1.000 0.000000E+00 0.000000E+00	HCO3- 0.000000E+00 -4.927
ULF2_3A	1.000 6.00 2.588848E+01 LogK(25), drHO: MINEQL-PSI Mar-91	U+4 -2269.706 0.000000E+00	-2.000 -2534.387 -8.183224E+03	E- -887.744 0.000	-4.000 0.000 0.000000E+00	H+ 0.000 -0.000000E+00	5.000 0.000 0.000000E+00	H2O 0.000000E+00 0.000000E+00	2.000 0.000000E+00 0.000000E+00	F- 0.000000E+00 -1.558
ULF2CR	1.000 6.00 2.981619E+01 LogK(25), drHO: MINEQL-PSI Mar-91	U+4 -1557.316 0.000000E+00	-2.000 -1653.508 -9.404938E+03	E- -322.630 0.000	-4.000 0.000 0.000000E+00	H+ 0.000 -0.000000E+00	2.000 0.000 0.000000E+00	H2O 0.000000E+00 0.000000E+00	2.000 0.000000E+00 0.000000E+00	F- 0.000000E+00 -1.728
ULFOH_1	1.000 6.00 2.401511E+01 LogK(25), drHO: MINEQL-PSI Mar-91	U+4 -1721.650 0.000000E+00	-2.000 -1894.504 -9.160167E+03	E- -579.755 0.000	-5.000 0.000 0.000000E+00	H+ 0.000 -0.000000E+00	4.000 0.000 0.000000E+00	H2O 0.000000E+00 0.000000E+00	1.000 0.000000E+00 0.000000E+00	F- 0.000000E+00 -6.708

Table A.3

Nagra Data Base, 05/92 Minerals and Gases

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Table A.3

Nagra Data Base, 05/92 Minerals and Gases

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logK(25) logK(T):	OPV	$\Delta_f G^0$	$\Delta_f H^0$	$\Delta_f S^0$	$\Delta_f Cp^0$	CpA	CpB	Cpc	$\Delta_r Cp^0$	$\Delta_r H^0$
	A	B	C	D	E					
ULSO4_3	1.000 U+4 12.00 2.300914E+01	-2.000 E- -2416.533 -2755.329 -1136.327 0.000000E+00 -9.107671E+03 0.000000E+00 -0.000000E+00	-4.000 H+ 0.000 0.000000E+00	5.000 H2O 0.000 0.000000E+00 0.000000E+00	1.000 SO4-2 0.000000E+00 0.000000E+00				0.000 0.000	174.361 -7.538
ULSO4_35	1.000 U+4 12.00 2.249529E+01	1.000 SO4-2 -2535.559 -2901.633 -1227.818 0.000000E+00 -8.930648E+03 0.000000E+00 -0.000000E+00	5.500 H2O 0.000 0.000000E+00	-2.000 E- 0.000 0.000000E+00	-4.000 H+ 0.000 0.000000E+00				0.000 0.000	170.972 -7.458
ULSO4CR	1.000 U+4 12.00 2.884788E+01	-2.000 E- -1685.763 -1845.162 -534.627 0.000000E+00 -1.185923E+04 0.000000E+00 -0.000000E+00	-4.000 H+ 0.000 0.000000E+00	2.000 H2O 0.000 0.000000E+00	1.000 SO4-2 0.000000E+00 0.000000E+00				0.000 0.000	227.038 -10.928
ULU02CL3	2.000 U+4 11.00 4.473952E+01	-3.000 E- -2234.799 -2404.450 -569.012 0.000000E+00 -2.206963E+04 0.000000E+00 -0.000000E+00	-8.000 H+ 0.000 0.000000E+00	4.000 H2O 0.000 0.000000E+00	3.000 CL- 0.000000E+00 0.000000E+00				0.000 0.000	422.510 -29.282
UO2_AMOR	1.000 U+4 4.00 -1.000367E-01	-4.000 H+ -1003.569 -1162.860 -534.265 0.000000E+00 0.000000E+00 0.000000E+00 -0.000000E+00	2.000 H2O 0.000 0.000000E+00						0.000 0.000	0.000 -0.100
UO2_CRYs	1.000 U+4 4.00 1.858142E+01	-4.000 H+ -1032.337 -1084.996 -176.619 0.000000E+00 -4.067192E+03 0.000000E+00 -0.000000E+00	2.000 H2O 0.000 0.000000E+00						0.000 0.000	77.864 4.940
UO2CLCR	1.000 U+4 5.00 2.100823E+01	-1.000 E- -1095.323 -1169.990 -250.434 0.000000E+00 -8.354919E+03 0.000000E+00 -0.000000E+00	-4.000 H+ 0.000 0.000000E+00	2.000 H2O 0.000 0.000000E+00	1.000 CL- 0.000000E+00 0.000000E+00				0.000 0.000	159.950 -7.014
UO3_2H2O	1.000 U+4 6.00 2.017097E+01	-2.000 E- -1636.459 -1826.115 -636.109 0.000000E+00 -1.014578E+04 0.000000E+00 -0.000000E+00	-6.000 H+ 0.000 0.000000E+00	5.000 H2O 0.000 0.000000E+00					0.000 0.000	194.235 -13.858

LogK(25), drHO: MINEQL-PSI Mar-91

Table A.3

Nagra Data Base, 05/92 Minerals and Gases

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Table A.3

Nagra Data Base, 05/92 Minerals and Gases

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Table A.3

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Table A.4

Nagra Data Base, 05/92 Reactions to Calculate Pe

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Table A.4

Nagra Data Base, 05/92 Reactions to Calculate Pe

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APPENDIX B: Comparison Between Nagra Chemical Thermodynamic Data and Other Compilations

B.1 INTRODUCTION

A number of thermochemical data sets have been prepared for modelling the behaviour of solutions of interest in nuclear waste isolation studies. Several of these have been used as data sources for the 05/92 Nagra data set. These are:

- MINEQL-PSI version of March, 1991
- PHREEQE-PSI version of April, 1991
- HATCHES 3.0

This appendix gives tables comparing values in the Nagra data set with values for equivalent aqueous species (Table B.1) and minerals and gases (Table B.2) in the three source data bases. Tables B.3, B.4, and B.5 give reaction data as they appear in the original data sets. The original MINEQL-PSI and HATCHES data bases included more elements and organic ligands than appear in these tables. Only data for elements and minerals in the supplemental data set are included in Tables B.3, B.4, and B.5.

A fourth major data base developed for nuclear waste work was not included in this comparison. A recent version of the EQ3/EQ6 programme (2345.1090) includes a revised data base. These data were available while this version of the supplemental data base was being prepared, but the programming needed to read the data into PMATCH (see below) had not been completed.

B.2 COMPARISON PROCEDURE

The identities of the master species and the forms in which reactions are written differ among the data bases, so they could not readily be compared in their original forms. Therefore, the first step was to put each data base into the same format so they could be directly compared.

The data bases were received in PHREEQE format. After minor changes – to remove duplicate species' names, for example – the data were read into PMATCH, a Program to MAnage ThermoCHemical data (PEARSON & AVIS

1989). The Gibbs energies and enthalpies of formation of the master species in each data base were assigned the same values as the equivalent species in the Nagra data set. From those properties and the reaction data from the original data base, PMATCH calculated Gibbs energies and enthalpies of formation for each species, mineral, and gas in the data set.

Two sets of tables were generated from PMATCH. The first summarizes the properties of formation and other attributes of all species, and gives reactions and the logK(25) and $\Delta_f H^0$ of each product species, mineral, and gas. These are given here as Tables B.3, B.4, and B.5.

The second set of tables contains only the species, mineral, and gas names and their $\Delta_f G^0$ and $\Delta_f H^0$ values combined into two tables to compare the several data sets. These are attached as Table B.1 and B.2.

Three columns of data are given for each of the four data bases represented in Tables B.1 and B.2 containing the aqueous species or mineral name and the $\Delta_f G^0$ and $\Delta_f H^0$ values for the entity. These were calculated from the reaction properties given in the several data bases, and the values assigned to the properties of formation of the master species. The master species were given the same values in each data base, so the $\Delta_f G^0$ and $\Delta_f H^0$ values are directly comparable.

The last six columns in these tables represent the differences between the data sets. To make it more apparent how these differences would affect reaction calculations, they are expressed as differences in logK(25) values, using the equation:

$$\Delta_r G^0 = -RT \ln K(T)$$

For 25°C and $\Delta_r G^0$ in kJ/mol, this becomes

$$\Delta_r G^0 = -5.708 \log K(25)$$

B.3 DESCRIPTION AND COMPARISON OF DATA BASES

This section discusses the data bases shown in Tables B.3, B.4, and B.5, and the comparison Tables B.1 and B.2. The Nagra supplemental data base itself is given in Appendix A, Tables A.1 through A.4.

B.3.1 HATCHES 3.0 - Table B.3

This data set includes 52 elements, and 53 inorganic master species (52 elements plus the electron). It is a fully redox-coupled data base, in that it includes only one master species per element. This contrasts with the other data bases which have one master species per oxidation state, and are called redox-decoupled. A redox-coupled data base is useful for calculating the change in redox state accompanying reactions, and it may be appropriate for performance assessment work if the assumption of redox equilibrium can be justified. The HATCHES data base includes many supplemental elements that are also included in either or both the MINEQL-PSI or PHREEQE-PSI data sets, but often with different species identities. While there is general agreement between these three data bases, there are also areas of disagreement, which are mentioned below.

As Table B.2 suggests, the HATCHES 3.0 data base includes a very much larger group of minerals than the Nagra or either of the PSI data bases. This is because the HATCHES data set incorporates the mineral data from the EQ3/EQ6 2345.1090 data set.

B.3.2 MINEQL-PSI - Table B.4

This data set contains 58 elements, and 98 inorganic master species. There is one master species for each oxidation state represented in the data set, and, as there may be more than one oxidation state per element, there are more master species than elements. Redox decoupled data bases like this one are useful for the interpretation of field data because they can be used to calculate redox conditions from analyses of different redox states of individual elements. The data set includes a very large number of species of the elements it includes, perhaps more than are likely to be found under natural conditions, even in the vicinity of nuclear waste.

B.3.3 PHREEQE-PSI - Table B.5

This data base has 27 elements, and 37 master species. It also contains one master species per redox state, and therefore has more master species than elements. Users of this data base should be aware that it is intended for use with an earlier version of PHREEQE, in which the expression for logK as a function of T is:

$$\log K(T) = a + bT + \frac{c}{T} + dT^2 + \frac{e}{T^2}$$

The equivalent expression in current versions of PHREEQE is:

$$\log K(T) = A + BT + \frac{C}{T} + D \log(T) + \frac{E}{T^2}$$

Reactions such as those for HCO_3^- and H_2CO_3 , which include coefficients for the fourth term in these expressions, will give incorrect values if used with recent versions of PHREEQE. Data in Tables B.1, B.2 and B.5 are derived correctly from equations in the original data base.

B.4 COMPARISON OF DATA BASES - TABLES B.1 AND B.2

There is generally excellent agreement between values in the Nagra core data base and those of the other data bases. This is as expected because the core data base includes only species with well-known properties.

A number of differences between the supplemental data and the other data bases are evident from inspection of Tables B.1 and B.2. The following are of particular note:

Al^{+3} hydrolysis:

There has long been disagreement in the literature about the identity and stability of the hydrolysis products of Al^{+3} . Helgeson and a colleague are examining this at present, which should lead to a resolution of the problem.

S^{-2} :

The HATCHES data base includes the "old" value of -13 for the dissociation constant of HS^- . The MINEQL-PSI data base includes the "new" value, -19, which is also recommended by the NEA (GRENTHÉ *et al.* 1991).

PuO_2Cl ; PuOH_5^- ; SeO_3^- ; HSO_3^- ; UO_2OH_3^- :

Reasons for the differences among these species in the data bases have not been explored.

AsO_4^{3-} minerals:

There seems to be a consistent difference between the values for these minerals in the HATCHES and MINEQL-PSI data bases. These differences have not been explored.

CaHPO_4 ; FePO_4 ; NiSeO_3 ; Sn(OH)_2 ; Sn(OH)_4 ; TcO_2 :

The differences among these minerals appear to be due to differing numbers of water of hydration.

Graphite:

The reaction in HATCHES is incorrect.

Hematite; magnetite; manganite; Se_2O_5 :

Differences among these minerals have not been explored.

Nickel sulphide minerals; PdS :

The differences among these minerals have not been examined, but may be due to the differences in the S^2 data in the several data bases.

Complexes with organic ligands:

As discussed by HUMMEL (1991), some of these differences between HATCHES values and those in the other data sets arise from the use of different procedures for adjusting experimental data to zero ionic strength.

Many of these differences are described in more detail in the body of this report.

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Table B.1: Comparison of aqueous species in Nagra 05/92, HATCHES 3.0, MINEQL-PSI 03/91 and PHREEQE-PSI 04/91 Data Bases Page 1 of 18

Table B.1: Comparison of aqueous species in Nagra 05/92, HATCHES 3.0, MINEQL-PSI 03/91 and PHREEQE-PSI 04/91 Data Bases Page 2 of 18

Nagra 05/92			HATCHES 3.0			MINEQL-PSI 03/91			PHREEQE-PSI 04/91			Nagra-HATCHES	Nagra-MQ0391	Nagra-PP0491	HATCHES	HATCHES
Name	$\Delta_f G^\circ$	$\Delta_f H^\circ$	Name	$\Delta_f G^\circ$	$\Delta_f H^\circ$	Name	$\Delta_f G^\circ$	$\Delta_f H^\circ$	Name	$\Delta_f G^\circ$	$\Delta_f H^\circ$	$\Delta \log K$				
AMHEDTA	-726.39		AMHEDTA	-723.25	-616.70							0.55				
AMNTA	-673.30		AMHP04+	-1712.04	-1901.10											
AMNTA2-3	-724.67		AMO2+	-741.18	-805.11											
AMOH+2	-799.14		AMOH+2	-790.58	-844.79	AMOH+2	-799.14	-902.53				1.50	0.00	-1.50		
AMOH2+	-994.61		AMOH2+	-976.92	-1110.12	AMOH2+	-994.61	-1188.36				3.10	0.00	-3.10		
AMOH3	-1166.68		AMOH3	-1144.99	-1365.82	AMOH3	-1166.68	-1474.19				3.80	0.00	-3.80		
AMOH2C03	-1560.20					AM1838	-1560.20	-1863.67					0.00			
AMOHCO3	-1368.16					AM1836	-1368.16	-1577.84					0.00			
AMOHCO32	-1919.48					AM1837	-1919.48	-2253.16					0.00			
AMOHEDTA-2	-883.62															
AMOX+	-636.26		AMOX+	-632.38	-606.70							0.68				
AMOX2-	-659.20		AMOX2-	-655.89	-616.70							0.58				
AMOX3-3	-672.16		AMOX3-3	-669.59	-616.70							0.45				
AMS04+	-1365.93		AMS04+	-1366.50	-1505.12	AMS04+	-1365.93	-1526.04				-0.10	0.00	0.10		
AMS042-	-2119.64		AMS042-	-2118.49	-2391.03	AMS042-	-2119.64	-2435.38				0.20	0.00	-0.20		
AS04-3	-648.41	-888.14	AS04-3	-647.69	-888.43	AS04-3	-648.41	-888.14	AS04-3	-648.41	-888.14	0.13	0.00	-0.13	0.00	
HAS04-2	-714.60	-906.34	HAS04-2	-713.34	-900.15	HAS04-2	-714.62	-906.34	HAS04-2	-714.60	-906.34	0.22	-0.00	0.00	-0.23	-0.22
H2AS04-	-753.17	-909.56	H2AS04-1	-753.06	-905.80	H2AS04-	-753.15	-909.56	H2AS04-	-753.17	-909.56	0.02	0.00	-0.00	-0.02	-0.02
H3AS04	-766.00	-902.50	H3AS04	-765.85	-1000.69	H3AS04	-765.99	-902.49				0.03	0.00	-0.03		
AS(OH)3	-639.80	-742.20	AS0H3	-640.13	-742.39	HAS02	-639.78	-742.18	H3AS03	-639.80	-742.20	-0.06	0.00	0.00	0.06	-0.00
AS(OH)4-	-824.24	-1000.69	AS0H4-	-824.24	-1000.69	AS02-+2a	-824.24	-1000.69	H2AS03-+a	-824.27	-1000.62	0.00	0.00	-0.00	0.00	-0.00
B(OH)3	-969.30	-1072.80	H3B03	-969.30	-1072.80	BOH3	-969.27	-1072.81	H3B03	-969.30	-1072.80	0.00	0.01	0.00	0.01	-0.01
B(OH)4-	-1153.73	-1344.58	H2B03-+a	-1153.70	-1345.14	B(OH)4-	-1153.73	-1344.58	H2B03-+a	-1153.70	-1345.14	0.00	0.00	-0.00	0.00	0.00
			BF20H2	-1338.75	-143.93											
			BF30H-	-1417.61	-1513.80											
			BF4-	-1499.66	-1564.22											
			BF0H3-	-1248.54	-1400.41											
BA+2	-555.36	-532.50	BA+2	-555.36	-532.50	BA+2	-555.36	-532.50	BA+2	-555.36	-532.50	0.00	0.00	0.00	0.00	0.00
			BACIT-	-578.65	-532.50											
			BACL+	-685.84	-699.58											
BAC030	-1098.77	-1192.97				BAC03	-1098.75	-1192.96	BAC03	-1098.77	-1192.97	0.00	0.00		-0.00	
			BAEDTA-2	-613.58	-532.50											
			BAH2CIT+	-626.02	-532.50											
			BAHCIT	-606.79	-532.50											
BAHC03+	-1147.84	-1199.45				BAHC03+	-1147.84	-1199.45	BAHC03+	-1147.84	-1199.45	0.00	-0.00		-0.00	
			BAHEDTA-	-643.26	-532.50											
			BAN03+	-671.29	-739.35											
			BAN032	-782.65	-946.20											
			BANTA-	-592.46	-532.50											
BAOH+	-715.62		BAOH+	-716.24	-755.17	BAOH+	-715.62	-818.33	BAOH+	-715.62	-755.17	-0.11	0.00	0.00	0.11	0.00
			BAOX	-565.06	-532.50											
			BAS0203	-1087.78	-1181.00											
BAS040	-1314.77					BAS04	-1314.77	-1441.84	BAS04	-1312.37	-1435.69	0.00	0.42		0.42	
			BAS042-2	-2062.77	-2351.18											
BR-	-103.85	-121.41	BR-	-103.85	-121.41	BR-	-103.85	-121.41	BR-	-103.85	-121.41	0.00	0.00	0.00	0.00	0.00

Table B.1: Comparison of aqueous species in Nagra 05/92, HATCHES 3.0, MINEQL-PSI 03/91 and PHREEQE-PSI 04/91 Data Bases Page 3 of 18

Nagra 05/92			HATCHES 3.0			MINEQL-PSI 03/91			PHREEQE-PSI 04/91			Nagra-HATCHES	Nagra-MQ0391	Nagra-PP0491	HATCHES-MQ0391	HATCHES-PP0491
Name	$\Delta_f G^\circ$	$\Delta_f H^\circ$	Name	$\Delta_f G^\circ$	$\Delta_f H^\circ$	Name	$\Delta_f G^\circ$	$\Delta_f H^\circ$	Name	$\Delta_f G^\circ$	$\Delta_f H^\circ$	$\Delta \log K$	$\Delta \log K$	$\Delta \log K$	$\Delta \log K$	
CA+2	-552.81	-543.00	CA+2	-552.81	-543.00	CA+2	-552.81	-543.00	CA+2	-552.81	-543.00	0.00	0.00	0.00	0.00	0.00
CACIT-	-580.49		CACIT-	-579.52	-543.00	CACIT-	-579.52	-543.00	CACIT-	-579.52	-543.00	0.17	0.17	0.00		
CACO30	-1099.13	-1203.48	CACO3	-1098.71	-1201.48	CACO3	-1099.11	-1203.50	CACO3	-1099.13	-1203.48	0.07	0.00	0.00	-0.07	-0.07
CAEDTA-2	-623.01		CAEDTA-2	-615.59	-543.00	CAEDTA-2	-624.16	-543.00				1.30	-0.20	-1.50		
CAF+	-839.69	-861.11	CAF+	-839.69	-862.46	CAF+	-839.69	-861.11	CAF+	-839.69	-862.46	0.00	0.00	0.00	0.00	0.00
CAH2CIT+	-624.73		CAH2CIT+	-622.79	-543.00	CAH2CIT+	-622.79	-543.00	CAH2CIT+	-622.79	-543.00	0.34	0.34	0.00		
CAHCIT	-606.06		CAHCIT	-606.98	-543.00	CAHCIT	-606.98	-543.00						0.00		
CAHC03+	-1145.99	-1221.95	CAHC03+	-1145.51	-1210.76	CAHC03+	-1146.02	-1221.95	CAHC03+	-1145.99	-1221.95	-0.16	-0.16	0.00		
CAHEDTA-	-643.56					CAHEDTA-	-644.13	-543.00				0.08	-0.01	0.00	-0.09	-0.08
CAHOX+	-587.68		CAHOX+	-587.68	-543.00							-0.10		0.01		
CA(HOX)2	-615.02					CAHP04	-1664.44	-1828.36	CAHP040	-1664.49	-1829.49				-0.01	
			CAI2	-656.25	-656.56	CANH3+2	-578.90	-624.15								
						CANH32+2	-602.13	-705.30								
						CANH33+2	-624.22	-786.44								
						CANH34+2	-644.60	-867.59								
						CAN03+	-667.59	-749.85								
						CAN032	-777.81	-956.70								
						CANTA-	-599.61	-543.00					-0.59			
CANTA-	-596.24															
CANTA2-4	-606.69															
CAOH+	-717.00		CAOH+	-718.03	-768.02	CAOH+	-717.00	-762.30	CAOH+	-716.60	-768.02	-0.18	0.00	0.07	0.18	0.25
CAOX	-571.02		CAOX	-569.93	-543.00	CAOX	-573.36	-543.00				0.19	-0.41	-0.60		
CAOX2-2	-574.50					CAP04-	-1615.18	-1814.43	CAP04-	-1615.17	-1814.85				0.00	
						CAS203	-1082.94	-1191.50								
CAS040	-1309.94	-1445.44	CAS04	-1309.99	-1446.19	CAS04	-1309.94	-1445.44	CAS04	-1309.99	-1446.19	-0.01	0.00	-0.01	0.01	0.00
CIT-3	0.00	0.00	CIT3-	0.00	0.00	CIT-3	0.00	0.00							-0.01	-0.01
HCIT-2	-36.51		HCIT-2	-36.53	0.00	HCIT-2	-36.53	0.00				-0.00	-0.00	0.00		
H2CIT-	-63.68		H2CIT-	-63.70	0.00	H2CIT-	-63.70	0.00				-0.00	-0.00	0.00		
H3CIT	-81.54		H3CIT	-81.57	0.00	H3CIT	-81.57	0.00				-0.01	-0.01	0.00		
CL-	-131.22	-167.08	CL-	-131.22	-167.08	CL-	-131.22	-167.08	CL-	-131.22	-167.08	0.00	0.00	0.00	0.00	0.00
CH4(AQ)	-34.42	-88.61	CH4(AQ)	-34.54	1627.75	CH4(AQ)	-34.42	-88.61	CH4(AQ)	-34.42	-88.61	-0.02	0.00	0.00	0.02	0.02
C02(AQ) + a	-623.13	-699.32	H2C03	-623.13	-699.33	H2C03	-623.13	-699.32	H2C03	-623.13	-699.32	0.00	0.00	-0.00	-0.00	-0.00
HC03-	-586.88	-690.22	HC03-	-586.88	-689.96	HC03-	-586.88	-690.21	HC03-	-586.88	-690.21	-0.00	-0.00	-0.00	0.00	0.00
C03-2	-527.92	-675.31	C03-2	-527.92	-675.31	C03-2	-527.92	-675.31	C03-2	-527.92	-675.31	0.00	0.00	0.00	0.00	0.00
E-	0.00	0.00	E-	0.00	0.00	E-	0.00	0.00	E-	0.00	0.00					
EDTA-4	0.00	0.00	EDTA4-	0.00	0.00	EDTA-4	0.00	0.00								
HEDTA-3	-62.87		HEDTA-3	-62.84	0.00	HEDTA-3	-63.07	0.00				0.00	-0.04	-0.04		
H2EDTA-2	-98.94		H2EDTA-2	-98.92	0.00	H2EDTA-2	-101.72	0.00				0.00	-0.49	-0.49		
H3EDTA-	-116.67		H3EDTA-	-116.61	0.00	H3EDTA-	-119.52	0.00				0.01	-0.50	-0.51		
H4EDTA	-129.00		H4EDTA	-128.94	0.00	H4EDTA	-132.20	0.00				0.01	-0.56	-0.57		
H5EDTA+	-137.56		H5EDTA+	-137.56	0.00	H5EDTA+	-140.76	0.00				0.00	-0.56	-0.56		
H6EDTA+2	-136.42					H6EDTA+2	-139.05	0.00					-0.46			
F-	-281.52	-335.35	F-	-281.52	-335.35	F-	-281.52	-335.35	F-	-281.52	-335.35	0.00	0.00	0.00	0.00	0.00
HFO	-299.65	-322.04	HF(AQ)	-299.61	-321.96	HF	-299.67	-322.05	HF(AQ)	-299.61	-320.87	0.01	-0.00	0.01	-0.01	0.01
HF2-	-583.70	-655.50	HF2-	-584.39	-653.13							-0.12				

Table B.1: Comparison of aqueous species in Nagra 05/92, HATCHES 3.0, MINEQL-PSI 03/91 and PHREEQE-PSI 04/91 Data Bases Page 4 of 18

Table B.1: Comparison of aqueous species in Nagra 05/92, HATCHES 3.0, MINEQL-PSI 03/91 and PHREEQE-PSI 04/91 Data Bases Page 5 of 18

Nagra 05/92			HATCHES 3.0			MINEQL-PSI 03/91			PHREEQE-PSI 04/91			Nagra-HATCHES	Nagra-MQ0391	Nagra-PP0491	HATCHES-MQ0391	HATCHES-PP0491	MQ0391-PP0491
Name	$\Delta_f G^\circ$	$\Delta_f H^\circ$	Name	$\Delta_f G^\circ$	$\Delta_f H^\circ$	Name	$\Delta_f G^\circ$	$\Delta_f H^\circ$	Name	$\Delta_f G^\circ$	$\Delta_f H^\circ$	$\Delta \log K$	$\Delta \log K$	$\Delta \log K$	$\Delta \log K$		
FENTA2-3	-154.24		FE(HS)2	-105.01	-124.39	FENTA2-3	-159.27	-48.60					-0.88				
			FE(HS)3-	-104.16	-142.04												
FEOH+	-261.82	-319.70	FEOH+	-261.82	-319.70	FEOH+	-261.82	-319.71	FEOH+	-261.82	-319.71	0.00	0.00	0.00	0.00	0.00	0.00
FEOH+2	-229.22	-290.92	FEOH+2	-229.17	-289.58	FEOH+2	-229.22	-290.92	FEOH+2	-229.17	-289.59	0.01	0.00	0.01	-0.01	0.00	0.01
FE(OH)2+	-446.50	-548.71	FEOH2+	-446.44	-618.92	FEOH2+	-446.50	-548.71	FE(OH)2+	-446.44	-618.92	0.01	0.00	0.01	-0.01	0.00	0.01
			FEOH2	-435.77	-541.24				FE(OH)20	-435.60	-541.26					0.03	
FE(OH)30	-644.31	-802.33	FEOH3	-638.32	-904.75	FEOH3	-644.31	-802.33	FE(OH)30	-638.26	-904.75	1.05	0.00	1.06	-1.05	0.01	1.06
			FEOH3-	-613.38	-819.82				FE(OH)3-	-613.38	-819.79					0.00	
			FEOH4-2	-764.90	-1232.42												
FE(OH)4-	-829.85	-1058.45	FEOH4-	-829.80	-1190.58	FEOH4-	-829.85	-1058.45	FE(OH)4-	-829.80	-1190.58	0.01	0.00	0.01	-0.01	0.00	0.01
FEOHCl-	-303.88		FEClOH-	-303.71	-374.93							0.03					
FE(OH)2ClT-2	-495.70		FEClTOH2	-495.53	-660.76							0.03					
FE(OH)2ClT2-	-496.10		FEClT2OH	-495.93	-660.76							0.03					
FEOHDETA-3	-352.00																
FEOHDETA-2	-354.85															-1.08	
FE(OH)2EDTA-	-528.07															-1.48	
FE(OH)2NTA-2	-511.51															-0.58	
FEOHNTA-	-321.18															-0.68	
FEOHNTA-2	-310.90															-0.80	
FEOX	-102.30																
FEOX+	-56.64		FEOX+	-56.53	-89.10	FEOX+	-55.38	-48.60				0.02	0.22		0.20		
FEOX2-2	-114.29																
FEOX2-	-94.88		FEOX2-	-94.43	-89.10	FEOX2-	-94.20	-48.60				0.08	0.12		0.04		
FEOX3-3	-119.43		FEOX3-3	-119.08	-89.10	FEOX3-3	-121.02	-48.60				0.06	-0.28		-0.34		
						FES203+	-546.13	-697.10									
FESO40	-835.74	-984.93	FESO4	-835.74	-984.93	FESO4	-835.74	-984.93	FESO40	-835.74	-991.74	0.00	0.00	0.00	0.00	0.00	0.00
FESO4+	-771.64	-941.58	FESO4+	-770.90	-940.24	FESO4+	-771.64	-941.58	FESO4+	-770.90	-940.24	0.13	0.00	0.13	-0.13	0.00	0.13
FE(SO4)2-	-1523.29	-1848.03	FE(SO4)2	-1523.46	-1846.69	FESO42-	-1523.29	-1848.03	FE(SO4)2	-1523.46	-1846.69	-0.03	0.00	-0.03	0.03	0.00	-0.03
H+	0.00	0.00	H+	0.00	0.00	H+	0.00	0.00	H+	0.00	0.00						
H2(AQ)	17.73	-4.04	H2(AQ)	17.98	-7.36	H2(AQ)	17.73	-4.04	H2(AQ)	17.73	-4.04	0.04	0.00	0.00	-0.04	-0.04	0.00
H2O	-237.14	-285.83	H2O	-237.14	-285.83	H2O	-237.14	-285.83	H2O	-237.14	-285.83	0.00	0.00	0.00	0.00	0.00	0.00
I-	-51.72	-56.78	I-	-51.72	-56.78				I-	-51.72	-56.78	0.00				0.00	
I2	16.14		I2	15.86	19.41				I2	16.14	-113.56	-0.05		0.00		0.05	
			I2CL-	-116.51	-140.81												
			I2O-2	-82.58	-399.39												
			I2OH-	-230.42	-399.39												
I3-	-51.96		I3-	-51.85	-56.28				I3-	-51.96	-170.34	0.02		0.00		-0.02	
			ICL	-17.41	-223.86												
			ICL2-	-161.19	-390.94												
			IO-	-38.85	-109.10												
			HIO	-99.36	-139.69												
			H2IO10+	-106.78	-342.61												
			I03-	-127.85	-222.91												
			HIO3	-132.42	-212.91												
			I04-	-58.48	-153.10												
K+	-282.51	-252.14	K+	-282.51	-252.14	K+	-282.51	-252.14	K+	-282.51	-252.14	0.00	0.00	0.00	0.00	0.00	0.00

Table B.1: Comparison of aqueous species in Nagra 05/92, HATCHES 3.0, MINEQL-PSI 03/91 and PHREEQE-PSI 04/91 Data Bases Page 6 of 18

Nagra 05/92			HATCHES 3.0			MINEQL-PSI 03/91			PHREEQE-PSI 04/91			Nagra-HATCHES	Nagra-MQ0391	Nagra-PP0491	HATCHES-MQ0391	HATCHES-PP0491	MQ0391-PP0491		
Name	Δ_fG°	Δ_fH°	Name	Δ_fG°	Δ_fH°	Name	Δ_fG°	Δ_fH°	Name	Δ_fG°	Δ_fH°	$\Delta logK$	$\Delta logK$	$\Delta logK$	$\Delta logK$	$\Delta logK$			
KCIT-2	-289.47		KCIT-2	-289.47	-252.14	KCIT-2	-289.53	-252.14				0.00	-0.01		-0.01				
KEDTA-3	-291.64		KEDTA-3	-291.64	-252.14							0.00							
KNTA-2	-289.36																		
KOH	-437.11		KOH									0.00							
KOX-	-287.65																		
KS04-	-1031.36	-1152.07	KS04-	-1031.36	-1152.07	KS04-	-1031.36	-1152.07	KS04-	-1031.36	-1152.07	0.00	0.00	0.00	0.00	0.00	0.00		
LI+	-292.92	-278.47	LI+	-292.92	-278.47	LI+	-292.92	-278.47	LI+	-292.92	-278.47	0.00	0.00	0.00	0.00	0.00	0.00		
LIOH0	-452.20											0.00							
LIS04-	-1040.57		LIS04-	-1040.57	-1190.86	LIS04-	-1040.57	-1187.81				0.00	0.00		0.00				
MG+2	-455.40	-467.00	MG+2	-455.40	-467.00	MG+2	-455.40	-467.00	MG+2	-455.40	-467.00	0.00	0.00	0.00	0.00	0.00	0.00		
MGCIT-	-483.03		MGCIT-	-483.08	-467.00	MGCIT-	-482.11	-467.00				-0.01	0.16	0.17					
MGC030	-1000.33	-1130.96	MGC03	-1000.33	-1130.96	MGC03	-1000.33	-1130.98	MGC03	-1000.33	-1130.96	-0.00	-0.00	-0.00	0.00	0.00	0.00		
MGEDTA-2	-515.33		MGEDTA-2	-507.46	-467.00	MGEDTA-2	-515.33	-467.00				1.38	0.00	-1.38					
MGF+	-747.31	-788.96	MGF+	-747.31	-782.79	MGF+	-747.31	-788.96	MGF+	-747.31	-782.79	0.00	0.00	0.00	0.00	0.00	0.00		
MGH2CIT+	-525.61		MGH2CIT+	-525.04	-467.00	MGH2CIT+	-526.35	-467.00				0.10	-0.13	-0.23					
MGH2PO4+			MGH2PO4+	-1601.16	-1756.09														
MGHCIT	-506.77		MGHCIT	-507.17	-467.00	MGHCIT	-506.94	-467.00				-0.07	-0.03	0.04					
MGHCO3+	-1048.37	-1153.93	MGHCO3+	-1048.39	-1152.89	MGHCO3+	-1048.39	-1153.95	MGHCO3+	-1048.36	-1152.89	-0.00	-0.00	0.00	0.00	0.00	0.00		
MGHEDTA-	-539.88					MGHEDTA-	-539.88	-467.00					0.00			-0.04			
			MGHP04	-1567.77	-1752.36	MGHP04	-1567.99	-1753.49											
			MGI2	-559.01	-580.55														
			MGI03+	-587.82	-1381.27														
						MGNH3+2	-482.63	-548.15											
						MGNH32+2	-508.72	-629.30											
						MGNH33+2	-533.67	-710.44											
						MGNH34+2	-556.33	-791.59											
						MGNTA-	-496.50	-467.00					-0.70						
MGOH+	-627.24		MGOH+	-625.24	-688.32	MGOH+	-627.24	-752.83	MGOH+	-627.24	-686.16	0.35	0.00	0.00	-0.35	-0.35	0.00		
MGOX	-474.92		MGOX	-474.98	-467.00	MGOX	-471.95	-467.00				-0.01	0.52	0.53					
MGOX2-2	-484.40		MGOX2-2	-484.40	-467.00							0.00							
			MGP04-	-1518.51	-1738.43														
						MGS203	-984.96	-1115.50											
MGS040	-1212.93	-1357.30	MGS04	-1212.24	-1370.48	MGS04	-1212.93	-1357.30	MGS04	-1212.24	-1370.49	0.12	0.00	0.12	-0.12	0.00	0.12		
MN+2	-228.10	-220.75	MN+2	-228.10	-220.75	MN+2	-228.10	-220.75	MN+2	-228.10	-220.75	0.00	0.00	0.00	0.00	0.00	0.00		
			MN+3	-82.49	-112.97														
			MN20H+3	-633.07	-727.33														
			MN20H3+	-1031.20	-1298.99				MN2(OH)3	-1031.20	-1298.99								
MNCIT-	-257.21					MNCIT-	-258.35	-220.75					-0.20						
MNCL+	-362.80		MNCL+	-362.80	-387.83	MNCL+	-362.80	-387.83	MNCL+	-362.79	-387.83	0.00	0.00	0.00	0.00	0.00	0.00		
MNCL20	-491.97		MNCL2	-490.77	-554.89	MNCL2	-491.97	-554.91	MNCL20	-490.77	-554.91	0.21	0.00	0.21	-0.21	-0.00	0.21		
MNCL3-	-619.99		MNCL3-	-619.99	-721.99	MNCL3-	-619.99	-721.99	MNCL3-	-620.02	-721.99	0.00	0.00	-0.00	0.00	-0.00	-0.00		
MNC030	-783.99					MNC03	-783.99	-896.06				-0.00							
MNEDTA-2	-317.14					MNEDTA-2	-318.29	-220.75				-0.20							
MNF+	-514.42		MNF+	-514.47	-556.10	MNF+	-514.42	-556.10				-0.01	0.00	0.01					

Table B.1: Comparison of aqueous species in Nagra 05/92, HATCHES 3.0, MINEQL-PSI 03/91 and PHREEQE-PSI 04/91 Data Bases Page 7 of 18

Nagra 05/92			HATCHES 3.0			MINEQL-PSI 03/91			PHREEQE-PSI 04/91			Nagra-HATCHES	Nagra-MQ0391	Nagra-PP0491	HATCHES-PP0491	HATCHES-MQ0391	MQ0391-PP0491	
Name	$\Delta_f G^\circ$	$\Delta_f H^\circ$	Name	$\Delta_f G^\circ$	$\Delta_f H^\circ$	Name	$\Delta_f G^\circ$	$\Delta_f H^\circ$	Name	$\Delta_f G^\circ$	$\Delta_f H^\circ$	$\Delta \log K$	$\Delta \log K$	$\Delta \log K$	$\Delta \log K$			
MNHCl	-282.33		MNHCO3+	-822.23	-911.14	MNHCl	-281.98	-220.75	MNHCO3+	-822.23	-911.16	0.68	0.06	0.68	-0.68	0.00	0.68	
MNHCO3-	-826.11		MNHCO3+			MNHCO3+	-826.11	-910.96	MNHCO3+				-0.00	0.68	-0.68	0.00	0.68	
MNHDETA-	-337.12		MNHDETA-			MNHDETA-	-338.26	-220.75	MNHDETA-				-0.20					
MNNH3			MNNH3+2	-1346.06	-1505.15	MNNH3+2	-258.76	-301.90	MNNH3+2									
MNNH3+2			MNNH3+2	-288.27	-383.05	MNNH3+2			MNNH3+2									
MNNTA-	-277.02		MN(N03)2	-453.11	-636.11	MNNTA-	-280.61	-220.75	MNNTA-				-0.63					
MNO4-	-447.08	-625.09	MNO4-	-500.62	-736.39	MNO4-	-404.79	-446.33	MNO4-	-404.79	-446.33	0.00	0.00	0.00	0.00	0.00	0.00	
MNO4-2			MNO4-2	-575.66	-792.41	MNO4-2	-744.31	-1078.24	MNO4-2	-740.89	-1078.24	MNO4-2			-0.60	0.00	0.60	
MNOH+	-404.79	-446.33	MNOH+	-740.89	-1078.24	MNOH+	-744.31	-1078.24	MNOH+	-740.89	-1078.24	MNOH+						
MNOH3-			MNOH3-	-900.97	-1364.07	MNOH3-			MNOH3-			MNOH3-						
MNOX	-250.65		MNOX	-246.37	-220.75	MNOX	-256.07	-220.75	MNOX	-985.00	-1121.01	MNOX			0.75			
MNOX2-2	-257.78		MNOX2-2			MNOX2-2	-758.24	-869.25	MNOX2-2			MNOX2-2			0.30			
MNSO40	-984.94	-1115.99	MNSO4	-985.00	-1121.01	MNSO4	-984.94	-1115.99	MNSO4	-985.00	-1121.01	MNSO4	-0.01	0.00	-0.01	0.01	0.00	-0.01
M004-2	-836.30	-997.90	M004-2	-836.30	-997.90	M004-2	-860.84	-997.90	M004-2			M004-2	0.00					
N2(AQ)	18.19	-10.44	N2(AQ)	19.27	-4.67	N2(AQ)	18.19	-10.44	N2(AQ)	18.19	-10.44	N2(AQ)	0.19	0.00	0.00	-0.19	-0.19	0.00
NH3(AQ)	-26.66	-81.15	NH3(AQ)	-26.27	-79.80	NH3(AQ)	-26.66	-81.15	NH3(AQ)	-26.59	-81.07	NH3(AQ)	0.07	0.00	0.01	-0.07	-0.06	0.01
NH4+	-79.40	-133.26	NH4+	-79.07	-132.00	NH4+	-79.40	-133.28	NH4+	-79.40	-133.26	NH4+	0.06	0.00	0.00	-0.06	-0.06	0.00
NH4S04-			NH4S04-	-829.40	-1043.01	NH4S04-			NH4S04-			NH4S04-						
NO2-			NO2-	-36.73	-104.11	NO2-			NO2-			NO2-						
NO3-	-110.79	-206.85	NO3-	-110.79	-206.85	NO3-	-110.79	-206.85	NO3-	-110.79	-206.85	NO3-	0.00	0.00	0.00	0.00	0.00	0.00
HN03	-102.63	-209.19	HN03			HN03			HN03			HN03						
NA+	-261.95	-240.34	NA+	-261.95	-240.34	NA+	-261.95	-240.34	NA+	-261.95	-240.34	NA+	0.00	0.00	0.00	0.00	0.00	0.00
NACIT-2	-269.60		NACIT-2	-269.37	-240.34	NACIT-2	-269.60	-240.34	NACIT-2	-269.37	-240.34	NACIT-2	0.04	0.00	0.00	-0.04		
NAC03-	-797.12	-878.38	NAC03-	-797.12	-878.37	NAC03-	-797.12	-878.38	NAC03-	-797.11	-878.37	NAC03-	-0.00	-0.00	0.00	0.00	0.00	0.00
NAEDTA-3	-277.36		NAEDTA-3	-276.11	-240.34	NAEDTA-3	-276.79	-240.34	NAEDTA-3	-276.11	-240.34	NAEDTA-3	0.22	0.10	0.10	-0.12		
NAF0	-542.10		NAF0	-540.90	-588.24	NAF0	-542.10	-575.69	NAF0	-542.10	-575.69	NAF0	0.21	0.00	0.00	-0.21		
NAHCO30	-847.40		NAHCO30	-847.41	-930.73	NAHCO30	-847.41	-930.55	NAHCO30	-847.41	-930.73	NAHCO30	-0.00	-0.00	-0.00	0.00	0.00	0.00
NANTA-2	-272.22		NANTA-2			NANTA-2	-275.65	-240.34	NANTA-2			NANTA-2	-0.60					
NAOHO	-418.15		NAOHO			NAOHO	-418.15	-526.17	NAOHO			NAOHO	0.00					
NAOX-	-267.66		NAOX-			NAOX-			NAOX-			NAOX-						
NAS04-	-1009.95	-1144.99	NAS04-	-1009.95	-1144.99	NAS04-	-1009.95	-1144.99	NAS04-	-1009.95	-1144.99	NAS04-	0.00	0.00	0.00	0.00	0.00	0.00
NBO3-	-932.10	0.00	NBO3-			NBO3-			NBO3-			NBO3-						
NBOH4+	-1208.60		NBOH4+			NBOH4+			NBOH4+			NBOH4+						
NBOH5	-1448.30		NBOH5			NBOH5			NBOH5			NBOH5						
NI+2	-45.60	-54.00	NI+2	-45.60	-54.00	NI+2	-45.60	-54.00	NI+2	-45.60	-54.00	NI+2	0.00	0.00	0.00	0.00	0.00	0.00
NI2OH3+	-267.27		NI2OH3+	-267.27	-393.83	NI2OH3+	-267.27	-393.83	NI2OH3+	-267.27	-393.83	NI2OH3+	0.00	0.00	0.00	0.00	0.00	0.00
NI4(OH)4	-972.62		NI4(OH)4	-972.85	-1359.32	NI4(OH)4	-972.62	-1359.32	NI4(OH)4	-972.62	-1359.32	NI4(OH)4	-0.04	0.00	0.00	0.04	0.04	0.00
NICIT-	-82.70		NICIT-	-83.84	-54.00	NICIT-	-83.44	-54.00	NICIT-			NICIT-	-0.20	-0.13	0.07			

Table B.1: Comparison of aqueous species in Nagra 05/92, HATCHES 3.0, MINEQL-PSI 03/91 and PHREEQE-PSI 04/91 Data Bases Page 8 of 18

Nagra 05/92			HATCHES 3.0			MINEQL-PSI 03/91			PHREEQE-PSI 04/91			Nagra-HATCHES	Nagra-MQ0391	Nagra-PP0491	HATCHES-MQ0391	HATCHES-PP0491	MQ0391-PP0491	
Name	ΔG°	ΔH°	Name	ΔG°	ΔH°	Name	ΔG°	ΔH°	Name	ΔG°	ΔH°	$\Delta \log K$	$\Delta \log K$	$\Delta \log K$	$\Delta \log K$			
NICIT2-4	-95.26					NICL+	-179.10	-221.08	NICL+	-179.10	-221.08	0.00	0.00			0.00		
NICL+	-179.10					NICL2	-313.52	-388.14	NICL2	-313.52	-388.16	0.99	-0.02	0.00	-1.01	-0.99	0.02	
NICL2	-313.52		NICL2	-307.87	-388.14	NIC03	-606.51	-729.31	NIC03	-606.51	-729.31	-0.00	-0.00			0.00		
NICO3	-606.51					NIC032-2	-1159.15	-1404.63	NI(CO3)2	-1159.15	-1404.63	-0.00	-0.00			0.00		
NICO32	-1159.14					NIEDTA-2	-160.39	-54.00	NIEDTA-2	-165.47	-54.00	-0.01	-0.90		-0.89			
NIF+	-334.54					NIF+	-334.54	-389.35	NIF+	-334.54	-389.35	0.07	0.06			0.00		
NIH2CIT+	-122.09		NIH2CIT+	-121.69	-54.00	NIH2CIT+	-121.74	-54.00	NIH2PO4+	-1191.53	-1338.40	NIH2PO4+	-1191.53	-1338.40	0.01	0.00	-0.01	
NIH2PO4+	-1191.56					NIHCIT	-105.53	-54.00	NIHCIT	-105.88	-54.00	0.00	-0.06			-0.00		
NIHCIT	-105.53		NIHCIT	-105.53	-54.00	NIHC03+	-650.06	-729.31	NIHC03+	-650.06	-729.31	-0.00	-0.00			0.00		
NIHC03+	-650.06					NIHEDTA-	-180.31	-54.00	NIHEDTA-	-187.16	-54.00	-1.20						
NIHP207-	-2053.28					NIHP207-	-2053.24	-2336.97				0.01						
NIHPO4	-1158.34					NIHPO4	-1158.31	-1338.40	NIHPO4	-1158.31	-1338.40	0.01	0.00			-0.00		
NINH32	-128.09	-247.97				NINH32+2	-128.20	-248.14	NI(NH3)2	-128.09	-247.97	-0.02	0.00			0.02		
NINH36	-256.24	-634.70				NINH36+2	-256.64	-635.20	NI(NH3)6	-256.24	-634.70	-0.07	0.00			0.07		
NINO3+	-158.67					NINO3+	-158.67	-260.85	NINO3+	-158.67	-260.85	0.00	0.00			0.00		
NINO32	-263.76					NINO32	-263.76	-467.70	NI(NO3)2	-263.76	-467.70	0.00	0.00			0.00		
NINTA-	-118.43					NINTA-	-120.37	-54.00				-0.34						
NINTA2-4	-142.35																	
NOH+	-227.32	-287.91	NOH+	-226.46	-287.91	NOH+	-227.32	-287.91	NOH+	-227.32	-287.91	0.15	0.00	0.00	-0.15	-0.15	0.00	
NOH2	-405.72		NOH2	-411.43	-513.78	NOH2	-405.72	-625.66	NI(OH)2	-405.72	-625.66	-1.00	0.00	0.00	1.00	1.00	0.00	
NOH3-	-585.78		NOH3-	-585.78	-911.49	NOH3-	-585.78	-911.49	NI(OH)3-	-585.78	-911.49	0.00	0.00	0.00	0.00	0.00	0.00	
NOH4-	-743.01		NOH4-2	-743.01	-1197.32	NOH4-2	-743.01	-1197.32	NI(OH)4-	-743.01	-1197.32	0.00	0.00	0.00	0.00	0.00	0.00	
NOHDETA-3	-326.12																	
NOHNTA-2	-291.19																	
NOX	-74.88					NOX	-71.86	-54.00				0.53						
NIOX2-2	-95.37					NIOX2-2	-91.26	-54.00				0.72						
NIP207-2	-2018.07	-2356.25				NIOX3-4	-99.25	-54.00										
NIP04-	-1118.90								NIP207-2	-2018.02	-2356.59	0.01						
NIS04	-802.79	-949.37	NIS04	-803.30	-949.37	NIS04	-802.79	-949.37	NIP04-	-1118.87	-1338.40	0.01	0.00			-0.00		
NIS042	-1551.87					NIS203	-577.45	-702.50	NIPO4-	-1118.87	-1338.40							
NP+3	-517.10	-527.20	NP+3	-517.17	-527.19	NP+3	-517.10	-527.20	NIS042-2	-1551.87	-1872.68	NIS04-	-802.79	-949.37	-0.09	0.00	0.09	0.00
NP+4	-502.90	-556.10	NP+4	-502.90	-556.10	NP+4	-502.90	-556.10	NI(SO4)2	-1551.87	-1872.68	0.00	0.00	0.00	0.01	0.00	0.00	
NP20H2+4	-1428.57		NP20H2+4	-1434.42	-1683.86	NP20H2+4	-1428.57	-1626.06				-0.01	0.00	0.00	0.00	0.00	0.00	
NP3OH5+4	-2554.35					NP20H2+6	-1468.66	-1683.86	NP30H5+4	-2554.35	-3010.75							
NPCIT+	-594.23											0.00						
			NPCL+2	-634.69	-723.18													
			NPCL+3	-633.49	-723.18	NPCL+3	-640.97	-723.18				1.31	0.00		-1.31			
			NPCL2+	-751.07	-890.26													
			NPCL2+2	-763.91	-890.26	NPCL2+2	-776.19	-890.26				2.15	0.00		-2.15			
			NPCL3+	-892.96	-1057.34													
			NPC03+	-1099.82	-1231.41	NPC03+	-1099.82	-1202.51				3.09	0.00		-3.09			
			NPC032-	-1646.57	-1906.73	NPC032-	-1646.57	-1877.83				1.89	0.00		-1.89			
			NPC033-3	-2193.33	-2582.04	NPC033-3	-2193.33	-2553.14				1.69	0.00		-1.69			

Table B.1: Comparison of aqueous species in Nagra 05/92, HATCHES 3.0, MINEQL-PSI 03/91 and PHREEQE-PSI 04/91 Data Bases Page 9 of 18

Table B.1: Comparison of aqueous species in Nagra 05/92, HATCHES 3.0, MINEQL-PSI 03/91 and PHREEQE-PSI 04/91 Data Bases Page 10 of 18

Nagra 05/92			HATCHES 3.0			MINEQL-PSI 03/91			PHREEQE-PSI 04/91			Nagra-HATCHES ΔlogK			Nagra-MQ0391 ΔlogK			Nagra-PP0491 ΔlogK			HATCHES -MQ0391 ΔlogK			HATCHES -PP0491 ΔlogK		
Name	Δ _r G°	Δ _r H°	Name	Δ _r G°	Δ _r H°	Name	Δ _r G°	Δ _r H°	Name	Δ _r G°	Δ _r H°	Name	Δ _r G°	Δ _r H°	Name	Δ _r G°	Δ _r H°	Name	Δ _r G°	Δ _r H°	Name	Δ _r G°	Δ _r H°			
NP020X-	-940.00		NP020X-	-940.08	-1127.76																		-0.01			
NP020X	-836.33																									
NP020X2-3	-957.01		NP020X2-	-957.20	-1127.76																		-0.03			
NP020X2-2	-859.73																									
NP02S04	-1558.64		NP02S04	-1558.51	-2037.10	NP02S04	-1558.64	-1769.94															0.02	0.00	-0.02	
NP02S042	-2310.63		NP02S042	-2309.35	-2946.44	NP02S042	-2310.63	-2679.28															0.22	0.00	-0.22	
NP0H+2	-714.29		NP0H+2	-712.07	-841.93	NP0H+2	-714.29	-813.03															0.39	0.00	-0.39	
NP0H+3	-731.48		NP0H+3	-731.48	-841.93	NP0H+3	-731.48	-841.93															0.00	0.00	0.00	
NP0H2+	-905.76		NP0H2+	-897.27	-1127.76	NP0H2+	-905.76	-1098.86															1.49	0.00	-1.49	
NP0H2+2	-954.35		NP0H2+2	-960.06	-1127.76	NP0H2+2	-954.35	-1127.76															-1.00	0.00	1.00	
NP0H3	-1085.82		NP0H3	-1077.33	-1413.59	NP0H3	-1085.82	-1384.69															1.49	0.00	-1.49	
NP0H3+	-1168.66		NP0H3+	-1180.07	-1413.59	NP0H3+	-1168.66	-1413.59															-2.00	0.00	2.00	
NP0H3C03	-1736.53		NP0H3C03	-1742.24	-2088.90	NP0H3C03	-1736.53	-2088.90															-1.00	0.00	1.00	
NP0H4	-1377.26		NP0H4	-1400.09	-1699.42	NP0H4	-1377.26	-1699.42															-4.00	0.00	4.00	
NP0H4-	-1265.88		NP0H4-	-1251.68	-1699.42	NP0H4-	-1265.88	-1670.52															2.49	0.00	-2.49	
NP0H5-	-1574.44		NP0H5-	-1547.62	-1985.25	NP0H5-	-1574.44	-1985.25															4.70	0.00	-4.70	
NP0X+2	-570.25																									
NP0S04+2	-1269.16		NPS04+2	-1266.36	-1465.44	NPS04+2	-1269.16	-1465.44															0.49	0.00	-0.49	
NP0S042	-2023.44		NP(S04)2	-2021.84	-2374.78	NPS042	-2023.44	-2374.78															0.28	0.00	-0.28	
NTA-3	0.00	0.00				NTA-3	0.00	0.00																		
HNTA-2	-58.99					HNTA-2	-59.93	0.00																-0.17		
H2NTA-	-75.77					H2NTA-	-78.20	0.00																-0.43		
H3NTA-	-85.19					H3NTA	-90.76	0.00																-0.98		
H4NTA+	-90.76																									
O2(AQ)	16.52	-12.06	O2(AQ)	17.06	-7.70	O2(AQ)	16.52	-12.06	O2(AQ)	16.52	-12.06	O2(AQ)	16.52	-12.06	O2(AQ)	16.52	-12.06	O2(AQ)	16.52	-12.06	O2(AQ)	0.09	0.00	-0.09	-0.09	0.00
OH-	-157.23	-229.93	OH-	-157.23	-230.00	OH-	-157.23	-229.93	OH-	-157.24	-230.00	OH-	-157.24	-230.00	OH-	-157.24	-230.00	OH-	-157.24	-230.00	OH-	0.00	0.00	-0.00	0.00	-0.00
OX-2	0.00	0.00	OX2-	0.00	0.00	OX-2	0.00	0.00	OX-2	0.00	0.00	OX-2	0.00	0.00	OX-2	0.00	0.00	OX-2	0.00	0.00	OX-2					
HOX-	-24.35		HOX-	-24.37	0.00	HOX-	-23.97	0.00	HOX-	-23.97	0.00	HOX-	-23.97	0.00	HOX-	-23.97	0.00	HOX-	-23.97	0.00	HOX-	-0.00	0.07	0.07	0.07	
H2OX	-31.50		H2OX	-31.51	0.00	H2OX	-29.11	0.00	H2OX	-29.11	0.00	H2OX	-29.11	0.00	H2OX	-29.11	0.00	H2OX	-29.11	0.00	H2OX	-0.00	0.42	0.42	0.42	
PD+2	176.50	149.00				PD+2	176.50	149.00	PD+2	176.50	149.00	PD+2	176.50	149.00	PD+2	176.50	149.00	PD+2	176.50	149.00	PD+2	0.00	0.00	0.00	0.00	0.00
PDBR+	31.44					PDBR+	31.33	27.59	PDBR+	31.44	27.59	PDBR+	31.33	27.59	PDBR+	31.44	27.59	PDBR+	31.33	27.59	PDBR+	-0.02	0.00	0.02	0.02	
PDBR3-	-203.89					PDBR3-	-203.89	-215.23	PDBR3-	-203.89	-215.23	PDBR3-	-203.89	-215.23	PDBR3-	-203.89	-215.23	PDBR3-	-203.89	-215.23	PDBR3-	0.00	0.00	0.00	0.00	
PDBR4-2	-317.56	-384.34				PDBR4-2	-317.56	-384.34	PDBR4-2	-317.56	-384.34	PDBR4-2	-317.56	-384.34	PDBR4-2	-317.56	-384.34	PDBR4-2	-317.56	-384.34	PDBR4-2	0.00	0.00	0.00	0.00	
PDCL+	22.62	-37.91				PDCL+	22.62	-37.91	PDCL+	22.62	-37.91	PDCL+	22.62	-37.91	PDCL+	22.62	-37.91	PDCL+	22.62	-37.91	PDCL+	0.00	0.00	0.00	0.00	
PDCL2	-128.81					PDCL2	-128.81	-185.16	PDCL2	-128.81	-185.16	PDCL2	-128.81	-185.16	PDCL2	-128.81	-185.16	PDCL2	-128.81	-185.16	PDCL2	0.00	0.00	0.00	0.00	
PDCL3-	-276.07					PDCL3-	-276.07	-352.24	PDCL3-	-276.07	-352.24	PDCL3-	-276.07	-352.24	PDCL3-	-276.07	-352.24	PDCL3-	-276.07	-352.24	PDCL3-	0.00	0.00	0.00	0.00	
PDCL4-2	-417.10	-549.86				PDCL4-2	-417.10	-549.86	PDCL4-2	-417.10	-549.86	PDCL4-2	-417.10	-549.86	PDCL4-2	-417.10	-549.86	PDCL4-2	-417.10	-549.86	PDCL4-2	0.00	0.00	0.00	0.00	
PDEDTA-2	18.96																									
PDHDETA-	-1.02																									
PDHNTA	24.10																									
PDI+	65.30					PDI+	65.19	92.22	PDI+	65.30	92.22	PDI+	65.19	92.22	PDI+	65.30	92.22	PDI+	65.30	92.22	PDI+	-0.02	0.00	0.02	0.02	
PDI4-2	-159.61					PDI4-2	-159.61	-78.12	PDI4-2	-159.61	-78.12	PDI4-2	-159.61	-78.12	PDI4-2	-159.61	-78.12	PDI4-2	-159.61	-78.12	PDI4-2	0.00	0.00	0.00	0.00	
PDNH3+2	95.11					PDNH3+2	95.05	67.85	PDNH3+2	95.11	15.74	PDNH3+2	95.05	67.85	PDNH3+2	95.11	15.74	PDNH3+2	95.05	67.85	PDNH3+2	-0.01	0.00	0.01	0.01	
PDNH32+2	17.72					PDNH32+2	17.59	-13.30	PDNH32+2	17.72	-117.52	PDNH32+2	17.59	-13.30	PDNH32+2	17.72	-117.52	PDNH32+2	17.59	-13.30	PDNH32+2	-0.02	0.00	0.02	0.02	
PDNH33+2	-51.68					PDNH33+2	-51.88	-94.44	PDNH33+2	-51.68	-250.78	PDNH33+2	-51.88	-94.44	PDNH33+2	-51.68	-250.78	PDNH33+2	-51.88	-94.44	PDNH33+2	-0.04	0.00	0.04	0.04	
PDNH34+2	-117.08					PDNH34+2	-117.36	-175.59	PDNH34+2	-117.08	-384.04	PDNH34+2	-117.36	-175.59	PDNH34+2	-117.08	-384.04	PDNH34+2	-117.36	-175.59	PDNH34+2	-0.05	0.00	0.05	0.05	
						PDN034-2	-385.96	-678.40				PDN034-2	-385.96	-678.40				PDN034-2	-385.96	-678.40						

Table B.1: Comparison of aqueous species in Nagra 05/92, HATCHES 3.0, MINEQL-PSI 03/91 and PHREEQE-PSI 04/91 Data Bases Page 11 of 18

Table B.1: Comparison of aqueous species in Nagra 05/92, HATCHES 3.0, MINEQL-PSI 03/91 and PHREEQE-PSI 04/91 Data Bases Page 12 of 18

Table B.1: Comparison of aqueous species in Nagra 05/92, HATCHES 3.0, MINEQL-PSI 03/91 and PHREEQE-PSI 04/91 Data Bases Page 13 of 18

Table B.1: Comparison of aqueous species in Nagra 05/92, HATCHES 3.0, MINEQL-PSI 03/91 and PHREEQE-PSI 04/91 Data Bases Page 14 of 18

Nagra 05/92			HATCHES 3.0			MINEQL-PSI 03/91			PHREEQE-PSI 04/91			Nagra-HATCHES	Nagra-MQ0391	Nagra-PP0491	HATCHES	HATCHES	MQ0391
Name	$\Delta_f G^\circ$	$\Delta_f H^\circ$	Name	$\Delta_f G^\circ$	$\Delta_f H^\circ$	Name	$\Delta_f G^\circ$	$\Delta_f H^\circ$	Name	$\Delta_f G^\circ$	$\Delta_f H^\circ$	$\Delta \log K$					
						H6SI208-	-2507.02	-2763.92									
						H7SI208-	-2569.24	-2763.92									
			SIF6-2	-2220.56	-2393.77	SIF6-2	-2220.56	-2393.79									0.00
SN+2	-27.60	-8.90	SN+2	-27.60	-8.90	SN+2	-27.60	-8.90				0.00	0.00	0.00			
SN+4	2.37	0.50	SN+4	2.37	30.43	SN+4	2.37	0.50				0.00	0.00	0.00			
SN2OH2+2	-502.25		SN2OH2+2	-502.25	-589.46							0.00					
SN3OH4+2	-992.09		SN3OH4+2	-992.09	-1170.02							0.00					
						SNBR+	-137.73	-130.31									
						SNBR2	-245.00	-251.72									
						SNBR3-	-347.14	-373.13									
SNCL+	-162.36	-173.31	SNCL+	-162.36	-164.81							0.00					
SNCL2	-298.20	-339.85	SNCL2	-298.20	-329.63							0.00					
SNCL3-	-426.28	-504.58	SNCL3-	-426.28	-486.88							0.00					
SNEDTA-2	-144.04					SNEDTA-2	-168.01	-8.90					-4.20				
SNHEDTA-	-161.17					SNF+	-348.51	-344.25									
						SNF2	-646.01	-679.60									
						SNF3-	-930.38	-1014.95									
SN03-2	-575.20		SN03-2	-575.20	-866.39							0.00					
HSN02-	-410.27		HSN02-	-410.27	-580.56							0.00					
SNOH+	-255.89	-292.72	SNOH+	-255.89	-286.32	SNOH+	-246.48	-294.73				0.00	1.65	1.65			
SNOH2	-461.58		SNOH2	-461.58	-580.56							0.00					
SNOH3-	-644.21		SNOH3-	-644.21	-866.39							0.00					
SNOH5-	-1130.54		SNOH5-	-1130.54	-1438.05							0.00					
SNOH6-2	-1299.12		SNOH6-2	-1299.12	-1723.88							0.00					
SNOX2-2	-101.23																
SR+2	-563.83	-550.90	SR+2	-563.83	-550.90	SR+2	-563.83	-550.90	SR+2	-563.83	-550.90	0.00	0.00	0.00	0.00	0.00	0.00
SR CIT-	-588.37		SR CIT-	-587.29	-550.90	SR CIT-	-587.29	-550.90				0.19	0.19	0.00			
			SRCL+	-696.14	-726.35												
						SRCL2	-826.27	-885.06						0.00			
SRC030	-1107.76	-1204.39	SRC03	-1107.79	-1226.21	SRC03	-1107.79	-1204.37	SRC03	-1107.76	-1204.39	-0.00	-0.00	0.00	0.00	0.00	0.00
SREDTA-2	-623.19		SREDTA-2	-619.08	-550.90	SREDTA-2	-623.19	-550.90				0.72	0.00	-0.72			
			SRF+	-848.20	-869.51												
SRHC03+	-1157.47	-1215.81				SRHC03+	-1157.45	-1215.80	SRHC03+	-1157.47	-1215.81	0.00	-0.00			-0.00	
SRHEDTA-	-648.31					SRHEDTA-	-647.74	-550.90				0.10					
SRHOX+	-596.94																
SR(HOX)2	-625.48																
			SRN03+	-679.30	-757.75	SRHP04	-1669.80	-1835.30						0.02			
						SRN03+	-679.19	-757.75									
SRNTA-	-599.50					SRN032	-789.98	-964.60									
SROH+	-725.11		SROH+	-725.68	-780.50	SRNTA-	-603.22	-550.90				-0.65					
						SROH+	-725.11	-776.06	SROH+	-725.11	-776.08	-0.10	0.00	0.00	0.10	0.10	0.00
SROX	-578.33					SROX	-574.68	-550.90				0.64					
SROX2-2	-579.24															-1.82	
			SRP04-	-1613.19	-1835.30	SRP04-	-1623.57	-1835.30									
						SRS203	-1094.54	-1199.40									
SRS040	-1320.90	-1451.54	SRS04	-1322.39	-1460.24	SRS04	-1320.90	-1451.54	SRS04	-1320.90	-1468.94	-0.26	0.00	0.00	0.26	0.26	0.00

Table B.1: Comparison of aqueous species in Nagra 05/92, HATCHES 3.0, MINEQL-PSI 03/91 and PHREEQE-PSI 04/91 Data Bases Page 15 of 18

Table B.1: Comparison of aqueous species in Nagra 05/92, HATCHES 3.0, MINEQL-PSI 03/91 and PHREEQE-PSI 04/91 Data Bases Page 16 of 18

Table B.1: Comparison of aqueous species in Nagra 05/92, HATCHES 3.0, MINEQL-PSI 03/91 and PHREEQE-PSI 04/91 Data Bases Page 17 of 18

Nagra 05/92			HATCHES 3.0			MINEQL-PSI 03/91			PHREEQE-PSI 04/91			Nagra-HATCHES ΔlogK	Nagra-MQ0391 ΔlogK	Nagra-PP0491 ΔlogK	HATCHES-MQ0391 ΔlogK	HATCHES-PP0491 ΔlogK	MQ0391-PP0491 ΔlogK
Name	Δ,G°	Δ,H°	Name	Δ,G°	Δ,H°	Name	Δ,G°	Δ,H°	Name	Δ,G°	Δ,H°						
UL20H+3	-2126.72		UL20H+3	-2124.98	-2309.05	UO220H+3	-2126.72	-2323.83				0.30	0.00		-0.30		
UL20H2+2	-2347.19		UL20H+2	-2345.00	-2565.59	UO220H2+	-2347.19	-2572.00				0.38	0.00		-0.38		
UL3C36-6	-6333.28		UL3C036-	-6327.20	-7170.18	UO23C036	-6333.28	-7177.59				1.07	0.00		-1.07		
UL30H4+2	-3738.12		UL30H4+2	-3734.95	-4115.18	UO230H4+	-3738.12	-4200.32				0.56	0.00		-0.56		
UL30H5+	-3954.42		UL30H5+	-3951.54	-4380.09	UO230H5+	-3954.42	-4389.08				0.51	0.00		-0.51		
UL30H3CO			UL30H3CO	-4109.63	-4518.05												
UL20HC3	-3139.42																
UL30H5C+	-4338.47																
UL30H7-	-4340.52		UL30H7-1	-4313.37	-4826.23	UO230H5C	-4338.47	-4875.63				0.00					
UL40H7+	-5345.18		UL40H7+	-5341.49	-5917.54	UO230H7-	-4340.52	-5057.81				4.76	0.00		-4.76		
			UL4EDTA2	-4858.38	-5794.76	UO240H7+	-5345.18	-6076.81				0.65	0.00		-0.65		
ULCIT-	-1002.21		ULCIT-	-1001.29	-1162.86	UO2BR+	-1057.54	-1140.41				0.16					
ULCIT)-2-2	-2026.00																
ULCL+	-1084.17		ULCL+	-1082.28	-1329.94	UO2CL+	-1084.17	-1178.09				0.33	0.00		-0.33		
ULCL2	-1208.71		ULCL2	-1210.07	-1497.02	UO2CL2	-1208.71	-1338.14				-0.24	0.00		0.24		
			ULCL3-	-1331.59	-1664.10												
ULC030	-1535.38		ULC03	-1533.77	-1702.19	UO2C03	-1535.38	-1689.29	ULC03	-1536.91	-1705.55	0.28	0.00	-0.27	-0.28	-0.55	-0.27
ULC032-2	-2105.37		ULC032-2	-2102.22	-2354.50	UO2C032-	-2105.37	-2351.18	ULC032-2	-2104.50	-2354.08	0.55	0.00	0.15	-0.55	-0.40	0.15
ULC033-4	-2659.71		ULC033-4	-2656.96	-3080.44	ULC033-4	-2659.71	-3083.23	ULC033-4	-2657.53	-3085.04	0.48	0.00	0.38	-0.48	-0.10	0.38
						ULC033-	-2587.19	-3051.07									
ULEDTA-2	-1027.33					UO2EDTA-	-1021.05	-1019.00				1.10					
ULF+	-1263.12		ULF+	-1261.12	-1498.21	UO2F+	-1263.12	-1352.64				0.35	0.00		-0.35		
ULF2	-1564.79		ULF2	-1563.76	-1833.56	UO2F2	-1564.79	-1687.61				0.18	0.00		-0.18		
ULF3-	-1859.33		ULF3-	-1860.12	-2168.91	UO2F3-	-1859.33	-2022.71				-0.14	0.00		0.14		
ULF4-2	-2145.47		ULF4-2	-2148.49	-2504.26	UO2F4-2	-2145.47	-2360.11				-0.53	0.00		0.53		
ULH2P04	-2108.35		ULH2P4+	-2106.12	-2317.97	UO2H2P04	-2108.35	-2303.40				0.39	0.00		-0.39		
			ULH2P43-	-4404.27	-4990.37												
ULH3P04	-2106.36					UO2H3P04	-2106.36	-2303.40				0.00					
ULH4P04	-3256.39		ULH4P42	-3257.19	-3656.77	UO2H4P04	-3256.39	-3587.80				-0.14	0.00		0.14		
ULH5P04	-3261.07					UO2H5P04	-3261.07	-3587.80				0.00					
ULHEDTA-	-1062.14		ULHEDTA-	-1056.08	-1162.86	UO2HEDTA	-1065.00	-1019.00				1.06	-0.50		-1.56		
ULHP04	-2092.60		ULHP04	-2092.42	-2312.12	UO2HP04	-2092.60	-2303.40				0.03	0.00		-0.03		
ULN03+	-1065.00		ULN03+	-1062.99	-1369.71	UO2N03+	-1065.00	-1225.85				0.35	0.00		-0.35		
ULNTA-	-1014.20																
ULOH+	-1159.95		ULOH+	-1158.52	-1261.25	UO2OH+	-1159.95	-1261.69	ULOH+	-1155.66	-1258.32	0.25	0.00	0.75	-0.25	0.50	0.75
ULOH2	-1367.93		ULOH2	-1357.98	-1517.37	UO2OH2	-1367.93	-1590.66	UL(OH)2	-1357.41	-1517.37	1.74	0.00	1.84	-1.74	0.10	1.84
ULOH3-	-1554.32					UO2OH3-	-1554.32	-1876.49				0.00					
ULOH4-2	-1712.69		ULOH4-2	-1692.42	-2009.53	UO2OH4-2	-1712.69	-2162.32				3.55	0.00		-3.55		
ULOX	-992.51		ULOX	-992.72	-1162.86							-0.04					
ULOX2-2	-1016.48		ULOX2-2	-1016.70	-1162.86							-0.04					
ULP04-	-2056.18					UO20HEDT	-1221.08	-1304.83				0.00					
						UO2P04-	-2056.18	-2303.40									
						UO2S203	-1487.82	-1667.50									
						UO2S03	-1477.64	-1654.50									
ULS04	-1714.47		ULS04	-1712.18	-1906.10	UO2S04	-1714.47	-1908.88				0.40	0.00		-0.40		
ULS042-2	-2464.18		ULS042-2	-2464.17	-2981.54	UO2S042-	-2464.18	-2802.66				0.00	0.00		-0.00		

Table B.1: Comparison of aqueous species in Nagra 05/92, HATCHES 3.0, MINEQL-PSI 03/91 and PHREEQE-PSI 04/91 Data Bases Page 18 of 18

Nagra 05/92			HATCHES 3.0			MINEQL-PSI 03/91			PHREEQE-PSI 04/91			Nagra-HATCHES	Nagra-MQ0391	Nagra-PP0491	HATCHES	HATCHES	MQ0391
Name	Δ_fG°	Δ_fH°	Name	Δ_fG°	Δ_fH°	Name	Δ_fG°	Δ_fH°	Name	Δ_fG°	Δ_fH°	Δ_fG°	Δ_fH°	Δ_fG°	Δ_fH°	Δ_fG°	Δ_fH°
UO2C033-5	-2587.19		UO20H	-1147.67	-1448.69												
UOH+3	-763.98	-830.13	UO20H2-	-1330.01	-1734.52	UO2C033-	-2636.41	-3188.80									
UOH4	-1452.56		UO4H+	-761.29	-827.66	UO4H2+	-992.72	-1088.39	UO4H3+	-1195.62	-1448.69						
UOH5-	-1621.15		UO5H-	-1567.15	-2020.35	UO4H4	-1409.93	-1734.52	UO4H5-	-1621.15	-2020.35	U(OH)4	-1429.90	-1630.76	7.47	0.00	3.97
UOHEDTA-	-905.13					UOHEDTA-	-905.70	-877.03	UOHEDTA-EDTA	-1830.24	-1754.06	U(OH)5-	-1640.50	-1904.87	9.46	0.00	-3.39
UOHEDTA)2-2	-1825.67														-0.10	-9.46	-12.85
UOX+2	-593.22														-0.80		-3.39
USO4+2	-1311.42	-1492.59	USO4+2	-1302.40	-1495.52	USO4+2	-1311.42	-1492.59									
USO42	-2077.85	-2377.29	U(SO4)2	-2074.94	-2386.87	USO42	-2077.85	-2377.29									
ZR+4	-524.50	0.00	ZR+4	-524.50	0.00												
ZR30H4+8	-2518.64		ZR30H4+8	-2518.64	-1143.32												
ZR4OH8+8	-4029.37		ZR4OH8+8	-4029.37	-2286.64												
ZRCIT+	-621.53																
ZRCL+3	-656.86		ZRCL+3	-656.86	-167.08												
ZREDTA	-711.72																
ZRHClT+2	-634.66																
ZRNTA+	-662.06																
ZROH+3	-763.35		ZROH+3	-763.35	-285.83												
ZROH4	-1417.69		ZROH4	-1417.69	-1143.32												
ZROH5-	-1618.87		ZROH5-	-1618.87	-1429.15												
ZROHEDTA-	-912.33																
ZROX+2	-595.28																
ZRSO4+2	-1285.91		ZRSO4+2	-1285.91	-909.34												

0.00

0.00

0.00

1.58

0.51

0.00

7.47

9.46

0.00

-8.62

0.47

0.00

-0.47

3.97

-3.39

-7.47

-9.46

-3.50

-12.85

3.97

-0.10

-0.80

-0.51

Table B.2: Comparison of minerals and gases in Nagra 05/92, HATCHES 3.0, MINEQL-PSI 03/91 and PHREEQE-PSI 04/91 Data Bases Page 1 of 16

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Table B.2: Comparison of minerals and gases in Nagra 05/92, HATCHES 3.0, MINEQL-PSI 03/91 and PHREEQE-PSI 04/91 Data Bases Page 2 of 16

Table B.2: Comparison of minerals and gases in Nagra 05/92, HATCHES 3.0, MINEQL-PSI 03/91 and PHREEQE-PSI 04/91 Data Bases Page 3 of 16

Nagra 05/92			HATCHES 3.0			MINEQL-PSI 03/91			PHREEQE-PSI 04/91			Nagra-HATCHES	Nagra-MQ0391	Nagra-PP0491	HATCHES	HATCHES	MQ0391			
	Name	Δ_fG°	Δ_fH°	Name	Δ_fG°	Δ_fH°	Name	Δ_fG°	Δ_fH°	Name	Δ_fG°	Δ_fH°	HATCHES	-MQ0391	-PP0491	-PP0491	$\Delta logK$			
	C5S6.3.5	-9414.52	-10456.4																	
	C5S6.3H	-9264.27	-10313.4																	
	C5S6.5.5	-9878.24	-11028.0																	
	C6S6.H2	-9449.29	-10570.6																	
	CA-AL	-3109.71	-3648.42																	
	CA(I03)2	-838.19	-1005.88																	
	CA2CL2(O	-1929.07	-2277.65																	
	CA2SI3O8	-4539.89	-5028.14																	
	CA2SiO4.	-2479.41	-2876.52																	
	CA2SiO4(-2199.25	-2542.96																	
	CA3AS042	-3061.23	-3405.87	CA3AS042	-3085.95	-3405.28									-4.33					
	CA3Si2O7	-4404.38	-5114.58																	
	CA3SiO5	-2780.85	-3371.79																	
	CA4CL2(O	-6588.62	-7936.93																	
				CA4HP043	-5555.40	-6025.20														
				CACL2.2H	-1243.29	-1448.82														
				CACL2.4H	-1735.90	-2020.48														
				CACL2.H2	-1005.41	-1162.99														
				CAHPO4(C	-1687.04	-1821.54	CAHPO4-2a	-1686.35	-1846.23						0.12					
				CAI2(C)	-528.39	-536.86														
CALCITE	-1129.13	-1208.71		CALCITE	-1129.07	-1207.52	CALCIT	-1129.13	-1208.69	CALCITE	-1129.13	-1208.69	0.01	-0.00	-0.00	-0.01	-0.01	0.00		
				CALCIUM	-1735.84	-2020.48														
				CAO	-603.70	-635.28	CAM004	-1431.35	-1540.90											
CAOX.3H2O	-1311.72			CAOX.H2O	-840.06		CAOXAL	-598.47	-543.00											
				CARNALLI	-2528.90	-2935.36														
				CASECR	-363.43	-368.11	CASE	-363.48	-368.23						-0.01					
				CASE03	-954.00	-1052.20	CASE03_2	-1427.94	-1623.86	CASE03AQ	-1427.94	-1623.87				0.14	0.14	-0.00		
				CASE03.2	-1423.09	-1623.74														
				CASE04	-1011.74	-1142.10	CASE04_H	-1486.65	-1706.65	CASE04_2	-1486.02	-1706.86	CASE04AQ	-1486.02	-1706.86	0.11	0.11	0.00		
				CAST205.	-2874.23	-3171.09	CAS03	-1077.38	-1178.50											
				CAS04.HY	-1435.18	-1595.26														
				CAU(P04)	-3916.74	-4274.66														
				CAUL2Si3	-4974.50	-5328.34														
				CAU04	-1893.10	-2001.46	CAU04	-1888.08	-2001.70						0.88					
				CCHL-7A	-8195.42	-9497.66														
				CCHL-14A	-8214.65	-9497.66														
CELESTITE	-1345.68	-1455.90	CH4(G)	-50.72	-74.81	CELESTIT	-1344.76	-1458.27	CELESTIT	-1345.67	-1455.89	CELESTIT	-1345.67	-1462.75	0.16	0.00	0.00	-0.16	-0.16	0.00
						CHABAZIT	-7163.23	-8019.30												
CHALCEDONY	-853.73	-905.06		CHALCEDY	-853.55	-904.63	CHALCEDO	-853.72	-905.07	CHALCEDO	-853.72	-905.05	(- H2O)	0.03	0.00	0.00	-0.03	-0.03	0.00	
CO2(G)	-394.37	-393.51		PCO2	-394.38	-392.79								-0.00						

Table B.2: Comparison of minerals and gases in Nagra 05/92, HATCHES 3.0, MINEQL-PSI 03/91 and PHREEQE-PSI 04/91 Data Bases Page 4 of 16

Nagra 05/92			HATCHES 3.0			MINEQL-PSI 03/91			PHREEQE-PSI 04/91			Nagra-HATCHES	Nagra-MQ0391	Nagra-PP0491	HATCHES-MQ0391	HATCHES-PP0491	MQ0391-PP0491
Name	Δ_fG°	Δ_fH°	Name	Δ_fG°	Δ_fH°	Name	Δ_fG°	Δ_fH°	Name	Δ_fG°	Δ_fH°	Δ_{logK}	Δ_{logK}	Δ_{logK}	Δ_{logK}	Δ_{logK}	Δ_{logK}
			CHAMOSIT	-3443.53	-4141.11												
			CHLOROMA	-592.27	-801.16												
			CHRYSOTI	-4038.73	-4600.75												
			CL'ZOISI	-6489.77	-7357.91												
			CLAUDETI	-577.11	-572.23												
			COLEMANI	-6324.01	-6951.14												
			CORD-HYD	-8885.23	-10086.6												
			CORD-ANH	-8633.94	-9800.74												
			CORUNDUM	-1572.39	-1934.29												
			CRIST	-853.15	-885.30												
			CRIST.BE	-850.64	-885.30												
			CRONSTED	-2568.10	-3158.83												
						CRYOLITE	-3159.63	-3309.55									
			DACH-NA	-24801.5	-27002.7												
			DACH-CA	-24900.6	-27158.5												
			DACH-K	-24941.9	-27061.7												
			DAPH-7A	-6403.10	-7608.16												
			DAPH-14A	-6422.34	-7608.16												
			DAWSONIT	-1787.90	-2040.36												
			DIASPORE	-915.84	-1110.06												
			DIOPSID	-3029.70	-3352.26												
DOLO_DIS	-2158.45	-2314.23	DOL-DIS	-2158.80	-2389.92	DOLO_DIS	-2158.45	-2314.23				-0.06	-0.00	0.06			
DOLO_ORD	-2161.59	-2321.15	DOLOMITE	-2161.19	-2325.94	DOLOMITE	-2161.59	-2321.13	DOLOMITE	-2161.08	-2325.94	0.07	-0.00	0.09	-0.07	0.02	0.09
			EDINGTON	-5831.96	-6551.84												
			ENSTATIT	-1460.53	-1638.13												
			EPID-ORD	-6063.64	-6866.77												
			EPIDOTE	-6063.64	-6866.77												
			EPISTILB	-8638.09	-9504.07												
			EPSOMITE	-2869.65	-3377.15												
			ERION-NA	-39760.1	-43774.1												
			ERION-CA	-39938.4	-44054.6												
			ERION-K	-40023.1	-43880.3												
			EUCRYPTI	-2012.59	-2273.83												
			FAUJ-NA	-7597.76	-8528.64												
			FAUJ-CA	-7637.45	-8590.96												
			FAYALITE	-1356.80	-1635.16	FAYALITE	-1366.22	-1469.37				-1.65					
FE(CR)	0.00	0.00				FE2SE032	-1298.94	-1624.80									
			FE2SO43	-2236.43	-2822.54												
			FE3PO42	-4390.30	-5122.74												
			FE3SE4	-219.70	-206.27				FE3SE4	-221.41	-209.62				-0.30		
			FEF2(C)	-655.87	-759.80				FEASO4CR	-772.86	-936.74						
			FEF3(C)	-959.36	-1053.31												
			FE0(C)	-251.20	-374.93												
			FEOH2(S)	-475.50	-569.05	FE(OH)2CR	-479.55	-569.55							-0.71		
FE(OH)3A	-698.88	-906.09				FE0H3AG	-711.44	-824.50				-2.20					
FE(OH)3B	-687.46	-906.09				FE0H3CR	-698.88	-824.50	FE(OH)3(-701.68	-823.16	-2.00	-2.49		-0.49		

Table B.2: Comparison of minerals and gases in Nagra 05/92, HATCHES 3.0, MINEQL-PSI 03/91 and PHREEQE-PSI 04/91 Data Bases Page 5 of 16

Nagra 05/92			HATCHES 3.0			MINEQL-PSI 03/91			PHREEQE-PSI 04/91			Nagra-HATCHES	Nagra-MQ0391	Nagra-PP0491	HATCHES-MQ0391	HATCHES-PP0491	MQ0391-PP0491														
Name	Δ_fG°	Δ_fH°	Name	Δ_fG°	Δ_fH°	Name	Δ_fG°	Δ_fH°	Name	Δ_fG°	Δ_fH°	$\Delta \log K$	$\Delta \log K$	$\Delta \log K$	$\Delta \log K$																
FLUORITE	-1176.35 -1233.34		FEOH3A	-688.03	-904.75	FEPO4(S)	-1655.16	-1895.20	FEPO4CR	-1651.62	-1904.66					0.62															
			FERR-MG	-1292.46	-1704.84	FERR-2-C	-1976.16	-2609.67	FERR-CA	-1387.36	-1780.84					-0.18															
			FERROSIL	-1107.14	-1260.23	FESCR	-90.63	-105.40																							
			FESE	-87.06	-64.95	FESE2	-96.37	-102.73	FESE2	-97.41	-102.91					11.50															
			FESO4(C)	-807.83	-998.44	FLUORAPA	-6524.45	-6947.86	FLUORAP	-6458.79	-6911.50	FLUORITE	-1176.35	-1233.37	FLUORITE	-1175.27 -1229.60	-0.36 -0.00 0.19 0.36														
			FLUORITE	-1178.41	-1233.41	FORSTERI	-2057.86	-2390.96	FLUORITE	-1176.35	-1233.37					0.55 0.19															
			GARRONIT	-18690.9	-20969.9	GAYLUSSI	-3372.01	-3832.75	GEHLENIT	-3784.42	-4477.25																				
GIBBS_CR	-1156.63	-1300.50	GIBBSITE	-1152.86	-1300.50	GIBBSI_C	-1156.63	-1300.50									0.00														
GIBBS_MC	-1149.55	-1293.38	GISMONDI	-4977.00	-5677.04	GIBBS_MC	-1149.55	-1293.38									0.00														
GOETHITE GRAPHITE	-484.57 0.00	-620.26 0.00	GOETHITE	-475.95	-558.34	GOETHITE	-476.01	-560.43	GOETHITE	-475.95	-558.34	1.51	1.50	1.51	-0.01	0.00	0.01														
			GRAPHITE	-103.74	750.54																										
			GREENALI	-2960.37	-3467.05																										
			GROSSULA	-6267.07	-7076.68																										
			GUMMITTE	-1129.35	-1304.34																										
GYPSUM H2(G)	-1797.23 0.00	-2023.55 0.00	GYPSUM	-1797.34	-2023.87	GYPSUM	-1797.23	-2023.54	GYPSUM	-1797.23	-2023.54	-0.02	0.00	0.00	0.02	0.02	0.00														
			H2-GAS	0.00	0.00	H2_GAS	-0.03	-0.02	H2S_GAS	-33.42	-16.30	H2TCO42	-576.37	-572.23																	
HAUSMANITE	-1284.51	-1384.49	H2SO4H6	-1433.43	-1723.88	HAIWEET	-9393.64	-10178.5	HALITE	-384.09	-407.42	HARMOTOM	-8874.13	-9779.40																	
			HAUSMANN	-1282.62	-1523.59	HAUSMANN	-1284.51	-1384.49					0.33	0.00																	
			HEDENBER	-2661.94	-2974.36																										
			HEMATITE	-743.36	-822.93	HEMATITE	-742.28	-826.66	HEMATITE	-816.88	-864.02					0.19 -12.88 -13.07															
			HERCYNIT	-1842.36	-2309.22																										
			HEUL-NA	-9691.59	-10612.9	HEUL-CA	-9731.23	-10675.2	HEUL	-9680.97	-10743.3	HEXAHYDR	-2631.14	-3091.32																	
			HTCO4(S)	-589.75	-857.49																										
			HUNTITE	-4205.17	-4703.83																										
			HYDROBOR	-6469.68	-7160.97																										

Table B.2: Comparison of minerals and gases in Nagra 05/92, HATCHES 3.0, MINEQL-PSI 03/91 and PHREEQE-PSI 04/91 Data Bases Page 6 of 16

Nagra 05/92			HATCHES 3.0			MINEQL-PSI 03/91			PHREEQE-PSI 04/91			Nagra-HATCHES	Nagra-MQ0391	Nagra-PP0491	HATCHES-MQ0391	HATCHES-PP0491	MQ0391-PP0491
Name	$\Delta_f G^\circ$	$\Delta_f H^\circ$	Name	$\Delta_f G^\circ$	$\Delta_f H^\circ$	Name	$\Delta_f G^\circ$	$\Delta_f H^\circ$	Name	$\Delta_f G^\circ$	$\Delta_f H^\circ$	$\Delta \log K$					
			HYDROMAG	-5867.17	-6809.81												
			HYDROPHI	-747.78	-877.16												
			HYDROXAP	-6308.67	-6747.05	HYDROXAP	-6323.09	-6746.92									-2.53
			I2(S)	-0.13	-3.19												
			ILLITE	-5460.66	-6034.05												
			JADEITE	-2844.87	-3121.00												
			JAROS-K	-3257.61	-3927.58												
			JAROS-NA	-3214.11	-3915.78												
			K-SODIUM	-2495.16	-2897.42												
			K-FELD	-3748.20	-4018.10												
			K-SEQUI	-6332.40	-7014.36												
			K-CARBON	-1430.67	-1622.98												
			K(UO2)(A)	-2009.97	-2159.09												
			K2CO3.3/	-1430.73	-1622.98												
			K2SE	-371.41	-1001.81	K2SE	-369.93	-383.78	K2SE	-369.98	-383.90				0.26	0.25	-0.01
						K2SE03	-877.97	-966.62	K2SE03	-877.97	-966.50				-0.00		
						K2SE04CR	-1009.97	-1128.07	K2SE04	-1009.97	-1127.98				0.00		
						K4PUS044	-4690.38	-5182.32									
			K8H4(CO3)	-6332.46	-7014.36												
			KAINITE	-2325.12	-2653.05												
			KALICINI	-867.51	-942.10												
			KALSILIT	-2017.47	-2247.50												
			KALSO42	-2240.55	-2609.22												
			KALSO42.	-187.36	-6039.18												
KAOLINITE	-3793.17	-4128.86	KAOLINIT	-3783.78	-4113.50	KAOLINIT	-3793.20	-4128.89				1.65	-0.00		-1.65		
			KBR	-380.02	-373.55												
			KIESERIT	-1437.17	-1662.17												
			KMGCL3	-1009.14	-1220.38												
			KMGCL3.2	-1525.08	-1792.04												
			KNACO3.6	-2495.28	-2897.42												
KTC04	-918.84		KTC04	-918.84	-1109.63							0.00					
			KYANITE	-2434.84	-2819.59												
			LAB.SALT	-4339.59	-4804.04												
			LANSFORD	-2199.84	-2586.11												
			LARNITE	-2190.86	-2542.96	LARNITE	-2191.08	-2295.58					-0.04				
			LAUMONTI	-6685.98	-7447.64												
			LAWRENCI	-289.74	-423.26												
			LAWSONIT	-4495.93	-5105.38												
			LEONHARD	-2152.76	-2519.66												
			LEONITE	-3478.90	-3933.28												
			LEVYNE	-7163.23	-8019.30												
			LI(UO2)(-2001.26	-2185.42												
			LI2SE	-394.06	-1054.47	LI2SE	-392.46	-400.88	LI2SE	-392.52	-401.00				0.28	0.27	-0.01
						LI2SE03	-969.40	-1057.77	LI2SE03	-969.40	-1057.99				-0.00		
						LI2SE04	-1020.01	-1138.05	LI2SE04	-1020.01	-1138.01				0.00		
						LI2U04	-1846.46	-1961.50									
			MAGNESIU	-2552.85	-3101.89												
			MAGNETIT	-977.72	-1326.94	MAGNETIT	-1013.22	-1120.42	MAGNETIT	-1161.12	-1195.69				-6.22	-32.13	-25.91

Table B.2: Comparison of minerals and gases in Nagra 05/92, HATCHES 3.0, MINEQL-PSI 03/91 and PHREEQE-PSI 04/91 Data Bases Page 7 of 16

Table B.2: Comparison of minerals and gases in Nagra 05/92, HATCHES 3.0, MINEQL-PSI 03/91 and PHREEQE-PSI 04/91 Data Bases Page 8 of 16

Nagra 05/92			HATCHES 3.0			MINEQL-PSI 03/91			PHREEQE-PSI 04/91			Nagra-HATCHES	Nagra-MQ0391	Nagra-PP0491	HATCHES-MQ0391	HATCHES-PP0491	MQ0391-PP0491
Name	Δ, G°	Δ, H°	Name	Δ, G°	Δ, H°	Name	Δ, G°	Δ, H°	Name	Δ, G°	Δ, H°	$\Delta \log K$					
			MONOHYDR	-1361.36	-1518.79												
			MONT-NA	-5322.44	-5817.07												
			MONT-MG	-5311.60	-5814.81												
			MONT-K	-5331.17	-5820.96												
			MONT-CA	-5327.21	-5827.35												
			MONTICEL	-2146.13	-2466.96												
MO-ELEM	0.00	0.00															
MO02(CR)	-533.01	-588.94															
MO03(CR)	-667.97	-745.09															
			MORD-K	-6169.51	-6646.19												
			MORD-NA	-6128.91	-6634.39												
			MUSCOVIT	-5597.11	-6238.22												
N2(G)	0.00	0.00															
			NA2C03	-1048.00	-1170.64												
			NA2SE	-327.44	-978.21	NA2SE	-327.10	-343.03	NA2SE	-327.15	-343.15		0.06	0.05	-0.01		
			NA2SE2	-370.82	-1193.77	NA2SE2	-370.03	-388.21	NA2SE2	-370.13	-388.03		0.14	0.12	-0.02		
			NA2SE04	-962.35	-1080.20	NA2SE03	-871.27	-959.76	NA2SE03	-871.27	-959.80				-0.00		
			NA2SI205	-2324.29	-2537.11	NA2SE04	-962.29	-1079.99	NA2SE04	-962.29	-1079.99		0.01	0.01	0.00		
			NA2U207	-2995.88	-3194.61	NA2U207	-3011.31	-3203.79							-2.70		
A_NA2U04	-1679.15	-1899.00	NA2U04	-1769.67	-1889.18	A_NA2U04	-1679.15	-1899.00				-15.86	0.00		15.86		
			NA3H(SO4)	-2278.36	-2539.70												
			NA3U04	-1897.25	-2022.08	NA3U04	-1899.74	-2024.01							-0.44		
			NA4SiO4	-1975.67	-2418.32												
			NA6Si2O7	-3369.37	-4070.13												
			NABR	-349.08	-361.75												
			NABR.ZH2	-828.04	-933.41												
			NAFE02(C)	-627.28	-859.26												
			NAHCOLIT	-849.40	-930.30												
			NAMP02CO	-2600.58	-2902.83												
NATC04(S)	-876.71		NATC04(S)	-876.71	-1097.83							0.00					
			NATROLIT	-5320.91	-5928.36												
			NATRON	-3427.56	-4028.94												
			NAU03	-1411.05	-1494.14												
NB205CR	-1766.00	-1899.50	NEPHELIN	-1980.53	-2235.70												
NB02CR	-740.50	-796.20	NESQUEHO	-1724.36	-2014.45												
			NH4HSE	-23.53	-629.53	NH42PU02	-1988.21	-2335.12									
						NI-SPINE	-1280.72	-1386.62									
						NI_ELEM	-1.19	-1.91	NI.METAL	-1.19	-1.91						0.00
						NI2OH3CL	-824.25	-1132.57									
						NI2P207	-2096.61	-2420.51									
						NI2SI04	-1317.08	-1564.96	NI-OLIVI	-1288.72	-1393.31						
NI2SiO4	-1288.72	-1523.97				NI2Si04S	-1280.72	-1522.35	NI3AS042	-1606.00	-1938.28						-0.02
NI2Si04S	-1280.72	-1522.35													4.97	4.97	0.00

Table B.2: Comparison of minerals and gases in Nagra 05/92, HATCHES 3.0, MINEQL-PSI 03/91 and PHREEQE-PSI 04/91 Data Bases Page 9 of 16

Nagra 05/92			HATCHES 3.0			MINEQL-PSI 03/91			PHREEQE-PSI 04/91			Nagra-HATCHES	Nagra-MQ0391	Nagra-PP0491	HATCHES-MQ0391	HATCHES-PP0491	MQ0391-PP0491
Name	Δ_rG°	Δ_rH°	Name	Δ_rG°	Δ_rH°	Name	Δ_rG°	Δ_rH°	Name	Δ_rG°	Δ_rH°	$\Delta logK$	$\Delta logK$	$\Delta logK$	$\Delta logK$	$\Delta logK$	
NI3S2	-310.33	-229.10	NI3P042	-2366.45	-2760.34	NI3P042CR	-2356.73	-2578.50	NI3P04.2	-2356.75	-2578.50				1.70	1.70	-0.00
NI3S4	-671.82	-325.20	NI3S2	-196.41	-311.91	NI3S2	-196.63	-181.63	NI3S2	-310.10	-196.94	19.96	19.92	0.04	-0.04	-19.92	-19.88
			NI3S4	-310.54	384.12	NI3S4	-331.17	-218.00	NI3S4	-671.82	-353.22	63.29	59.68	0.00	-3.61	-63.29	-59.68
			NI3SE4	-249.31	-1870.15	NI40H7CL	-1722.45	-2383.89									
			NI8022	-1454.15	-1599.83	NI(B02)2	-1454.10	-1627.94									0.01
			NIBR2	-199.53	-213.98	NIBR2S	-199.53	-213.98									0.00
			NICL2.2H	-759.83	-959.82	NICL2_2H	-760.12	-922.16	NICL22AQ	-760.12	-922.04						
			NICL2.4H	-1234.57	-1531.48	NICL2_4H	-1234.91	-1516.42	NICL24AQ	-1234.91	-1516.54						
			NICL2.6H	-1712.73	-2103.14	NICL2_6H	-1713.24	-2103.14	NICL26AQ	-1713.24	-2103.06						
			NICL2(S)	-258.95	-305.15	NICL2CR	-260.32	-307.41	NICL2S	-260.32	-307.41						
NICO3S	-613.30	-720.22	NICO3(S)	-612.73	-729.31	NICO3CR	-613.30	-691.24	NICO3S	-613.30	-691.24	0.10	-0.00	-0.00	-0.10	-0.10	0.00
			NIF2.4H	-1580.49	-1901.49	NIF2_4H2	-1586.48	-1868.02	NIF2.4AQ	-1586.48	-1868.02				-1.05	-1.05	0.00
NIF2S	-610.64	-709.00	NIF2(S)	-603.79	-724.70	NIF2CR	-610.64	-659.01	NIF2S	-610.64	-659.01	1.20	0.00	0.00	-1.20	-1.20	0.00
NIFE204	-972.96	-1305.12	NIFE204	-947.73	-1291.84	NIFE204	-973.07	-1083.65	NIFE204	-972.96	-1080.97	4.42	-0.02	0.00	-4.44	-4.42	0.02
			NI12	-81.74	-80.11	NI12S	-81.74	-80.11									0.00
NIO	-211.68	-315.90	NINGYOIT	-3917.08	-4304.20												
			NIO	-211.68	-339.83	NIO	-211.68	-239.71	NIO	-211.68	-239.71	0.00	0.00	0.00	0.00	0.00	0.00
NI(OH)2S	-447.22	-602.73	NIOH2(S)	-458.24	-529.72	NI(OH)2CR	-447.22	-529.72	NI(OH)2S	-447.22	-529.72	-1.93	0.00	0.00	1.93	1.93	0.00
			NI(OH)2B0H	-2526.80	-2743.15	NI(OH)2B	-2526.75	-2771.26	NI(OH)2B	-2526.75	-2771.26						0.01
NIS	-85.99	-70.46	MILLERIT	-79.06	12.03	MILLERIT	-86.04	-83.52	NIOHCL50	-452.09	-510.45				-1.22	-1.21	0.01
			NIS	-79.06	12.03	NIS_ALPH	-64.75	-70.30	NIOHCL75	-490.56	-540.14				2.51		
			NIS_BETA	-96.15	-70.30	NIS	-85.99	0.03	NIS	-85.99	0.03	1.21	3.72				
NIS2	-248.59	-130.90	NIS2	-125.25	360.05	NIS2	-105.85	-70.30									0.00
NISI03	-1127.95		NISE2	-106.56	-767.09	NIS2	-135.11	-140.57	NIS2	-248.58	-129.95	21.61	19.88	0.00	-1.73	-21.61	-19.88
			NISE03.2	-913.14	-1134.74	NISE03CR	-445.65	-563.20				178.94					
			NIS04.6H	-2223.80	-2678.32	NIS04.6H	-1127.95	-1150.13	NISI03	-1127.95	-1225.13						
			NIS04.7H	-2460.94	-2964.15	NIS04.7H	-2223.91	-2682.92	NIS046AQ	-2223.91	-2682.88						
			NIS04(S)	-759.18	963.34	NIS04(S)	-759.18	-872.97	NIS047AQ	-2461.11	-2976.37	0.03	0.00	0.00	-0.02	-0.02	0.00
			NITER	-393.81	-458.99	NIS04CR	-759.18	-872.97	NIS04S	-759.18	-872.97				-0.03	-0.03	0.00
			NITROBAR	-790.13	-946.20												
			NONT-NA	-4487.01	-4932.52												
			NONT-MG	-4476.17	-4930.27												
			NONT-CA	-4492.13	-4942.81												
			NONT-K	-4495.68	-4936.42												
			NP(HP04)	-2871.43	-3154.44												
			NP(S)	-0.43	-1120.06												
			NP205	-2012.50	-2259.37												
NP02	-992.59		NP02	-992.48	-1127.76	NP02	-992.59	-1127.76				0.02	0.00		-0.02		
NPO20HCR	-1124.17		NPO20H(S)	-1124.14	-1413.59	NPO20HCR	-1124.17	-1264.03				0.01	0.00		-0.01		
NPO20H2C	-1239.83		NPO20H2(S)	-1239.70	-1699.42	NPO20H2C	-1239.83	-1432.26				0.02	0.00		-0.02		
NP(OH)3CR	-1102.95		NPOH3(S)	-1103.07	-1384.68	NP(OH)3CR	-1102.95	-1384.69				-0.02	0.00		0.02		

Table B.2: Comparison of minerals and gases in Nagra 05/92, HATCHES 3.0, MINEQL-PSI 03/91 and PHREEQE-PSI 04/91 Data Bases Page 10 of 16

Nagra 05/92			HATCHES 3.0			MINEQL-PSI 03/91			PHREEQE-PSI 04/91			Nagra-HATCHES	Nagra-MQ0391	Nagra-PP0491	HATCHES-MQ0391	HATCHES-PP0491	MQ0391-PP0491
Name	$\Delta_f G^\circ$	$\Delta_f H^\circ$	Name	$\Delta_f G^\circ$	$\Delta_f H^\circ$	Name	$\Delta_f G^\circ$	$\Delta_f H^\circ$	Name	$\Delta_f G^\circ$	$\Delta_f H^\circ$	$\Delta \log K$	$\Delta \log K$	$\Delta \log K$	$\Delta \log K$	$\Delta \log K$	
NP(OH)4CR O2(G)	-1446.89 0.00	0.00	NPOH4(S) O2-GAS ORPIMENT OXYCH-CA OXYCH-MG	-1447.24 0.16 -167.56 -5706.64 -0.91	-1699.42 0.00 483.36 -7936.93 -3101.89	NP(OH)4CR-1446.89 O2_GAS 0.03 -0.01						-0.06	0.00	0.06	-0.02		
			PARAGONI PARGASIT PD-OXYAN	-5554.17 -11920.8 -4713.13	-6226.42 -13551.3 -5303.20		P					-394.38	-393.49				
PD.METAL PD4S	-0.05 -72.14	0.05 427.10	PD_ELEM		-0.05 0.05	PD.METAL PD4S	-0.05 -72.14	0.05 12.23	PD.METAL PD4S	-0.05 -72.14	0.05 12.23	0.00	0.00	0.00	0.00	0.00	
			PDBR2CR PDCL2CR PDI2CR PDO PDOH2CR PDS	-107.17 -126.41 -62.62 -85.76 -306.97	-105.12 -173.03 -63.72 -85.37 -395.05	PDBR2S PDCL2S PDI2S PDO PD(OH)2S	-107.17 -126.41 -62.62 -85.76 -395.05	-105.28 -173.19 -63.60 -85.37 -395.05						0.00	0.00		
PDO PD(OH)2S	-85.76 -306.91	-124.53 -416.06	PDS2	-69.83	-73.15	PDS2	-80.99	-82.76	PDSS PDS2	-70.23 -194.87	10.40 -72.13	0.00	0.00	-0.01	0.00	0.01	
PDS2 PDSS	-194.87 -76.06	37.40 86.50	PENTAHYD PETALITE PHENGITE PHILL-K PHILL-NA PHILL-CA PHLOGOPI PICOMERI PIRSSONI POLYHALI PORTLANDITE	-2392.06 -9224.88 -5466.36 -9205.7 -9118.1 -9177.5 -5845.26 -3955.01 -2659.68 -5656.00	-2805.49 -9859.46 -5942.06 -10228.1 -10192.7 -10286.2 -6562.42 -4504.94 -2975.26 -6266.30 -985.04	PORTLAND PREHNITE PSD CAOH2(C) PU203 PUCL3CR PUF3CR PUF4CR PUH2P42C	-896.89 -5821.86 -1543.38 -896.89 -1594.71 -1037.37 -1483.36 -1683.02 -2831.80	-984.96 -6533.68 -1714.13 -985.04 -1656.24 -1093.29 -1598.10 -1846.00 -3085.37	PORTLAND PU203 PUCL3CR PUF3CR PUF4CR PUH2P42C	-897.75 -1594.07 -1037.33 -1480.24 -1681.88 -2833.39	-986.25 -1681.16 -1093.24 -1551.73 -1777.80 -3099.93	0.01	0.01	-0.14	0.00	-0.15	-0.15
			PUK4(SO4) PU02 PLC03CR PLHPO4CR PU020HCR	-4690.38 -995.84 -1364.73 -1927.37 -1055.55	-5182.32 -1056.18 -1497.44 -2110.62 -1157.75	PU02 PU02CO3 PU02HP4 PU020H(S) PU020H(2)	-998.12 -1363.36 -1924.01 -1058.31 -1205.84	-1056.18 -1497.44 -2103.30 -1158.16 -1356.84	PU02 PLC03CR PLHPO4CR PU020HCR	-995.84 -1364.73 -1927.37 -1055.55 -1157.75	-1055.97 -1497.51 -2110.62 -1157.75 -121.70	-0.11 -0.01 -0.55 -0.20 0.28	0.00 0.00 0.00 0.00 0.00	0.11 0.01 0.55 0.20 -0.28			
PU(OH)3CR PU(OH)4CR PU03	-1162.73 -1424.45 -974.06	-1301.17 -1610.81 -1072.13	PUOH3(S) PUOH4(S) PYRITE	-1164.48 -1427.88 -159.40	-1296.82 -1615.29 -4.31	PU(OH)3CR-1162.73 PU(OH)4CR-1424.45 PU03-a	-1301.17 -1610.81 -974.06				-0.31 -0.60 -0.00	0.00 0.00 0.89	0.31 0.60				

Table B.2: Comparison of minerals and gases in Nagra 05/92, HATCHES 3.0, MINEQL-PSI 03/91 and PHREEQE-PSI 04/91 Data Bases Page 11 of 16

Table B.2: Comparison of minerals and gases in Nagra 05/92, HATCHES 3.0, MINEQL-PSI 03/91 and PHREEQE-PSI 04/91 Data Bases Page 12 of 16

Table B.2: Comparison of minerals and gases in Nagra 05/92, HATCHES 3.0, MINEQL-PSI 03/91 and PHREEQE-PSI 04/91 Data Bases Page 13 of 16

Nagra 05/92			HATCHES 3.0			MINEQL-PSI 03/91			PHREEQE-PSI 04/91			Nagra-HATCHES	Nagra-MQ0391	Nagra-PP0491	HATCHES-MQ0391	HATCHES-PP0491	MQ0391
Name	Δ_fG°	Δ_fH°	Name	Δ_fG°	Δ_fH°	Name	Δ_fG°	Δ_fH°	Name	Δ_fG°	Δ_fH°	HATCHES	$\Delta \log K$	$\Delta \log K$	HATCHES	$\Delta \log K$	$\Delta \log K$
			TACHYHYD	-4996.89	-5909.44												
TC(C)	-0.79	49.95	TALC	-5525.52	-6085.52	TC(C)	-0.79	-701.10	TC_ELEM	0.03	0.00		0.00	0.14		0.14	
TC207	-935.41	-1422.75	TC207	-935.41	-1402.37								0.00				
TC257	2051.93	1928.54	TC257	2051.93	1033.90								0.00				
TC304	-864.29	-319.53	TC304	-864.29	-426.82								0.00				
TC407	-1323.87		TC407	-1323.87	-857.49								0.00				
TCO2AM	-835.99		TCO2AM	-835.99	-857.49	TCO2 +2a	-817.16	-857.49					0.00	3.30		3.30	
TC03	-460.15		TC03	-460.15	-571.66								0.00				
TCOH(S)	-234.96	-67.40	TCOH(S)	-234.96	-281.98								0.00				
TCOH2(S)	-461.20	-319.53	TCOH2(S)	-461.20	-426.82								0.00				
TCOH3(S)	-658.56		TCOH3(S)	-658.56	-571.66								0.00				
TCS2	-215.15	673.51	TCS2	-215.15	417.90								0.00				
TCS3	1103.54	867.35	TCS3	1103.54	483.93								0.00				
			TEPHTOIT	-1632.25	-1898.46												
			TH2S3	-1076.01	-1621.88												
			TH2SE3	-932.25	-3312.58												
			TH7S12	-4116.45	-5154.55												
			THBR4(C)	-926.50	-1254.64												
			THCL4(C)	-1094.60	-1186.70												
			THENARDI	-1269.27	-1390.02												
			THERMONA	-1285.19	-1456.47												
THF4_AQ	-2612.86	-2854.89	THF4_2.5	-2606.58	-2824.98	THF4_AQ	-2612.86	-2854.89					1.10	0.00		-1.10	
THF4CR	-2002.89	-2098.69	THF4(S)	-2003.46	-2097.85	THF4CR	-2002.89	-2098.69					-0.10	0.00		0.10	
THH2P42C	-3998.50	-4489.49	THHP042(-3050.52	-3347.42	THH2P42C	-3998.50	-4489.49					0.00				
			THI4(S)	-654.40	-996.12												
			THN034(S	-2322.50	-3025.55												
TH02	-1143.32	-1226.86	TH02	-1143.04	-1340.66	TH02	-1143.32	-1226.86					0.05	0.00		-0.05	
			TH02(C)	-1169.01	-1226.44												
			THOCL2(S	-1156.06	-1232.09												
			THOH4(A)	-1599.91	-1912.32												
TH(OH)4CR	-1574.79	-1880.94	THOH4(C)	-1589.06	-1912.32	TH(OH)4CR-1574.79	-1880.94						-2.50	0.00		2.50	
			THORIANI	-1168.72	-1340.66												
			THS2	-619.18	-636.93												
			THSO42(S	-2308.87	-2542.91	THS032	-1796.95	-2040.00									
			TODOROKI	-3862.16	-4422.80												
			TREMOLIT	-11595.4	-12790.0												
			TREVORIT	-947.67	-1291.84												
			TRIDYMITE	-855.32	-885.30												
			TROILITE	-87.87	-23.07												
			U-ALPH	0.63	-1155.16												
			U(SO4)2(-2082.70	-2409.88												
U203F6	-3373.92	-3580.38	U203F6	-3373.92	-3580.38								0.00				
U305F8	-4889.51	-5199.46	U305F8	-4889.51	-5199.46								0.00				
U307-BE	-3241.72	-3426.00	MIN41506	-3241.98	-3427.00	B_U307	-3241.75	-3426.06					-0.01				

Table B.2: Comparison of minerals and gases in Nagra 05/92, HATCHES 3.0, MINEQL-PSI 03/91 and PHREEQE-PSI 04/91 Data Bases Page 14 of 16

Nagra 05/92			HATCHES 3.0			MINEQL-PSI 03/91			PHREEQE-PSI 04/91			Nagra-HATCHES	Nagra-MQ0391	Nagra-PP0491	HATCHES	HATCHES	MQ0391
Name	Δ_fG°	Δ_fH°	Name	Δ_fG°	Δ_fH°	Name	Δ_fG°	Δ_fH°	Name	Δ_fG°	Δ_fH°	$\Delta logK$					
U308	-3369.47	-3574.80	U308	-3366.66	-3574.39	MIN32521	-3369.37	-3574.78				0.49	0.02		-0.47		
A_U308	-3369.42	-3574.85	U3SE4	-988.09	-4327.69	A_U308	-3369.42	-3574.85				0.00					
U409	-4276.33	-4509.60	U409	-4273.11	-4509.83	MIN41511	-4277.86	-4513.21							-0.83		
U5012CL	-5517.97	-5854.42				B_U409	-4277.91	-4513.27	U5012CL	-5517.97	-5854.42				-0.28		
						UBR2CL	-715.68	-750.59						0.00			
						UBR3CR	-674.32	-698.69									
						UBR4CR	-767.29	-802.12									
						UBR5	-769.06	-810.44									
						UBRCL2	-761.65	-812.08									
						UCL2BR2	-850.80	-907.85									
UCL2F2	-1376.06	-1465.98				UCL2F2	-1376.06	-1465.98					0.00				
						UCL2I2	-723.42	-768.01									
						UCL3BR	-893.46	-963.06									
UCL3CR	-800.27	-866.03				UCL3CR	-800.27	-866.03					0.00				
UCL3F	-1146.65	-1242.94				UCL3F	-1146.65	-1242.94					0.00				
						UCL3I	-829.97	-898.22									
						UCL4CR	-929.62	-1018.73					0.18	0.00		-0.18	
UCL4CR	-929.62	-1018.73	UCL4(S)	-928.60	-1259.52	UCL5CR	-949.80	-1058.54						0.00			
UCL5CR	-949.80	-1058.54				UCL6	-951.37	-1091.88						0.00			
UCL6	-951.37	-1091.88				UCLBR3	-806.99	-852.27									
						UCLF3	-1606.44	-1689.98					0.00				
						UCLI3	-672.91	-643.77									
UCLF3	-1606.44	-1689.98				UF3CR	-1434.62	-1502.10						0.00			
						UF4_2.5A	-2440.35	-2671.48					6.00	0.00		-6.00	
UF3CR	-1434.62	-1502.10				UF4(C)	-1823.58	-1914.19					5.83	0.00		-5.83	
UF4_2.5A	-2440.35	-2671.48				UF4CR	-1823.58	-1914.19									
UF4CR	-1823.58	-1914.19				A_UF5	-1968.77	-2075.32									
A_UF5	-1968.77	-2075.32				B_UF5	-1970.71	-2083.23									
						UF6_CRYs	-2068.59	-2197.02					0.00				
UF6_CRYs	-2068.59	-2197.02				UH2P424H	-3844.65	-4337.88					0.00				
						UHP042(S	-3823.43	-4332.86									
						UI3CR	-468.04	-467.39									
						UI4	-513.22	-518.79									
UL3P424H	-6138.99	-6742.09				UL3P424H	-6138.99	-6742.09					0.00				
UL3P426H	-6618.07					UL3P426H	-6618.07	-7340.78					0.00				
UL3P42CR	-5116.06	-5494.30	U023P042	-5186.13	-5564.63	UL3P42CR	-5116.06	-5494.30					-12.28	0.00		12.28	
ULN032_H	-1362.93	-1663.89				ULN032_H	-1362.93	-1663.89						0.00			
ULN0322H	-1620.44	-1978.59	U02N032.	-1618.61	-2003.87	ULN0322H	-1620.44	-1978.59					0.32	0.00		-0.32	
ULN0323H	-1864.60	-2280.32	U02N03.H	-1863.34	-2289.70	ULN0323H	-1864.60	-2280.32					0.22	0.00		-0.22	
ULN0326H	-2584.13	-3167.39	U02N03.6	-2583.26	-3147.19	ULN0326H	-2584.13	-3167.39					0.15	0.00		-0.15	
ULN032CR	-1106.04	-1350.90	U02N032(-1119.15	-1432.21	ULN032CR	-1106.04	-1350.90					-2.30	0.00		2.30	
ULS04_25	-2298.48	-2607.56	U02S0425	-2297.38	-2642.43	ULS03CR	-1530.38	-1654.50									
ULS04_3	-2416.53	-2755.33	U02S0430	-2449.97	-2785.34	U02S04_2	-2298.48	-2607.56					0.19	0.00		-0.19	
ULS04_35	-2535.56	-2901.63	U02S0435	-2534.58	-2928.26	ULS04_3	-2416.53	-2755.33					-5.86	0.00		5.86	
ULS04CR	-1685.76	-1845.16	U02S04(C	-1724.17	-1927.85	ULS04_35	-2535.56	-2901.63					0.17	0.00		-0.17	
			U02S04.	-1966.79	-2213.68	ULS04CR	-1685.76	-1845.16					-6.73	0.00		6.73	

Table B.2: Comparison of minerals and gases in Nagra 05/92, HATCHES 3.0, MINEQL-PSI 03/91 and PHREEQE-PSI 04/91 Data Bases Page 15 of 16

Nagra 05/92			HATCHES 3.0			MINEQL-PSI 03/91			PHREEQE-PSI 04/91			Nagra-HATCHES	Nagra-MQ0391	Nagra-PP0491	HATCHES-PP0491	HATCHES-PP0491	MQ0391-PP0491			
Name	Δ_fG°	Δ_fH°	Name	Δ_fG°	Δ_fH°	Name	Δ_fG°	Δ_fH°	Name	Δ_fG°	Δ_fH°	$\Delta \log K$	$\Delta \log K$	$\Delta \log K$	$\Delta \log K$					
ULUO2CL3	-2234.80	-2404.45				U02U02CL	-2234.80	-2404.45					0.00							
U02_AMOR	-1003.57	-1162.86	U02(AM)	-981.31	-1162.86	U02_AMOR	-1003.57	-1162.86				3.90	0.00		-3.90					
U02_CRYs	-1032.34	-1085.00	U02(AM)	-981.31	-1162.86	URANINIT	-1030.57	-1162.86	U02_CRYs	-1032.34	-1085.00	URANINIT	-1030.40	-1084.62	0.31	0.00	0.34	-0.31	0.03	0.34
			U022HP04	-4226.52	-4592.85				U02BR2	-1066.24	-1137.39									
						U02BR2_1	-1328.44	-1455.90												
						U02BR2_3	-1818.36	-2058.01												
						U02BROH	-1744.08	-1957.99												
ULCL2_1	-1404.98	-1559.75				U02CL2_1	-1404.98	-1559.75					0.00							
ULCL2_3	-1894.62	-2163.96				U02CL2_3	-1894.62	-2163.96					0.00							
ULCL2CR	-1145.81	-1243.54	U02CL2(S)	-1144.43	-1352.67	U02CL2CR	-1145.81	-1243.54				0.24	0.00		-0.24					
U02CLCR	-1095.32	-1169.99				U02CLCR	-1095.32	-1169.99					0.00							
ULCLOH	-1782.18	-2010.39				U02CLOH	-1782.18	-2010.39					0.00							
ULC03CR	-1562.89	-1689.63	ULC03(S)	-1561.74	-1672.45	U02C03CR	-1562.89	-1689.63				0.20	0.00		-0.20					
ULF2_3A	-2269.71	-2534.39				U02F2_3A	-2269.71	-2534.39					0.00							
ULF2CR	-1557.32	-1653.51	U02F2(C)	-1571.92	-1689.21	U02F2CR	-1557.32	-1653.51				-2.56	0.00		2.56					
ULFOH_1	-1721.65	-1894.50				U02FOH_1	-1721.65	-1894.50					0.00							
ULFOH_2	-1960.96	-2190.29				U02FOH_2	-1960.96	-2190.29					0.00							
ULHP04_	-3064.79	-3471.49				U02HP04	-3064.79	-3471.49					0.00							
			U02HP04(-2111.26	-2447.26															
			U020H(S)	-1176.21	-1318.15															
			U020H2(S)	-1393.37	-1533.27	B_U020H2	-1398.63	-1533.80								-0.92				
U03_2H20	-1636.46	-1826.12	U032H20	-1631.08	-1826.46	U03_2H20	-1636.46	-1826.12				0.94	0.00		-0.94					
U03_ALF	-1140.38	-1217.51	U03	-1144.82	-1223.80	U03_ALF	-1140.38	-1217.51				-0.78	0.00		0.78					
U03_ALF_	-1374.58	-1506.30				U03_ALF_	-1374.58	-1506.30					0.00							
U03_BETA	-1142.26	-1220.31				U03_BETA	-1142.26	-1220.31					0.00							
U03_GAMM	-1145.63	-1223.79				U03_GAMM	-1145.63	-1223.79					0.00							
						U0BR2	-929.49	-973.62												
						U0BR3	-901.35	-954.03												
UOCL2CR	-996.11	-1066.84				UOCL2CR	-996.11	-1066.84					0.00							
UOCL3	-1068.85	-1162.97				UOCL3	-1068.85	-1162.97					0.00							
UOCLR	-787.13	-832.89				UOCLR	-787.13	-832.89					0.00							
UOF2_1AQ	-1674.49	-1802.01	UOF2.H20	-1667.47	-1833.56	UOF2_1AQ	-1674.49	-1802.01				1.23	0.00		-1.23					
UOF2CR	-1434.10	-1504.59				UOF2CR	-1434.10	-1504.59					0.00							
UOF4	-1816.32	-1924.62				UOF4	-1816.32	-1924.62					0.00							
UOF0H	-1342.63	-1426.71				UOF0H	-1342.63	-1426.71					0.00							
UOF0H_0.	-1458.11	-1576.11				UOF0H_0.	-1458.11	-1576.11					0.00							
UOH2SO4	-1766.23	-2072.20				UOH2SO4	-1766.23	-2072.20					0.00							
			URANOCIR	-4763.15	-5167.86															
			URANOPHA	-4972.39	-5493.94															
			USE2	-426.66	-1586.27															
USIO4	-1882.29	-1973.16	USIO4(S)	-1881.55	-1990.30	USIO4	-1882.29	-1973.16				0.13	0.00		-0.13					
			COFFINIT	-1884.86	-2048.16															
						US032	-1712.80	-1862.20												
US042_4A	-3033.26	-3483.29				US042_4A	-3033.26	-3483.29					0.00							
US042_8A	-3987.87	-4662.67				US042_8A	-3987.87	-4662.67					0.00							
US042CR	-2084.47	-2309.67				US042CR	-2084.47	-2309.67					0.00							

Table B.2: Comparison of minerals and gases in Nagra 05/92, HATCHES 3.0, MINEQL-PSI 03/91 and PHREEQE-PSI 04/91 Data Bases Page 16 of 16

Nagra 05/92			HATCHES 3.0			MINEQL-PSI 03/91			PHREEQE-PSI 04/91			Nagra-HATCHES	Nagra-MQ0391	Nagra-PP0491	HATCHES	HATCHES	MQ0391
Name	Δ_fG°	Δ_fH°	Name	Δ_fG°	Δ_fH°	Name	Δ_fG°	Δ_fH°	Name	Δ_fG°	Δ_fH°	$\Delta logK$					
UU3F17	-7464.23	-7849.73				UU3F17	-7464.23	-7849.73				0.00					
UUF9	-3812.16	-4015.91				UUF9	-3812.16	-4015.91				0.00					
UU02CL5	-2037.33	-2197.34	VIVIANIT	-4390.64	-5152.28	VIVIANIT	-4390.29	-5122.74				0.00				0.06	
			WAIRAKIT	-6186.53	-6875.98												
			WEEKSITE	-9040.34	-9853.91												
			WHITLOCK	-3906.91	-4227.34												
WITHERITE	-1132.15	-1210.75	WITHERIT	-1159.48	-1207.81	WITHERIT	-1132.14	-1210.74	WITHERIT	-1132.14	-1210.74	-4.79	0.00	0.00	4.79	4.79	0.00
			WOLLAST	-1545.66	-1714.13												
			WUSTITE	-233.31	-365.77												
			YUGAWARA	-7545.01	-8332.94												
			ZOISITE	-6489.54	-7357.91												
ZRCL4(S)	-835.16		ZRCL4(S)	-835.16	-668.32							0.00					
ZRO2	-1009.63		ZRO2	-1009.63	-571.66							0.00					

Table B.3: Selected aqueous species and minerals in HATCHES 3.0 data base. Page 1 of 50

	Charge	OPV	DH a	DH b	$\Delta_f G^\circ$	$\Delta_f H^\circ$	$\Delta_f S^\circ$	$\Delta_f H^\circ$	logK(25)
MASTER SPECIES									
AL+3	3.0	0.00	6.65	0.19	-491.500	-538.400	-157.303		
AM+3	3.0	0.00	9.00	0.00	-599.100	-616.700	-59.031		
ASOH4-	-1.0	3.00	4.00	0.00	-824.240	-1000.690	-591.816		
BA+2	2.0	0.00	4.55	0.09	-555.360	-532.500	76.673		
BR-	-1.0	0.00	3.00	0.00	-103.850	-121.410	-58.897		
CA+2	2.0	0.00	4.86	0.15	-552.807	-543.000	32.893		
CIT3-	-3.0	0.00	0.00	0.00	0.000	0.000	0.000		
CL-	-1.0	0.00	3.71	0.01	-131.220	-167.080	-120.275		
CO3-2	-2.0	4.00	5.40	0.00	-527.919	-675.314	-494.365		
E-	-1.0	-1.00	0.00	0.00	0.000	0.000	0.000		
EDTA4-	-4.0	0.00	0.00	0.00	0.000	0.000	0.000		
F-	-1.0	0.00	3.46	0.08	-281.520	-335.350	-180.547		
FE+2	2.0	2.00	5.08	0.16	-78.900	-89.100	-34.211		
H+	1.0	0.00	9.00	0.00	0.000	0.000	0.000		
H2O	0.0	0.00	0.00	0.00	-237.140	-285.830	-163.307		
H3BO3	0.0	0.00	0.00	0.00	-969.300	-1072.800	-347.141		
H4SiO4	0.0	0.00	0.00	0.00	-1307.735	-1456.960	-500.503		
I-	-1.0	0.00	3.00	0.00	-51.720	-56.780	-16.971		
K+	1.0	0.00	3.71	0.01	-282.510	-252.140	101.861		
Li+	1.0	0.00	4.76	0.20	-292.920	-278.470	48.466		
MG+2	2.0	0.00	5.46	0.22	-455.400	-467.000	-38.907		
MN+2	2.0	2.00	7.04	0.22	-228.100	-220.750	24.652		
MOO4-2	-2.0	0.00	5.00	0.00	-836.300	-997.900	-542.009		
NA+	1.0	0.00	4.32	0.06	-261.950	-240.340	72.480		
NI+2	2.0	0.00	5.51	0.22	-45.600	-54.000	-28.174		
NO3-	-1.0	5.00	3.00	0.00	-110.790	-206.850	-322.187		
NP+4	4.0	4.00	11.00	0.00	-502.900	-556.100	-178.434		
NTA-3	-3.0	0.00	0.00	0.00	0.000	0.000	0.000		
OX2-	-2.0	0.00	0.00	0.00	0.000	0.000	0.000		
PD+2	2.0	0.00	5.50	0.00	176.500	149.000	-92.235		
PO4-3	-3.0	0.00	4.00	0.00	-1025.497	-1284.400	-868.365		
PU+4	4.0	4.00	11.00	0.00	-481.600	-536.400	-183.800		
SEO4-2	-2.0	6.00	4.00	0.00	-441.300	-599.100	-529.264		
SN+2	2.0	2.00	6.00	0.00	-27.600	-8.900	62.720		
SO4-2	-2.0	6.00	5.31	-0.07	-744.000	-909.340	-554.553		
SR+2	2.0	0.00	5.48	0.11	-563.830	-550.900	43.367		
TCO+2	2.0	2.00	5.00	0.00	-100.600	0.000	337.414		
TH+4	4.0	0.00	11.00	0.00	-705.000	-769.000	-214.657		
U+4	4.0	4.00	11.00	0.00	-529.860	-591.200	-205.735		
ZR+4	4.0	0.00	11.00	0.00	-524.500	0.000	1759.182		

Table B.3: Selected aqueous species and minerals in HATCHES 3.0 data base. Page 2 of 50

	Charge	OPV	DH a	DH b	$\Delta_f G^\circ$	$\Delta_f H^\circ$	$\Delta_f S^\circ$	$\Delta_f H^\circ$	logK(25)	
PRODUCT SPECIES										
ALF+2		2.0	0.00	0.00	0.00	-813.032	-873.750	-203.648	0.000	7.010
1.00	AL+3		1.00	F-						
ALF2+		1.0	0.00	0.00	0.00	-1127.316	-1125.420	6.359	83.680	12.750
1.00	AL+3		2.00	F-						
ALF3		0.0	0.00	0.00	0.00	-1433.209	-1533.990	-338.023	10.460	17.020
1.00	AL+3		3.00	F-						
ALF4-		-1.0	0.00	0.00	0.00	-1730.140	-1879.800	-501.962	0.000	19.720
1.00	AL+3		4.00	F-						
ALOH+2		2.0	0.00	0.00	0.00	-700.158	-774.440	-249.146	49.790	-4.990
1.00	AL+3		1.00	H2O		-1.00	H+			
ALOH2+		1.0	0.00	0.00	0.00	-908.130	-1110.060	-677.276	0.000	-10.100
1.00	AL+3		2.00	H2O		-2.00	H+			
ALOH3		0.0	0.00	0.00	0.00	-1111.594	-1395.890	-953.535	0.000	-16.000
1.00	AL+3		3.00	H2O		-3.00	H+			
ALOH4-		-1.0	0.00	0.00	0.00	-1308.778	-1497.373	-632.550	184.347	-23.000
1.00	AL+3		4.00	H2O		-4.00	H+			
ALSO4+		1.0	6.00	0.00	0.00	-1252.738	-1438.744	-623.869	8.996	3.020
1.00	AL+3		1.00	SO4-2						
ALSO42-		-1.0	12.00	0.00	0.00	-2007.583	-2345.197	-1132.365	11.883	4.920
1.00	AL+3		2.00	SO4-2						
AM+4		4.0	4.00	0.00	0.00	-346.811	-405.826	-197.940	210.874	-44.200
1.00	AM+3		-1.00	E-						
AMCIT		0.0	3.00	0.00	0.00	-654.067	-616.700	125.330	0.000	9.630
1.00	CIT3-		1.00	AM+3						
AMCIT2-3		-3.0	3.00	0.00	0.00	-672.161	-616.700	186.018	0.000	12.800
2.00	CIT3-		1.00	AM+3						
AMCL+2		2.0	3.00	0.00	0.00	-737.169	-799.261	-208.255	-15.481	1.200
1.00	AM+3		1.00	CL-						
AMCL2+		1.0	3.00	0.00	0.00	-870.673	-982.658	-375.602	-31.798	1.600
1.00	AM+3		2.00	CL-						
AMCO3+		1.0	7.00	0.00	0.00	-1164.120	-1275.278	-372.824	16.736	6.500
1.00	AM+3		1.00	CO3-2						
AMCO32-		-1.0	11.00	0.00	0.00	-1734.849	-1953.521	-733.430	13.807	14.000
1.00	AM+3		2.00	CO3-2						
AMCO33-3		-3.0	15.00	0.00	0.00	-2259.229	-2642.642	-1285.974	0.000	13.380
1.00	AM+3		3.00	CO3-2						
AMEDTA-		-1.0	3.00	0.00	0.00	-700.301	-616.700	280.400	0.000	17.730
1.00	EDTA4-		1.00	AM+3						
AMEDTA2-		-5.0	3.00	0.00	0.00	-734.377	-616.700	394.692	0.000	23.700
1.00	AM+3		2.00	EDTA4-						
AMF+2		2.0	3.00	0.00	0.00	-898.257	-922.762	-82.189	29.288	3.090
1.00	AM+3		1.00	F-						
AMH2P4+2		2.0	3.00	0.00	0.00	-1741.324	-1901.100	-535.892	0.000	20.450
1.00	AM+3		1.00	PO4-3		2.00	H+			

Table B.3: Selected aqueous species and minerals in HATCHES 3.0 data base. Page 3 of 50

		Charge	OFV	DH a	DH b	$\Delta_f G^\circ$	$\Delta_f H^\circ$	$\Delta_f S^\circ$	$\Delta_f H^\circ$	logK(25)
AMHCIT+	1.00	CIT3-	1.0	3.00	0.00	0.00 -668.337	-616.700	173.191	0.000	12.130
					1.00 H+	1.00 AM+3				
AMHCIT2-	2.00	CIT3-	-2.0	3.00	0.00	0.00 -705.838	-616.700	298.970	0.000	18.700
					1.00 H+	1.00 AM+3				
AMHCO3+2	1.00	AM+3	2.0	7.00	0.00	0.00 -1217.775	-1335.109	-393.542	-43.095	15.900
					1.00 H+	1.00 CO3-2				
AMHCO32+	1.00	AM+3	1.0	11.00	0.00	0.00 -1826.746	-2056.447	-770.422	-89.119	30.100
					2.00 CO3-2	2.00 H+				
AMHEDTA	1.00	EDTA4-	0.0	3.00	0.00	0.00 -723.247	-616.700	357.360	0.000	21.750
					1.00 H+	1.00 AM+3				
AMHPO4+	1.00	AM+3	1.0	3.00	0.00	0.00 -1712.042	-1901.100	-634.103	0.000	15.320
					1.00 PO4-3	1.00 H+				
AMO2+	1.00	AM+3	1.0	5.00	0.00	0.00 -741.180	-805.106	-214.408	383.254	-58.200
					2.00 H2O	-4.00 H+	-2.00 E-			
AMO2+2	1.00	AM+3	2.0	6.00	0.00	0.00 -587.066	-651.971	-217.692	536.389	-85.200
					2.00 H2O	-4.00 H+	-3.00 E-			
AMOH+2	1.00	AM+3	2.0	3.00	0.00	0.00 -790.577	-844.791	-181.835	57.739	-8.000
					1.00 H2O	-1.00 H+				
AMOH2+	1.00	AM+3	1.0	3.00	0.00	0.00 -976.916	-1110.119	-446.764	78.241	-16.900
					2.00 H2O	-2.00 H+				
AMOH2CO3	1.00	AM+3	-1.0	7.00	0.00	0.00 -1036.216	-1863.674	-2775.307	0.000	-99.000
					1.00 CO3-2	2.00 H2O	-2.00 H+			
AMOH3	1.00	AM+3	0.0	3.00	0.00	0.00 -1144.991	-1365.824	-740.680	108.366	-29.000
					3.00 H2O	-3.00 H+				
AMOHCO3	1.00	AM+3	0.0	7.00	0.00	0.00 -799.076	-1577.844	-2612.000	0.000	-99.000
					1.00 CO3-2	1.00 H2O	-1.00 H+			
AMOHCO32	1.00	AM+3	-2.0	11.00	0.00	0.00 -1326.995	-2253.158	-3106.365	0.000	-99.000
					2.00 CO3-2	1.00 H2O	-1.00 H+			
AMOX	1.00	AM+3	1.0	3.00	0.00	0.00 -632.377	-616.700	52.581	0.000	5.830
					1.00 OX2-					
AMOX2-	1.00	AM+3	-1.0	3.00	0.00	0.00 -655.894	-616.700	131.456	0.000	9.950
					2.00 OX2-					
AMOX3-3	1.00	AM+3	-3.0	3.00	0.00	0.00 -669.593	-616.700	177.403	0.000	12.350
					3.00 OX2-					
AMSO4+	1.00	AM+3	1.0	9.00	0.00	0.00 -1366.502	-1505.120	-464.926	20.920	4.100
					1.00 SO4-2					
AMSO42-	1.00	AM+3	-1.0	15.00	0.00	0.00 -2118.493	-2391.030	-914.091	44.350	5.500
					2.00 SO4-2					
ASO4-3	1.00	ASOH4-	-3.0	5.00	0.00	0.00 -647.694	-888.433	-807.442	112.257	-30.930
					-4.00 H+	-2.00 E-				
ASOH3	1.00	ASOH4-	0.0	3.00	0.00	0.00 -640.126	-742.391	-342.996	-27.531	9.290
					1.00 H+	-1.00 H2O				
BAOH+	1.00	BA+2	1.0	0.00	0.00	0.00 -716.242	-755.173	-130.572	63.157	-13.360
					1.00 H2O	-1.00 H+				
BF2OH2	1.00	H3BO3	-1.0	0.00	0.00	0.00 -1338.751	-1450.829	-375.911	6.841	7.630
					2.00 F-	1.00 H+	-1.00 H2O			

Table B.3: Selected aqueous species and minerals in HATCHES 3.0 data base. Page 4 of 50

		Charge	OPV	DH a	DH b	$\Delta_f G^\circ$	$\Delta_f H^\circ$	$\Delta_f S^\circ$	$\Delta_f H^\circ$	logK(25)
BF3OH-	1.00	-1.0	0.00	0.00	0.00	-1417.607	-1513.801	-322.635	-6.611	13.670
	H3BO3		2.00	H+	3.00	F-	-2.00	H2O		
BF4-	1.00	-1.0	0.00	0.00	0.00	-1499.659	-1564.220	-216.539	-7.510	20.270
	H3BO3		3.00	H+	4.00	F-	-3.00	H2O		
BFOH3-	1.00	-1.0	0.00	0.00	0.00	-1248.537	-1400.410	-509.384	7.740	-0.400
	H3BO3		1.00	F-						
CACIT-	1.00	-1.0	0.00	0.00	0.00	-579.520	-543.000	122.489	0.000	4.680
	CA+2		1.00	CIT3-						
CACO3	1.00	0.0	4.00	0.00	0.00	-1098.706	-1201.482	-344.712	16.832	3.150
	CA+2		1.00	CO3-2						
CAEDTA-2	1.00	-2.0	0.00	0.00	0.00	-615.594	-543.000	243.481	0.000	11.000
	CA+2		1.00	EDTA4-						
CAF+	1.00	1.0	0.00	0.00	0.00	-839.692	-862.459	-76.360	15.891	0.940
	CA+2		1.00	F-						
CAH2CIT+	1.00	1.0	0.00	0.00	0.00	-622.786	-543.000	267.603	0.000	12.260
	CA+2		1.00	CIT3-	2.00	H+				
CAH2PO4+	1.00	1.0	0.00	0.00	0.00	-1697.942	-1832.086	-449.922	-4.686	20.960
	CA+2		2.00	H+	1.00	PO4-3				
CAHCIT	1.00	0.0	0.00	0.00	0.00	-606.975	-543.000	214.573	0.000	9.490
	CA+2		1.00	CIT3-	1.00	H+				
CAHCO3+	1.00	1.0	4.00	0.00	0.00	-1145.511	-1210.758	-218.839	7.556	11.350
	CA+2		1.00	CO3-2	1.00	H+				
CAHOX+	1.00	1.0	0.00	0.00	0.00	-587.682	-543.000	149.865	0.000	6.110
	CA+2		1.00	OX2-	1.00	H+				
CAHPO4	1.00	0.0	0.00	0.00	0.00	-1664.436	-1828.362	-549.811	-0.962	15.090
	CA+2		1.00	H+	1.00	PO4-3				
CAI2	1.00	0.0	-2.00	0.00	0.00	-656.247	-656.560	-1.050	0.000	0.000
	CA+2		2.00	I-						
CAOH+	1.00	1.0	0.00	0.00	0.00	-718.027	-768.016	-167.661	60.814	-12.600
	CA+2		1.00	H2O	-1.00	H+				
CAOX	1.00	0.0	0.00	0.00	0.00	-569.931	-543.000	90.326	0.000	3.000
	CA+2		1.00	OX2-						
CAPO4-	1.00	-1.0	0.00	0.00	0.00	-1615.177	-1814.430	-668.296	12.970	6.460
	CA+2		1.00	PO4-3						
CASO4	1.00	0.0	6.00	0.00	0.00	-1309.992	-1446.190	-456.808	6.150	2.310
	CA+2		1.00	SO4-2						
CH4(AQ)	1.00	0.0	-4.00	0.00	0.00	-34.541	1627.748	5575.345	1445.572	38.200
	CO3-2		10.00	H+	8.00	E-	-3.00	H2O		
FE(HS)2	1.00	0.0	-2.00	0.00	0.00	-105.008	-124.392	-65.013	-503.252	76.250
	FE+2		2.00	SO4-2	18.00	H+	16.00	E-	-8.00	H2O
FE(HS)3-	1.00	-1.0	-4.00	0.00	0.00	-104.163	-142.037	-127.031	-754.877	111.940
	FE+2		3.00	SO4-2	27.00	H+	24.00	E-	-12.00	H2O
FE(SO4)2	1.00	-1.0	15.00	0.00	0.00	-1523.463	-1846.694	-1084.121	61.086	-7.610
	FE+2		2.00	SO4-2	-1.00	E-				
FE+3	1.00	3.0	3.00	0.00	0.00	-4.526	-47.260	-143.331	41.840	-13.030
	FE+2		-1.00	E-						

Table B.3: Selected aqueous species and minerals in HATCHES 3.0 data base. Page 5 of 50

	Charge	OPV	DH a	DH b	$\Delta_f G^\circ$	$\Delta_f H^\circ$	$\Delta_f S^\circ$	$\Delta_f H^\circ$	logK(25)
FE2CIT2O 2.00	-2.0 CIT3-	6.00 2.00	0.00 FE+2	0.00 -2.00	-609.305 H+	-749.860 -2.00	-471.422 E-	0.000 2.00	-3.990 H2O
FE2OH2+4 2.00	4.0 FE+2	6.00 2.00	0.00 H2O	0.00 -2.00	-466.494 H+	-609.696 -2.00	-480.303 E-	140.164	-29.010
FE3OH4+5 3.00	5.0 FE+2	9.00 4.00	0.00 H2O	0.00 -4.00	-926.121 H+	-1225.269 -3.00	-1003.346 E-	185.351	-45.400
FECIT 1.00	0.0 FE+2	3.00 -1.00	0.00 E-	0.00 1.00	-76.674 CIT3-	-89.100	-41.677	0.000	-0.390
FECIT2-3 2.00	-3.0 CIT3-	3.00 1.00	0.00 FE+2	0.00 -1.00	-107.896 E-	-89.100	63.043	0.000	5.080
FECIT2OH 2.00	-5.0 CIT3-	3.00 1.00	0.00 FE+2	0.00 -2.00	-495.930 H+	-660.760 -1.00	-552.844 E-	0.000 2.00	-10.030 H2O
FECITOH- 1.00	-1.0 CIT3-	3.00 1.00	0.00 FE+2	0.00 -1.00	-303.711 H+	-374.930 -1.00	-238.870 E-	0.000 1.00	-2.160 H2O
FECITOH2 1.00	-2.0 FE+2	3.00 -1.00	0.00 E-	0.00 1.00	-495.530 CIT3-	-660.760 -2.00	-554.184 H+	0.000 2.00	-10.100 H2O
FECL+2 1.00	2.0 FE+2	3.00 1.00	0.00 CL-	0.00 -1.00	-144.194 E-	-190.910	-156.686	65.270	-11.550
FECL2+ 1.00	1.0 FE+2	3.00 2.00	0.00 CL-	0.00 -1.00	-279.124 E-	-381.420	-343.103	41.840	-10.900
FECL3 1.00	0.0 FE+2	3.00 3.00	0.00 CL-	0.00 -1.00	-404.636 E-	-548.500	-482.522	41.840	-11.900
FEEDTA- 1.00	-1.0 FE+2	3.00 1.00	0.00 EDTA4-	0.00 -1.00	-161.665 E-	-89.100	243.383	0.000	14.500
FEF+2 1.00	2.0 FE+2	3.00 1.00	0.00 F-	0.00 -1.00	-321.606 E-	-371.313	-166.718	53.137	-6.800
FEF2+ 1.00	1.0 FE+2	3.00 2.00	0.00 F-	0.00 -1.00	-629.383 E-	-698.295	-231.134	61.505	-2.200
FEF3 1.00	0.0 FE+2	3.00 3.00	0.00 F-	0.00 -1.00	-928.997 E-	-1030.716	-341.170	64.434	0.970
FEH2CIT2 2.00	-1.0 CIT3-	3.00 1.00	0.00 FE+2	0.00 2.00	-154.530 H+	-89.100 -1.00	219.452 E-	0.000	13.250
FEH2P4+ 1.00	1.0 FE+2	2.00 2.00	0.00 H+	0.00 1.00	-1231.398 PO4-3	-1392.412	-540.043	-18.912	22.250
FEH2P4+2 1.00	2.0 FE+2	3.00 2.00	0.00 H+	0.00 1.00	-1172.606 PO4-3	-1350.572 -1.00	-596.898 E-	22.928	11.950
FEHCIT+ 1.00	1.0 CIT3-	3.00 1.00	0.00 FE+2	0.00 1.00	-85.521 H+	-89.100 -1.00	-12.003 E-	0.000	1.160
FEHCIT2- 2.00	-2.0 CIT3-	3.00 1.00	0.00 FE+2	0.00 1.00	-117.600 H+	-89.100 -1.00	95.588 E-	0.000	6.780
FEHEDTA 1.00	0.0 EDTA4-	3.00 1.00	0.00 FE+2	0.00 1.00	-170.226 H+	-89.100 -1.00	272.100 E-	0.000	16.000
FEHOX+2 1.00	2.0 OX2-	3.00 1.00	0.00 FE+2	0.00 -1.00	-58.180 E-	-89.100 1.00	-103.705 H+	0.000	-3.630
FEHPO4 1.00	0.0 FE+2	2.00 1.00	0.00 H+	0.00 1.00	-1195.438 PO4-3	-1388.270	-646.760 -14.770	0.000	15.950

Table B.3: Selected aqueous species and minerals in HATCHES 3.0 data base. Page 6 of 50

		Charge	OPV	DH a	DH b	$\Delta_f G^\circ$	$\Delta_f H^\circ$	$\Delta_f S^\circ$	$\Delta_f H^\circ$	logK(25)
FEHPO4+		1.0	3.00	0.00	0.00 -1131.452	-1322.330	-640.205	51.170	4.740	
1.00	FE+2		1.00	H+	1.00 PO4-3	-1.00	E-			
FEOH+		1.0	2.00	0.00	0.00 -261.815	-319.701	-194.152	55.229	-9.500	
1.00	FE+2		1.00	H2O	-1.00 H+					
FEOH+2		2.0	3.00	0.00	0.00 -229.166	-289.576	-202.619	85.354	-15.220	
1.00	FE+2		1.00	H2O	-1.00 E-	-1.00	H+			
FEOH2		0.0	2.00	0.00	0.00 -435.768	-541.244	-353.767	119.516	-20.570	
1.00	FE+2		2.00	H2O	-2.00 H+					
FEOH2+		1.0	3.00	0.00	0.00 -446.442	-618.920	-578.494	41.840	-18.700	
1.00	FE+2		2.00	H2O	-2.00 H+	-1.00	E-			
FEOH3-		-1.0	2.00	0.00	0.00 -613.375	-819.815	-692.403	126.775	-31.000	
1.00	FE+2		3.00	H2O	-3.00 H+					
FEOH3		0.0	3.00	0.00	0.00 -638.318	-904.750	-893.616	41.840	-26.630	
1.00	FE+2		3.00	H2O	-3.00 H+	-1.00	E-			
FEOH4-2		-2.0	2.00	0.00	0.00 -764.896	-1232.420	-1568.082	0.000	-46.000	
1.00	FE+2		4.00	H2O	-4.00 H+					
FEOH4-		-1.0	3.00	0.00	0.00 -829.795	-1190.580	-1210.078	41.840	-34.630	
1.00	FE+2		4.00	H2O	-4.00 H+	-1.00	E-			
FEOX+		1.0	3.00	0.00	0.00 -56.525	-89.100	-109.257	0.000	-3.920	
1.00	OX2-		1.00	FE+2	-1.00 E-					
FEOX2-		-1.0	3.00	0.00	0.00 -94.426	-89.100	17.862	0.000	2.720	
2.00	OX2-		1.00	FE+2	-1.00 E-					
FEOX3-3		-3.0	3.00	0.00	0.00 -119.084	-89.100	100.566	0.000	7.040	
3.00	OX2-		1.00	FE+2	-1.00 E-					
FESO4		0.0	8.00	0.00	0.00 -835.743	-984.926	-500.362	13.514	2.250	
1.00	FE+2		1.00	SO4-2						
FESO4+		1.0	9.00	0.00	0.00 -770.901	-940.241	-567.968	58.199	-9.110	
1.00	FE+2		1.00	SO4-2	-1.00 E-					
H2(AQ)		0.0	-2.00	0.00	0.00 17.980	-7.360	-84.989	-7.360	-3.150	
2.00	H+		2.00	E-						
H2ASO4-1		-1.0	5.00	0.00	0.00 -753.062	-905.797	-512.274	94.893	-12.470	
1.00	ASOH4-		-2.00	H+	-2.00 E-					
H2BO3-		-1.0	0.00	0.00	0.00 -916.559	-1059.311	-478.792	13.489	-9.240	
1.00	H3BO3		-1.00	H+						
H2CIT-		-1.0	0.00	0.00	0.00 -63.700	0.000	213.652	0.000	11.160	
1.00	CIT3-		2.00	H+						
H2CO3		0.0	4.00	0.00	0.00 -623.127	-698.326	-252.219	-23.012	16.680	
1.00	CO3-2		2.00	H+						
H2EDTA-2		-2.0	0.00	0.00	0.00 -98.918	0.000	331.773	0.000	17.330	
1.00	EDTA4-		2.00	H+						
H2IO+		1.0	1.00	0.00	0.00 -106.778	-342.610	-790.985	0.000	-31.900	
1.00	I-		1.00	H2O	-2.00 E-					
H2OX		0.0	0.00	0.00	0.00 -31.508	0.000	105.677	0.000	5.520	
1.00	OX2-		2.00	H+						
H2PO4-		-1.0	0.00	0.00	0.00 -1137.087	-1303.312	-557.522	-18.912	19.550	
1.00	PO4-3		2.00	H+						

Table B.3: Selected aqueous species and minerals in HATCHES 3.0 data base. Page 7 of 50

		Charge	OPV	DH a	DH b	$\Delta_f G^\circ$	$\Delta_f H^\circ$	$\Delta_f S^\circ$	$\Delta_f H^\circ$	logK(25)
H2S		0.0	-2.00	0.00	0.00	-27.409	-39.821	-41.629	-273.801	40.640
1.00	SO4-2		10.00	H+	8.00	E-	-4.00	H2O		
H2SE		0.0	-2.00	0.00	0.00	22.659	19.128	-11.842	-525.092	84.900
1.00	SEO4-2		10.00	H+	8.00	E-	-4.00	H2O		
H2SEO3		0.0	4.00	0.00	0.00	-426.198	-507.408	-272.380	-194.138	38.900
1.00	SEO4-2		4.00	H+	2.00	E-	-1.00	H2O		
H2SiO4-2		-2.0	0.00	0.00	0.00	-1184.330	-1332.624	-497.381	124.336	-21.620
1.00	H4SiO4		-2.00	H+						
H2TCO4		0.0	6.00	0.00	0.00	-616.239	-857.490	-809.160	0.000	-34.300
1.00	TCO+2		-4.00	H+	3.00	H2O	-2.00	E-		
H3ASO4		0.0	5.00	0.00	0.00	-765.848	-1000.690	-787.664	0.000	-10.230
1.00	ASOH4-		-1.00	H+	-2.00	E-				
H3CIT		0.0	0.00	0.00	0.00	-81.566	0.000	273.574	0.000	14.290
1.00	CIT3-		3.00	H+						
H3EDTA-		-1.0	0.00	0.00	0.00	-116.613	0.000	391.120	0.000	20.430
1.00	EDTA4-		3.00	H+						
H3PO4		0.0	0.00	0.00	0.00	-1149.359	-1294.860	-488.014	-10.460	21.700
1.00	PO4-3		3.00	H+						
H3SiO4-		-1.0	0.00	0.00	0.00	-1251.055	-1419.572	-565.206	37.388	-9.930
1.00	H4SiO4		-1.00	H+						
H4EDTA		0.0	0.00	0.00	0.00	-128.942	0.000	432.472	0.000	22.590
1.00	EDTA4-		4.00	H+						
H5EDTA+		1.0	0.00	0.00	0.00	-137.561	0.000	461.380	0.000	24.100
1.00	EDTA4-		5.00	H+						
HASO4-2		-2.0	5.00	0.00	0.00	-713.335	-900.148	-626.574	100.542	-19.430
1.00	ASOH4-		-3.00	H+	-2.00	E-				
HCIT-2		-2.0	0.00	0.00	0.00	-36.531	0.000	122.524	0.000	6.400
1.00	CIT3-		1.00	H+						
HCO3-		-1.0	4.00	0.00	0.00	-586.882	-689.958	-345.720	-14.644	10.330
1.00	CO3-2		1.00	H+						
HEDTA-3		-3.0	0.00	0.00	0.00	-62.844	0.000	210.780	0.000	11.010
1.00	EDTA4-		1.00	H+						
HF(AQ)		0.0	0.00	0.00	0.00	-299.614	-321.961	-74.953	13.389	3.170
1.00	H+		1.00	F-						
HF2-		-1.0	0.00	0.00	0.00	-584.388	-653.127	-230.554	17.573	3.740
1.00	H+		2.00	F-						
HI		0.0	-1.00	0.00	0.00	-51.720	-56.780	-16.971	0.000	0.000
1.00	I-		1.00	H+						
HIO		0.0	1.00	0.00	0.00	-99.358	-139.686	-135.262	202.924	-33.200
1.00	I-		1.00	H2O	-1.00	H+	-2.00	E-		
HIO3		0.0	5.00	0.00	0.00	-132.416	-212.906	-269.964	701.364	-110.500
1.00	I-		3.00	H2O	-5.00	H+	-6.00	E-		
HNO3		0.0	5.00	0.00	0.00	-102.628	-209.193	-357.422	-2.343	-1.430
1.00	NO3-		1.00	H+						
HOX-		-1.0	0.00	0.00	0.00	-24.373	0.000	81.747	0.000	4.270

Table B.3: Selected aqueous species and minerals in HATCHES 3.0 data base. Page 8 of 50

		Charge	OPV	DH a	DH b	$\Delta_f G^\circ$	$\Delta_f H^\circ$	$\Delta_f S^\circ$	$\Delta_f H^\circ$	logK(25)
1.00	OX2-		1.00	H+						
HPO4-2		-2.0	0.00	0.00	0.00	-1095.990	-1299.170	-681.469	-14.770	12.350
1.00	PO4-3		1.00	H+						
HS-		-1.0	-2.00	0.00	0.00	12.489	66.034	179.592	-167.946	33.650
1.00	SO4-2		9.00	H+	8.00	E-	-4.00	H2O		
HSE-		-1.0	-2.00	0.00	0.00	44.349	15.781	-95.818	-528.439	81.100
1.00	SEO4-2		9.00	H+	8.00	E-	-4.00	H2O		
HSEO3-		-1.0	4.00	0.00	0.00	-411.357	-514.520	-346.012	-201.250	36.300
1.00	SEO4-2		3.00	H+	2.00	E-	-1.00	H2O		
HSEO4-		-1.0	6.00	0.00	0.00	-452.145	-581.527	-433.950	17.573	1.900
1.00	SEO4-2		1.00	H+						
HSNO2-		-1.0	2.00	0.00	0.00	-410.268	-580.560	-571.162	0.000	-16.050
1.00	SN+2		2.00	H2O	-3.00	H+				
HSO4-		-1.0	6.00	0.00	0.00	-755.359	-886.746	-440.676	22.594	1.990
1.00	SO4-2		1.00	H+						
HTCO4-		-1.0	6.00	0.00	0.00	-614.526	-857.490	-814.904	0.000	-34.600
1.00	TCO+2		-5.00	H+	3.00	H2O	-2.00	E-		
I2		0.0	0.00	0.00	0.00	15.855	19.408	11.914	132.968	-20.900
2.00	I-		-2.00	E-						
I2CL-		-1.0	0.00	0.00	0.00	-116.506	-140.811	-81.517	139.829	-20.700
2.00	I-		1.00	CL-	-2.00	E-				
I2O-2		-2.0	0.00	0.00	0.00	-82.583	-399.390	-1062.577	0.000	-45.200
2.00	I-		1.00	H2O	-2.00	H+	-2.00	E-		
I2OH-		-1.0	0.00	0.00	0.00	-230.417	-399.390	-566.737	0.000	-19.300
2.00	I-		1.00	H2O	-1.00	H+	-2.00	E-		
I3-		-1.0	-1.00	0.00	0.00	-51.847	-56.284	-14.883	114.056	-18.100
3.00	I-		-2.00	E-						
ICL		0.0	1.00	0.00	0.00	-17.411	-223.860	-692.434	0.000	-29.000
1.00	I-		1.00	CL-	-2.00	E-				
ICL2-		-1.0	1.00	0.00	0.00	-161.188	-390.940	-770.592	0.000	-26.800
1.00	I-		2.00	CL-	-2.00	E-				
IO-		-1.0	1.00	0.00	0.00	-38.854	-109.101	-235.610	233.509	-43.800
1.00	I-		1.00	H2O	-2.00	H+	-2.00	E-		
IO3-		-1.0	5.00	0.00	0.00	-127.850	-222.906	-318.819	691.364	-111.300
1.00	I-		3.00	H2O	-6.00	H+	-6.00	E-		
IO4-		-1.0	7.00	0.00	0.00	-58.475	-153.096	-317.358	1047.004	-165.000
1.00	I-		4.00	H2O	-8.00	H+	-8.00	E-		
KCIT-2		-2.0	0.00	0.00	0.00	-289.474	-252.140	125.218	0.000	1.220
1.00	CIT3-		1.00	K+						
KEDTA-3		-3.0	0.00	0.00	0.00	-281.643	-252.140	132.493	0.000	1.600
1.00	EDTA4-		1.00	K+						
KHPO4-		-1.0	0.00	0.00	0.00	-1380.155	-1551.310	-574.055	-14.770	12.640
1.00	K+		1.00	H+	1.00	PO4-3				
KSO4-		-1.0	6.00	0.00	0.00	-1031.362	-1152.066	-404.844	9.414	0.850
1.00	K+		1.00	SO4-2						

Table B.3: Selected aqueous species and minerals in HATCHES 3.0 data base. Page 9 of 50

		Charge	OPV	DH a	DH b	$\Delta_f G^\circ$	$\Delta_f H^\circ$	$\Delta_f S^\circ$	$\Delta_f H^\circ$	logK(25)
LISO4-		-1.0	6.00	0.00	0.00	-1040.573	-1190.864	-504.079	-3.054	0.640
1.00	LI+		1.00	SO4-2						
MGCIT-		-1.0	0.00	0.00	0.00	-483.083	-467.000	53.944	0.000	4.850
1.00	MG+2		1.00	CIT3-						
MGCO3		0.0	4.00	0.00	0.00	-1000.329	-1130.963	-438.149	11.351	2.980
1.00	MG+2		1.00	CO3-2						
MGEDTA-2		-2.0	0.00	0.00	0.00	-507.456	-467.000	135.690	0.000	9.120
1.00	MG+2		1.00	EDTA4-						
MGF+		1.0	0.00	0.00	0.00	-747.308	-782.794	-119.019	19.556	1.820
1.00	MG+2		1.00	F-						
MGH2CIT+		1.0	0.00	0.00	0.00	-525.036	-467.000	194.655	0.000	12.200
1.00	MG+2		1.00	CIT3-		2.00	H+			
MGH2PO4+		1.0	0.00	0.00	0.00	-1601.163	-1756.086	-519.616	-4.686	21.070
1.00	MG+2		2.00	H+		1.00	PO4-3			
MGHCIT		0.0	0.00	0.00	0.00	-507.171	-467.000	134.733	0.000	9.070
1.00	MG+2		1.00	CIT3-		1.00	H+			
MGHCO3+		1.0	4.00	0.00	0.00	-1048.389	-1152.887	-350.487	-10.573	11.400
1.00	MG+2		1.00	H+		1.00	CO3-2			
MGHPO4		0.0	0.00	0.00	0.00	-1567.771	-1752.362	-619.121	-0.962	15.220
1.00	MG+2		1.00	H+		1.00	PO4-3			
MGI2		0.0	-2.00	0.00	0.00	-559.011	-580.552	-72.247	0.008	0.030
1.00	MG+2		2.00	I-						
MGIO3+		1.0	5.00	0.00	0.00	-587.816	-1381.270	-2661.256	0.000	-110.500
1.00	I-		3.00	H2O		1.00	MG+2	-6.00	H+	-6.00 E-
MGOH+		1.0	0.00	0.00	0.00	-625.244	-688.317	-211.548	64.513	-11.790
1.00	MG+2		1.00	H2O		-1.00	H+			
MGOX		0.0	0.00	0.00	0.00	-474.978	-467.000	26.759	0.000	3.430
1.00	MG+2		1.00	OX2-						
MGOX2-2		-2.0	0.00	0.00	0.00	-484.396	-467.000	58.347	0.000	5.080
1.00	MG+2		2.00	OX2-						
MGP04-		-1.0	0.00	0.00	0.00	-1518.512	-1738.430	-737.607	12.970	6.590
1.00	MG+2		1.00	PO4-3						
MGS04		0.0	6.00	0.00	0.00	-1212.243	-1370.482	-530.738	5.858	2.250
1.00	MG+2		1.00	SO4-2						
MN(NO3)2		0.0	12.00	0.00	0.00	-453.105	-636.107	-613.792	-1.657	0.600
1.00	MN+2		2.00	NO3-						
MN+3		3.0	3.00	0.00	0.00	-82.491	-112.970	-102.227	107.780	-25.510
1.00	MN+2		-1.00	E-						
MN2OH+3		3.0	4.00	0.00	0.00	-633.065	-727.330	-316.168	0.000	-10.560
2.00	MN+2		1.00	H2O		-1.00	H+			
MN2OH3+		1.0	4.00	0.00	0.00	-1031.201	-1298.990	-898.169	0.000	-23.900
2.00	MN+2		3.00	H2O		-3.00	H+			
MNCL+		1.0	2.00	0.00	0.00	-362.802	-387.830	-83.945	0.000	0.610
1.00	MN+2		1.00	CL-						
MNCL2		0.0	2.00	0.00	0.00	-490.768	-554.889	-215.062	0.021	0.040
1.00	MN+2		2.00	CL-						

Table B.3: Selected aqueous species and minerals in HATCHES 3.0 data base. Page 10 of 50

		Charge	OPV	DH a	DH b	$\Delta_f G^\circ$	$\Delta_f H^\circ$	$\Delta_f S^\circ$	$\Delta_f H^\circ$	logK(25)
MNCL3-		-1.0	2.00	0.00	0.00	-619.991	-721.990	-342.108	0.000	-0.310
1.00	MN+2		3.00	CL-						
MNF+		1.0	2.00	0.00	0.00	-514.472	-556.100	-139.622	0.000	0.850
1.00	MN+2		1.00	F-						
MNHCO3+		1.0	6.00	0.00	0.00	-822.231	-911.143	-298.214	-15.079	11.600
1.00	MN+2		1.00	CO3-2	1.00	H+				
MNO4-		-1.0	7.00	0.00	0.00	-447.075	-625.092	-597.070	738.978	-127.820
1.00	MN+2		4.00	H2O	-8.00	H+	-5.00	E-		
MNO4-2		-2.0	6.00	0.00	0.00	-500.616	-736.386	-790.779	627.684	-118.440
1.00	MN+2		4.00	H2O	-8.00	H+	-4.00	E-		
MNOH+		1.0	2.00	0.00	0.00	-404.793	-446.330	-139.316	60.250	-10.590
1.00	MN+2		1.00	H2O	-1.00	H+				
MNOH2		0.0	2.00	0.00	0.00	-575.664	-792.410	-726.968	0.000	-22.200
1.00	MN+2		2.00	H2O	-2.00	H+				
MNOH3-		-1.0	2.00	0.00	0.00	-740.885	-1078.240	-1131.495	0.000	-34.800
1.00	MN+2		3.00	H2O	-3.00	H+				
MNOH4-2		-2.0	2.00	0.00	0.00	-900.968	-1364.070	-1553.251	0.000	-48.300
1.00	MN+2		4.00	H2O	-4.00	H+				
MNSO4		0.0	8.00	0.00	0.00	-985.000	-1121.011	-456.183	9.079	2.260
1.00	MN+2		1.00	SO4-2						
N2(AQ)		0.0	0.00	0.00	0.00	19.267	-4.672	-80.291	-1305.952	207.080
2.00	NO3-		12.00	H+	10.00	E-	-6.00	H2O		
NACIT-2		-2.0	0.00	0.00	0.00	-269.370	-240.340	97.368	0.000	1.300
1.00	CIT3-		1.00	NA+						
NACO3-		-1.0	4.00	0.00	0.00	-797.118	-878.370	-272.522	37.284	1.270
1.00	NA+		1.00	CO3-2						
NAEDTA-3		-3.0	0.00	0.00	0.00	-276.106	-240.340	119.958	0.000	2.480
1.00	EDTA4-		1.00	NA+						
NAF		0.0	0.00	0.00	0.00	-540.901	-588.242	-158.781	-12.552	-0.450
1.00	F-		1.00	NA+						
NAHCO3		0.0	4.00	0.00	0.00	-847.405	-930.733	-279.485	-15.079	10.080
1.00	NA+		1.00	H+	1.00	CO3-2				
NAHPO4-		-1.0	0.00	0.00	0.00	-1359.595	-1539.510	-603.436	-14.770	12.640
1.00	NA+		1.00	H+	1.00	PO4-3				
NASO4-		-1.0	6.00	0.00	0.00	-1009.946	-1144.994	-452.955	4.686	0.700
1.00	NA+		1.00	SO4-2						
NH3(AQ)		0.0	-3.00	0.00	0.00	-26.269	-79.803	-179.552	-730.443	109.830
1.00	NO3-		9.00	H+	8.00	E-	-3.00	H2O		
NH4+		1.0	-3.00	0.00	0.00	-79.067	-131.998	-177.530	-782.638	119.080
1.00	NO3-		10.00	H+	8.00	E-	-3.00	H2O		
NH4SO4-		-1.0	3.00	0.00	0.00	-829.403	-1043.012	-716.446	-784.312	120.190
1.00	NO3-		10.00	H+	8.00	E-	1.00	SO4-2	-3.00	H2O
NI2OH+3		3.0	0.00	0.00	0.00	-267.265	-393.830	-424.500	0.000	-10.700
2.00	NI+2		1.00	H2O	-1.00	H+				
NI4OH+4		4.0	0.00	0.00	0.00	-972.851	-1359.320	-1296.223	0.000	-27.700
4.00	NI+2		4.00	H2O	-4.00	H+				

Table B.3: Selected aqueous species and minerals in HATCHES 3.0 data base. Page 11 of 50

		Charge	OPV	DH a	DH b	$\Delta_f G^\circ$	$\Delta_f H^\circ$	$\Delta_f S^\circ$	$\Delta_f H^\circ$	logK(25)
NICIT-		-1.0	0.00	0.00	0.00	-83.843	-54.000	100.094	0.000	6.700
1.00	NI+2		1.00	CIT3-						
NICL2		0.0	0.00	0.00	0.00	-307.869	-388.139	-269.228	0.021	-0.030
1.00	NI+2		2.00	CL-						
NIEDTA-2		-2.0	0.00	0.00	0.00	-160.386	-54.000	356.820	0.000	20.110
1.00	NI+2		1.00	EDTA4-						
NIH2CIT+		1.0	0.00	0.00	0.00	-121.686	-54.000	227.021	0.000	13.330
1.00	NI+2		1.00	CIT3-	2.00	H+				
NIHCIT		0.0	0.00	0.00	0.00	-105.533	-54.000	172.843	0.000	10.500
1.00	NI+2		1.00	CIT3-	1.00	H+				
NIOH+		1.0	0.00	0.00	0.00	-226.460	-287.907	-206.093	51.923	-9.860
1.00	NI+2		1.00	H2O	-1.00	H+				
NIOH2		0.0	0.00	0.00	0.00	-411.430	-513.780	-343.284	111.880	-19.000
1.00	NI+2		2.00	H2O	-2.00	H+				
NIOH3-		-1.0	0.00	0.00	0.00	-585.783	-911.490	-1092.427	0.000	-30.000
1.00	NI+2		3.00	H2O	-3.00	H+				
NIOH4-2		-2.0	0.00	0.00	0.00	-743.012	-1197.320	-1523.756	0.000	-44.000
1.00	NI+2		4.00	H2O	-4.00	H+				
NISO4		0.0	6.00	0.00	0.00	-803.299	-949.365	-489.909	13.975	2.400
1.00	NI+2		1.00	SO4-2						
NO2-		-1.0	3.00	0.00	0.00	-36.725	-104.112	-226.017	-183.092	28.570
1.00	NO3-		2.00	H+	2.00	E-	-1.00	H2O		
NP(SO4)2		0.0	16.00	0.00	0.00	-2021.837	-2374.780	-1183.777	0.000	5.420
1.00	NP+4		2.00	SO4-2						
NP+3		3.0	3.00	0.00	0.00	-517.170	-527.189	-33.603	28.911	2.500
1.00	NP+4		1.00	E-						
NP2OH2+4		4.0	6.00	0.00	0.00	-1434.417	-1683.860	-836.637	0.000	-8.000
2.00	NP+4		-2.00	H+	2.00	E-	2.00	H2O		
NP2OH2+6		6.0	8.00	0.00	0.00	-1468.664	-1683.860	-721.770	0.000	-2.000
2.00	NP+4		-2.00	H+	2.00	H2O				
NPCL+2		2.0	3.00	0.00	0.00	-634.691	-723.180	-296.794	0.000	0.100
1.00	NP+4		1.00	E-	1.00	CL-				
NPCL+3		3.0	4.00	0.00	0.00	-633.492	-723.180	-300.815	0.000	-0.110
1.00	NP+4		1.00	CL-						
NPCL2+		1.0	3.00	0.00	0.00	-751.070	-890.260	-466.845	0.000	-2.500
1.00	NP+4		1.00	E-	2.00	CL-				
NPCL2+2		2.0	4.00	0.00	0.00	-763.913	-890.260	-423.770	0.000	-0.250
1.00	NP+4		2.00	CL-						
NPCL3+		1.0	4.00	0.00	0.00	-892.964	-1057.340	-551.320	0.000	-0.630
1.00	NP+4		3.00	CL-						
NPCO3+		1.0	7.00	0.00	0.00	-1082.190	-1231.414	-500.499	0.000	9.000
1.00	NP+4		1.00	E-	1.00	CO3-2				
NPCO32-		-1.0	11.00	0.00	0.00	-1635.795	-1906.728	-908.715	0.000	13.500
1.00	NP+4		1.00	E-	2.00	CO3-2				
NPCO33-3		-3.0	15.00	0.00	0.00	-2183.691	-2582.042	-1336.074	0.000	17.000
1.00	NP+4		1.00	E-	3.00	CO3-2				

Table B.3: Selected aqueous species and minerals in HATCHES 3.0 data base. Page 12 of 50

		Charge	OPV	DH a	DH b	$\Delta_f G^\circ$	$\Delta_f H^\circ$	$\Delta_f S^\circ$	$\Delta_f H^\circ$	logK(25)
NPEDTA		0.0	4.00	0.00	0.00	-676.991	-556.100	405.471	0.000	30.500
1.00	EDTA4-		1.00	NP+4						
NPF+3		3.0	4.00	0.00	0.00	-819.752	-874.714	-184.344	16.736	6.190
1.00	NP+4		1.00	F-						
NPF2+2		2.0	4.00	0.00	0.00	-1127.928	-1226.800	-331.619	0.000	10.860
1.00	NP+4		2.00	F-						
NPF3+		1.0	4.00	0.00	0.00	-1435.933	-1562.150	-423.335	0.000	15.500
1.00	NP+4		3.00	F-						
NPF4		0.0	4.00	0.00	0.00	-1741.997	-1897.500	-521.561	0.000	19.800
1.00	NP+4		4.00	F-						
NPO2+		1.0	5.00	0.00	0.00	-914.964	-1127.760	-713.722	0.000	-10.900
1.00	NP+4		2.00	H2O		-4.00	H+	-1.00	E-	
NPO2+2		2.0	6.00	0.00	0.00	-795.669	-1127.760	-1113.840	0.000	-31.800
1.00	NP+4		-4.00	H+		-2.00	E-	2.00	H2O	
NPO22OH+		3.0	12.00	0.00	0.00	-1803.362	-2541.350	-2475.223	0.000	-68.000
2.00	NP+4		-9.00	H+		-4.00	E-	5.00	H2O	
NPO22OH2		2.0	12.00	0.00	0.00	-2029.087	-2827.180	-2676.818	0.000	-70.000
2.00	NP+4		-10.00	H+		-4.00	E-	6.00	H2O	
NPO23OH5		1.0	18.00	0.00	0.00	-3472.817	-4812.430	-4493.083	0.000	-112.900
3.00	NP+4		-17.00	H+		-6.00	E-	11.00	H2O	
NPO2C-		-1.0	9.00	0.00	0.00	-1470.852	-1803.074	-1114.280	0.000	-6.000
1.00	NP+4		-4.00	H+		-1.00	E-	2.00	H2O	1.00 CO3-2
NPO2C2-3		-3.0	13.00	0.00	0.00	-2011.328	-2478.388	-1566.527	0.000	-3.800
1.00	NP+4		-4.00	H+		-1.00	E-	2.00	H2O	2.00 CO3-2
NPO2C2-2		-2.0	14.00	0.00	0.00	-1948.541	-2478.388	-1777.116	0.000	-14.800
1.00	NP+4		-4.00	H+		-2.00	E-	2.00	H2O	2.00 CO3-2
NPO2C3-4		-4.0	18.00	0.00	0.00	-2499.292	-3153.702	-2194.903	0.000	-10.800
1.00	NP+4		-4.00	H+		-2.00	E-	2.00	H2O	3.00 CO3-2
NPO2C3-5		-5.0	17.00	0.00	0.00	-2540.389	-3153.702	-2057.063	0.000	-3.600
1.00	NP+4		-4.00	H+		-1.00	E-	2.00	H2O	3.00 CO3-2
NPO2CIT-		-2.0	5.00	0.00	0.00	-946.357	-1127.760	-608.428	0.000	-5.400
1.00	CIT3-		1.00	NP+4		-4.00	H+	-1.00	E-	2.00 H2O
NPO2CL		0.0	5.00	0.00	0.00	-1043.901	-1294.840	-841.655	0.000	-11.300
1.00	NP+4		1.00	CL-		-4.00	H+	-1.00	E-	2.00 H2O
NPO2CL+		1.0	6.00	0.00	0.00	-928.030	-1294.840	-1230.286	0.000	-31.600
1.00	NP+4		2.00	H2O		1.00	CL-	-4.00	H+	-2.00 E-
NPO2CL2		0.0	6.00	0.00	0.00	-1082.082	-1461.920	-1273.984	0.000	-27.600
1.00	NP+4		2.00	H2O		2.00	CL-	-4.00	H+	-2.00 E-
NPO2CO3		0.0	10.00	0.00	0.00	-1380.667	-1803.074	-1416.761	0.000	-21.800
1.00	NP+4		-4.00	H+		-2.00	E-	2.00	H2O	1.00 CO3-2
NPO2EDTA		-3.0	5.00	0.00	0.00	-961.769	-1127.760	-556.738	0.000	-2.700
1.00	EDTA4-		1.00	NP+4		2.00	H2O	-4.00	H+	-1.00 E-
NPO2F		0.0	5.00	0.00	0.00	-1205.046	-1463.110	-865.552	0.000	-9.400
1.00	NP+4		2.00	H2O		-4.00	H+	-1.00	E-	1.00 F-
NPO2F+		1.0	6.00	0.00	0.00	-1104.016	-1463.110	-1204.408	0.000	-27.100
1.00	NP+4		2.00	H2O		-4.00	H+	-2.00	E-	1.00 F-

Table B.3: Selected aqueous species and minerals in HATCHES 3.0 data base. Page 13 of 50

		Charge	OPV	DH a	DH b	$\Delta_r G^\circ$	$\Delta_r H^\circ$	$\Delta_r S^\circ$	$\Delta_r H^\circ$	logK(25)
NPO2HEDT		-2.0	5.00	0.00	0.00 -1011.427	-1127.760	-390.181	0.000	6.000	
1.00	EDTA4-		-3.00	H+	1.00 NP+4	2.00	H2O	-1.00 E-		
NPO2HOX		0.0	5.00	0.00	0.00 -955.490	-1127.760	-577.797	0.000	-3.800	
1.00	NP+4		2.00	H2O	-3.00 H+	-1.00	E-	1.00 OX2-		
NPO2OH		0.0	5.00	0.00	0.00 -1086.463	-1413.590	-1097.190	0.000	-22.400	
1.00	NP+4		-5.00	H+	-1.00 E-	3.00	H2O			
NPO2OH+		1.0	6.00	0.00	0.00 -1003.698	-1413.590	-1374.784	0.000	-36.900	
1.00	NP+4		-5.00	H+	-2.00 E-	3.00	H2O			
NPO2OH2		0.0	6.00	0.00	0.00 -1204.308	-1699.420	-1660.615	0.000	-43.300	
1.00	NP+4		-6.00	H+	-2.00 E-	4.00	H2O			
NPO2OH2-		-1.0	5.00	0.00	0.00 -1258.533	-1699.420	-1478.743	0.000	-33.800	
1.00	NP+4		-6.00	H+	-1.00 E-	4.00	H2O			
NPO2OH3-		-1.0	6.00	0.00	0.00 -1388.935	-1985.250	-2000.051	0.000	-52.500	
1.00	NP+4		-7.00	H+	-2.00 E-	5.00	H2O			
NPO2OX-		-1.0	5.00	0.00	0.00 -940.079	-1127.760	-629.486	0.000	-6.500	
1.00	NP+4		2.00	H2O	-4.00 H+	-1.00 E-		1.00 OX2-		
NPO2OX2-		-3.0	5.00	0.00	0.00 -957.202	-1127.760	-572.053	0.000	-3.500	
1.00	NP+4		2.00	H2O	-4.00 H+	-1.00 E-		2.00 OX2-		
NPO2SO4		0.0	12.00	0.00	0.00 -1558.505	-2037.100	-1605.217	0.000	-28.500	
1.00	NP+4		-4.00	H+	-2.00 E-	2.00	H2O	1.00 SO4-2		
NPO2SO42		-2.0	18.00	0.00	0.00 -2309.354	-2946.440	-2136.796	0.000	-27.300	
1.00	NP+4		-4.00	H+	-2.00 E-	2.00	H2O	2.00 SO4-2		
NPOH+2		2.0	3.00	0.00	0.00 -712.071	-841.930	-435.548	0.000	-4.900	
1.00	NP+4		1.00	H2O	-1.00 H+	1.00 E-				
NPOH+3		3.0	4.00	0.00	0.00 -731.478	-841.930	-370.457	0.000	-1.500	
1.00	NP+4		-1.00	H+	1.00 H2O					
NPOH2+		1.0	3.00	0.00	0.00 -897.269	-1127.760	-773.070	0.000	-14.000	
1.00	NP+4		-2.00	H+	1.00 E-	2.00	H2O			
NPOH2+2		2.0	4.00	0.00	0.00 -960.056	-1127.760	-562.481	0.000	-3.000	
1.00	NP+4		-2.00	H+	2.00 H2O					
NPOH3		0.0	3.00	0.00	0.00 -1077.330	-1413.590	-1127.821	0.000	-24.000	
1.00	NP+4		-3.00	H+	1.00 E-	3.00	H2O			
NPOH3+		1.0	4.00	0.00	0.00 -1180.073	-1413.590	-783.221	0.000	-6.000	
1.00	NP+4		-3.00	H+	3.00 H2O					
NPOH3CO3		-1.0	8.00	0.00	0.00 -1742.239	-2088.904	-1162.720	0.000	0.000	
1.00	NP+4		-3.00	H+	3.00 H2O	1.00 CO3-2				
NPOH4-		-1.0	3.00	0.00	0.00 -1251.683	-1699.420	-1501.716	0.000	-35.000	
1.00	NP+4		-4.00	H+	1.00 E-	4.00	H2O			
NPOH4		0.0	4.00	0.00	0.00 -1400.089	-1699.420	-1003.962	0.000	-9.000	
1.00	NP+4		-4.00	H+	4.00 H2O					
NPOH5-		-1.0	4.00	0.00	0.00 -1547.615	-1985.250	-1467.836	0.000	-24.700	
1.00	NP+4		5.00	H2O	-5.00 H+					
NPSO4+2		2.0	10.00	0.00	0.00 -1266.364	-1465.440	-667.704	0.000	3.410	
1.00	NP+4		1.00	SO4-2						
O2(AQ)		0.0	4.00	0.00	0.00 17.057	-7.699	-83.029	563.961	-86.080	
2.00	H2O		-4.00	H+	-4.00 E-					

Table B.3: Selected aqueous species and minerals in HATCHES 3.0 data base. Page 14 of 50

		Charge	OPV	DH a	DH b	$\Delta_r G^\circ$	$\Delta_r H^\circ$	$\Delta_r S^\circ$	$\Delta_r H^\circ$	logK(25)
OH-		-1.0	0.00	0.00	0.00	-157.229	-229.995	-244.056	55.835	-14.000
	1.00 H2O		-1.00 H+							
PU(HP)4-		-4.0	4.00	0.00	0.00	-5112.140	-5722.116	-2045.869	-48.116	92.600
	1.00 PU+4		4.00 H+		4.00 PO4-3					
PU(SO4)2		0.0	16.00	0.00	0.00	-2028.106	-2299.391	-909.894	55.689	10.250
	1.00 PU+4		2.00 SO4-2							
PU(SO4)3		-2.0	22.00	0.00	0.00	-2779.241	-3264.420	-1627.299	0.000	11.500
	1.00 PU+4		3.00 SO4-2							
PU+3		3.0	3.00	0.00	0.00	-578.634	-592.047	-44.987	-55.647	17.000
	1.00 PU+4		1.00 E-							
PU2OH2+4		4.0	6.00	0.00	0.00	-1551.638	-1644.460	-311.326	0.000	20.000
	2.00 PU+4		-2.00 H+		2.00 E-	2.00	H2O			
PU2OH2+6		6.0	8.00	0.00	0.00	-1431.772	-1644.460	-713.359	0.000	-1.000
	2.00 PU+4		-2.00 H+		2.00 H2O					
PU2OH3+5		5.0	8.00	0.00	0.00	-1663.204	-1930.290	-895.810	0.000	-2.000
	2.00 PU+4		-3.00 H+		3.00 H2O					
PU2OH4+4		4.0	8.00	0.00	0.00	-1894.636	-2216.120	-1078.262	0.000	-3.000
	2.00 PU+4		-4.00 H+		4.00 H2O					
PU2OH5+3		3.0	8.00	0.00	0.00	-2108.945	-2501.950	-1318.146	0.000	-7.000
	2.00 PU+4		-5.00 H+		5.00 H2O					
PU3OH5+4		4.0	9.00	0.00	0.00	-2733.242	-3038.350	-1023.336	0.000	18.000
	3.00 PU+4		-5.00 H+		3.00 E-	5.00	H2O			
PUCIT+		1.0	4.00	0.00	0.00	-588.338	-536.400	174.200	0.000	18.700
	1.00 CIT3-		1.00 PU+4							
PUCIT2-2		-2.0	4.00	0.00	0.00	-675.669	-536.400	467.110	0.000	34.000
	2.00 CIT3-		1.00 PU+4							
PUCL+2		2.0	3.00	0.00	0.00	-715.562	-703.480	40.524	0.000	18.000
	1.00 PU+4		1.00 CL-		1.00 E-					
PUCL+3		3.0	4.00	0.00	0.00	-622.352	-703.480	-272.104	0.000	1.670
	1.00 PU+4		1.00 CL-							
PUCL2+		1.0	3.00	0.00	0.00	-812.535	-870.560	-194.617	0.000	12.000
	1.00 PU+4		2.00 CL-		1.00 E-					
PUCL2+2		2.0	4.00	0.00	0.00	-747.179	-870.560	-413.821	0.000	0.550
	1.00 PU+4		2.00 CL-							
PUCL3+		1.0	4.00	0.00	0.00	-873.034	-1037.640	-552.092	0.000	-0.390
	1.00 PU+4		3.00 CL-							
PUCO3+		1.0	7.00	0.00	0.00	-1143.655	-1211.714	-228.272	0.000	23.500
	1.00 PU+4		1.00 E-		1.00 CO3-2					
PUCO3+2		2.0	8.00	0.00	0.00	-1118.540	-1211.714	-312.507	0.000	19.100
	1.00 PU+4		1.00 CO3-2							
PUCO32-1		-1.0	11.00	0.00	0.00	-1697.259	-1887.028	-636.487	0.000	28.000
	1.00 PU+4		1.00 E-		2.00 CO3-2					
PUCO32		0.0	12.00	0.00	0.00	-1726.370	-1887.028	-538.851	0.000	33.100
	1.00 PU+4		2.00 CO3-2							
PUCO33-1		-3.0	15.00	0.00	0.00	-2245.156	-2562.342	-1063.847	0.000	31.500
	1.00 PU+4		1.00 E-		3.00 CO3-2					

Table B.3: Selected aqueous species and minerals in HATCHES 3.0 data base. Page 15 of 50

		Charge	OPV	DH a	DH b	$\Delta_f G^\circ$	$\Delta_f H^\circ$	$\Delta_f S^\circ$	$\Delta_f H^\circ$	logK(25)
PUCO33-2 1.00	PU+4	-2.0 3.00	16.00 CO3-2	0.00	0.00	-2306.801 -2562.342	-2562.342	-857.087	0.000	42.300
PUCO34-4 1.00	PU+4	-4.0 4.00	20.00 CO3-2	0.00	0.00	-2850.132 -3237.656	-3237.656	-1299.763	0.000	45.000
PUCO35-6 1.00	PU+4	-6.0 5.00	24.00 CO3-2	0.00	0.00	-3375.197 -3912.970	-3912.970	-1803.700	0.000	44.500
PUEDTA 1.00	EDTA4-	0.0 1.00	4.00 PU+4	0.00	0.00	-647.129 -536.400	-536.400	371.388	0.000	29.000
PUEDTA- 1.00	EDTA4-	-1.0 1.00	3.00 E-	0.00	0.00	-696.217 1.00 PU+4	-536.400	536.030	0.000	37.600
PUF+3 1.00	PU+4	3.0 1.00	4.00 F-	0.00	0.00	-811.637 -849.910	-849.910	-128.366	21.840	8.500
PUF2+2 1.00	PU+4	2.0 2.00	4.00 F-	0.00	0.00	-1132.542 -1207.100	-1207.100	-250.070	0.000	15.400
PUF3+ 1.00	PU+4	1.0 3.00	4.00 F-	0.00	0.00	-1444.314 -1542.450	-1542.450	-329.151	0.000	20.700
PUF4 1.00	PU+4	0.0 4.00	4.00 F-	0.00	0.00	-1749.807 -1877.800	-1877.800	-429.291	0.000	24.900
PUH2P4+2 1.00	PU+4	2.0 2.00	3.00 H+	0.00	0.00	-1729.705 1.00 PO4-3	-1844.356 1.00 E-	-384.540	-23.556	39.000
PUHEDTA 1.00	EDTA4-	0.0 1.00	3.00 E-	0.00	0.00	-704.208 1.00 H+	-536.400 1.00 PU+4	562.832	0.000	39.000
PUHOX+3 1.00	PU+4	3.0 1.00	4.00 OX2-	0.00	0.00	-552.378 1.00 H+	-536.400	53.591	0.000	12.400
PUHPO4+2 1.00	PU+4	2.0 1.00	4.00 H+	0.00	0.00	-1651.450 1.00 PO4-3	-1775.069 1.00 E-	-414.620	45.731	25.290
PUHPO42 1.00	PU+4	0.0 2.00	4.00 H+	0.00	0.00	-2809.199 2.00 PO4-3	-3069.971 2.00 E-	-874.632	35.229	48.460
PUHPO43- 1.00	PU+4	-2.0 3.00	4.00 H+	0.00	0.00	-3960.270 3.00 PO4-3	-4373.701 3.00 E-	-1386.653	15.899	70.460
PUHSO4+ 1.00	PU+4	1.0 1.00	15.00 E-	0.00	0.00	-2116.293 2.00 H+	-2355.080 2.00 SO4-2	-800.895	0.000	25.700
PUNO3+3 1.00	PU+4	3.0 1.00	9.00 NO3-	0.00	0.00	-602.664 -734.882	-734.882	-443.461	8.368	1.800
PUNO32+2 1.00	PU+4	2.0 2.00	14.00 NO3-	0.00	0.00	-711.000 -950.100	-950.100	-801.946	0.000	1.370
PUNO33+ 1.00	PU+4	1.0 3.00	19.00 NO3-	0.00	0.00	-820.819 -1156.950	-1156.950	-1127.387	0.000	1.200
PUO2+ 1.00	PU+4	1.0 2.00	5.00 H2O	0.00	0.00	-849.713 -4.00 H+	-914.592 -1.00 E-	-217.605	193.468	-18.600
PUO2+2 1.00	PU+4	2.0 -4.00	6.00 H+	0.00	0.00	-756.674 -2.00 E-	-822.125 2.00 H2O	-219.525	285.935	-34.900
PUO22OH2 2.00	PU+4	2.0 -10.00	12.00 H+	0.00	0.00	-1956.805 -4.00 E-	-2269.508 6.00 H2O	-1048.809	518.272	-75.200
PUO23OH5 3.00	PU+4	1.0 -17.00	18.00 H+	0.00	0.00	-3387.227 -6.00 E-	-4035.356 11.00 H2O	-2173.833	717.974	-116.700

Table B.3: Selected aqueous species and minerals in HATCHES 3.0 data base. Page 16 of 50

		Charge	OPV	DH a	DH b	$\Delta_f G^\circ$	$\Delta_f H^\circ$	$\Delta_f S^\circ$	$\Delta_f H^\circ$	logK(25)
PUO2C2-2		-2.0	14.00	0.00	0.00	-1896.989	-2149.909	-848.297	308.779	-20.100
1.00	PU+4		-4.00	H+		-2.00	E-	2.00	H2O	2.00 CO3-2
PUO2C3-2		-4.0	18.00	0.00	0.00	-2439.749	-3134.002	-2328.537	0.000	-17.500
1.00	PU+4		-4.00	H+		-2.00	E-	2.00	H2O	3.00 CO3-2
PUO2CL		0.0	5.00	0.00	0.00	-522.017	-1275.140	-2525.986	0.000	-99.000
1.00	PU+4		2.00	H2O		1.00	CL-	-4.00	H+	-1.00 E-
PUO2CL+		1.0	6.00	0.00	0.00	-888.465	-1275.140	-1296.915	0.000	-34.800
1.00	PU+4		2.00	H2O		1.00	CL-	-4.00	H+	-2.00 E-
PUO2CL2		0.0	6.00	0.00	0.00	-1016.260	-1442.220	-1428.676	0.000	-35.400
1.00	PU+4		2.00	H2O		2.00	CL-	-4.00	H+	-2.00 E-
PUO2CO3-		-1.0	9.00	0.00	0.00	-1432.428	-1783.374	-1177.079	0.000	-9.000
1.00	PU+4		-4.00	H+		-1.00	E-	2.00	H2O	1.00 CO3-2
PUO2CO3		0.0	10.00	0.00	0.00	-1337.106	-1783.374	-1496.791	0.000	-25.700
1.00	PU+4		-4.00	H+		-2.00	E-	2.00	H2O	1.00 CO3-2
PUO2CT-2		-2.0	5.00	0.00	0.00	-881.106	-1108.060	-761.206	0.000	-13.100
1.00	CIT3-		1.00	PU+4		-4.00	H+	-1.00	E-	2.00 H2O
PUO2CT-		-1.0	6.00	0.00	0.00	-808.045	-1108.060	-1006.254	0.000	-25.900
1.00	CIT3-		1.00	PU+4		-4.00	H+	-2.00	E-	2.00 H2O
PUO2CT2-		-4.0	6.00	0.00	0.00	-842.293	-1108.060	-891.388	0.000	-19.900
2.00	CIT3-		1.00	PU+4		-4.00	H+	-2.00	E-	2.00 H2O
PUO2ED-3		-3.0	5.00	0.00	0.00	-911.929	-1108.060	-657.826	0.000	-7.700
1.00	EDTA4-		1.00	PU+4		2.00	H2O	-4.00	H+	-1.00 E-
PUO2ED-2		-2.0	6.00	0.00	0.00	-857.704	-1108.060	-839.698	0.000	-17.200
1.00	EDTA4-		-2.00	E-		1.00	PU+4	2.00	H2O	-4.00 H+
PUO2F+		1.0	6.00	0.00	0.00	-1064.450	-1162.664	-329.409	280.746	-30.300
1.00	PU+4		2.00	H2O		-2.00	E-	-4.00	H+	1.00 F-
PUO2H2PO		1.0	6.00	0.00	0.00	-1915.736	-2107.279	-642.437	285.181	-11.500
1.00	PU+4		2.00	H2O		1.00	PO4-3	-2.00	E-	-2.00 H+
PUO2HED-		-2.0	5.00	0.00	0.00	-943.323	-1108.060	-552.532	0.000	-2.200
1.00	EDTA4-		-3.00	H+		1.00	PU+4	2.00	H2O	-1.00 E-
PUO2HPO4		-1.0	5.00	0.00	0.00	-1961.970	-2392.460	-1443.870	0.000	-3.400
1.00	PU+4		2.00	H2O		1.00	PO4-3	-1.00	E-	-3.00 H+
PUO2NO3+		1.0	11.00	0.00	0.00	-864.039	-1314.910	-1512.228	0.000	-35.500
1.00	PU+4		-4.00	H+		-2.00	E-	2.00	H2O	1.00 NO3-
PUO2OH		0.0	5.00	0.00	0.00	-1031.486	-1187.200	-522.268	206.690	-28.300
1.00	PU+4		-5.00	H+		-1.00	E-	3.00	H2O	
PUO2OH+		1.0	6.00	0.00	0.00	-963.562	-1118.583	-519.942	275.307	-40.200
1.00	PU+4		-5.00	H+		-2.00	E-	3.00	H2O	
PUO2OH2		0.0	6.00	0.00	0.00	-1159.605	-1679.720	-1744.473	0.000	-47.400
1.00	PU+4		-6.00	H+		-2.00	E-	4.00	H2O	
PUO2OH2-		-1.0	5.00	0.00	0.00	-1215.543	-1679.720	-1556.858	0.000	-37.600
1.00	PU+4		-6.00	H+		-1.00	E-	4.00	H2O	
PUO2OH3-		-1.0	6.00	0.00	0.00	-1328.250	-1965.550	-2137.513	0.000	-59.400
1.00	PU+4		-7.00	H+		-2.00	E-	5.00	H2O	
PUO2OX2-		-2.0	6.00	0.00	0.00	-814.895	-1108.060	-983.281	0.000	-24.700
1.00	PU+4		2.00	H2O		-2.00	E-	-4.00	H+	2.00 OX2-

Table B.3: Selected aqueous species and minerals in HATCHES 3.0 data base. Page 17 of 50

		Charge	OPV	DH a	DH b	$\Delta_f G^\circ$	$\Delta_f H^\circ$	$\Delta_f S^\circ$	$\Delta_f H^\circ$	logK(25)
PUO2SO4		0.0	12.00	0.00	0.00	-1518.939	-1715.315	-658.648	302.085	-31.700
1.00	PU+4		-4.00	H+		-2.00	E-	2.00	H2O	1.00 SO4-2
PUOH+2		2.0	3.00	0.00	0.00	-775.819	-324.752	1512.885	497.478	10.000
1.00	PU+4		-1.00	H+		1.00	E-	1.00	H2O	
PUOH+3		3.0	4.00	0.00	0.00	-713.603	-774.114	-202.955	48.116	-0.900
1.00	PU+4		-1.00	H+		1.00	H2O			
PUOH2+		1.0	3.00	0.00	0.00	-955.880	-1108.060	-510.414	0.000	0.000
1.00	PU+4		-2.00	H+		1.00	E-	2.00	H2O	
PUOH2+2		2.0	4.00	0.00	0.00	-943.323	-1033.585	-302.741	74.475	-2.200
1.00	PU+4		-2.00	H+		2.00	H2O			
PUOH3		0.0	3.00	0.00	0.00	-1138.795	-1393.890	-855.593	0.000	-9.500
1.00	PU+4		-3.00	H+		1.00	E-	3.00	H2O	
PUOH3+		1.0	4.00	0.00	0.00	-1163.910	-1297.240	-447.191	96.650	-5.100
1.00	PU+4		-3.00	H+		3.00	H2O			
PUOH4-		-1.0	3.00	0.00	0.00	-1316.002	-1679.720	-1219.917	0.000	-20.000
1.00	PU+4		-4.00	H+		1.00	E-	4.00	H2O	
PUOH4		0.0	4.00	0.00	0.00	-1369.999	-1570.518	-672.544	109.202	-10.540
1.00	PU+4		4.00	H2O		-4.00	H+			
PUOH5-		-1.0	4.00	0.00	0.00	-1102.217	-1965.550	-2895.632	0.000	-99.000
1.00	PU+4		5.00	H2O		-5.00	H+			
PUOX+2		2.0	4.00	0.00	0.00	-542.104	-536.400	19.131	0.000	10.600
1.00	PU+4		1.00	OX2-						
PUOX2		0.0	4.00	0.00	0.00	-596.900	-536.400	202.917	0.000	20.200
1.00	PU+4		2.00	OX2-						
PUOX3-2		-2.0	4.00	0.00	0.00	-632.289	-536.400	321.612	0.000	26.400
1.00	PU+4		3.00	OX2-						
PUSO4+		1.0	9.00	0.00	0.00	-1339.187	-1486.952	-495.606	-41.212	19.900
1.00	PU+4		1.00	E-		1.00	SO4-2			
PUSO4+2		2.0	10.00	0.00	0.00	-1258.249	-1433.188	-586.748	12.552	5.720
1.00	PU+4		1.00	SO4-2						
PUSO42-1		-1.0	15.00	0.00	0.00	-2095.174	-2355.080	-871.729	0.000	22.000
1.00	PU+4		1.00	E-		2.00	SO4-2			
S-2		-2.0	-2.00	0.00	0.00	86.235	116.661	102.048	-117.319	20.730
1.00	SO4-2		8.00	H+		8.00	E-	-4.00	H2O	
SE-2		-2.0	-2.00	0.00	0.00	129.397	544.220	1391.324	0.000	66.200
1.00	SEO4-2		8.00	H+		8.00	E-	-4.00	H2O	
SEO3-2		-2.0	4.00	0.00	0.00	-369.689	-509.081	-467.523	-195.811	29.000
1.00	SEO4-2		2.00	H+		2.00	E-	-1.00	H2O	
SIF6-2		-2.0	0.00	0.00	0.00	-2220.560	-2393.772	-580.957	-68.032	30.180
1.00	H4SiO4		4.00	H+		6.00	F-	-4.00	H2O	
SN+4		4.0	4.00	0.00	0.00	2.367	30.430	94.124	39.330	-5.250
1.00	SN+2		-2.00	E-						
SN2OH2+2		2.0	4.00	0.00	0.00	-502.253	-589.460	-292.493	0.000	-4.770
2.00	SN+2		2.00	H2O		-2.00	H+			
SN3OH4+2		2.0	6.00	0.00	0.00	-992.090	-1170.020	-596.781	0.000	-6.880
3.00	SN+2		4.00	H2O		-4.00	H+			

Table B.3: Selected aqueous species and minerals in HATCHES 3.0 data base. Page 18 of 50

		Charge	OPV	DH a	DH b	$\Delta_f G^\circ$	$\Delta_f H^\circ$	$\Delta_f S^\circ$	$\Delta_f H^\circ$	logK(25)
SNCL+		1.0	2.00	0.00	0.00	-162.359	-164.809	-8.217	11.171	0.620
	1.00 SN+2		1.00	CL-						
SNCL2		0.0	2.00	0.00	0.00	-298.202	-329.629	-105.407	13.431	1.430
	1.00 SN+2		2.00	CL-						
SNCL3-		-1.0	2.00	0.00	0.00	-426.283	-486.877	-203.233	23.263	0.880
	1.00 SN+2		3.00	CL-						
SNO3-2		-2.0	4.00	0.00	0.00	-575.203	-866.390	-976.646	0.000	-28.700
	1.00 SN+2		3.00	H2O		-6.00 H+	-2.00 E-			
SNOH+		1.0	2.00	0.00	0.00	-255.893	-286.320	-102.054	8.410	-1.550
	1.00 SN+2		1.00	H2O		-1.00 H+				
SNOH2		0.0	2.00	0.00	0.00	-461.582	-580.560	-399.054	0.000	-7.060
	1.00 SN+2		2.00	H2O		-2.00 H+				
SNOH3-		-1.0	2.00	0.00	0.00	-644.212	-866.390	-745.190	0.000	-16.610
	1.00 SN+2		3.00	H2O		-3.00 H+				
SNOH5-		-1.0	4.00	0.00	0.00	-1130.535	-1438.050	-1031.409	0.000	-14.500
	1.00 SN+2		5.00	H2O		-5.00 H+	-2.00 E-			
SNOH6-2		-2.0	4.00	0.00	0.00	-1299.123	-1723.880	-1424.641	0.000	-26.510
	1.00 SN+2		6.00	H2O		-6.00 H+	-2.00 E-			
SRCIT-		-1.0	0.00	0.00	0.00	-587.289	-550.900	122.051	0.000	4.110
	1.00 SR+2		1.00	CIT3-						
SRCL+		1.0	0.00	0.00	0.00	-696.135	-726.348	-101.337	-8.368	0.190
	1.00 SR+2		1.00	CL-						
SRCL2		0.0	0.00	0.00	0.00	-826.270	-885.039	-197.112	0.021	0.000
	1.00 SR+2		2.00	CL-						
SRCO3		0.0	4.00	0.00	0.00	-1107.788	-1226.214	-397.202	0.000	2.810
	1.00 SR+2		1.00	CO3-2						
SREDTA-2		-2.0	0.00	0.00	0.00	-619.083	-550.900	228.685	0.000	9.680
	1.00 SR+2		1.00	EDTA4-						
SRF+		1.0	0.00	0.00	0.00	-848.204	-869.514	-71.474	16.736	0.500
	1.00 SR+2		1.00	F-						
SRNO3+		1.0	5.00	0.00	0.00	-679.300	-757.750	-263.121	0.000	0.820
	1.00 SR+2		1.00	NO3-						
SROH+		1.0	0.00	0.00	0.00	-725.683	-780.497	-183.848	56.233	-13.190
	1.00 SR+2		1.00	H2O		-1.00 H+				
SROH2		0.0	0.00	0.00	0.00	-875.378	-1122.560	-829.054	0.000	-28.510
	1.00 SR+2		2.00	H2O		-2.00 H+				
SRPO4-		-1.0	0.00	0.00	0.00	-1613.186	-1835.300	-744.974	0.000	4.180
	1.00 SR+2		1.00	PO4-3						
SRSO4		0.0	6.00	0.00	0.00	-1322.385	-1460.240	-462.367	0.000	2.550
	1.00 SR+2		1.00	SO4-2						
TC+3		3.0	3.00	0.00	0.00	105.717	285.830	604.101	0.000	5.400
	1.00 TCO+2		2.00	H+		-1.00 H2O	1.00	E-		
TCO4-3		-3.0	5.00	0.00	0.00	-507.789	-857.490	-1172.904	0.000	-53.300
	1.00 TCO+2		-6.00	H+		3.00 H2O	-1.00	E-		
TCO4-1		-1.0	7.00	0.00	0.00	-623.659	-857.490	-784.273	0.000	-33.000
	1.00 TCO+2		-6.00	H+		3.00 H2O	-3.00	E-		

Table B.3: Selected aqueous species and minerals in HATCHES 3.0 data base. Page 19 of 50

		Charge	OPV	DH a	DH b	$\Delta_f G^\circ$	$\Delta_f H^\circ$	$\Delta_f S^\circ$	$\Delta_f H^\circ$	logK(25)
TCO4-2		-2.0	6.00	0.00	0.00	-564.868	-857.490	-981.460	0.000	-43.300
1.00	TCO+2		-6.00	H+	3.00	H2O	-2.00	E-		
TCOOH+		1.0	4.00	0.00	0.00	-331.461	-285.830	153.048	0.000	-1.100
1.00	TCO+2		1.00	H2O	-1.00	H+				
TCOOH2		0.0	4.00	0.00	0.00	-556.044	-571.660	-52.377	0.000	-3.300
1.00	TCO+2		-2.00	H+	2.00	H2O				
TCOOH22		0.0	8.00	0.00	0.00	-1149.189	-1143.320	19.685	0.000	-0.100
2.00	TCO+2		-4.00	H+	4.00	H2O				
TH(NO3)+		3.0	5.00	0.00	0.00	-824.923	-975.850	-506.213	0.000	1.600
1.00	TH+4		1.00	NO3-						
TH(NO3)2		2.0	10.00	0.00	0.00	-942.562	-1182.700	-805.426	0.000	2.800
1.00	TH+4		2.00	NO3-						
TH(NO3)3		1.0	15.00	0.00	0.00	-1048.786	-1389.550	-1142.929	0.000	2.000
1.00	TH+4		3.00	NO3-						
TH(NO3)4		0.0	20.00	0.00	0.00	-1153.868	-1601.002	-1499.696	-4.602	1.000
1.00	TH+4		4.00	NO3-						
TH(SO4)2		0.0	12.00	0.00	0.00	-2248.367	-2555.882	-1031.410	31.798	9.700
1.00	TH+4		2.00	SO4-2						
TH(SO4)3		-2.0	18.00	0.00	0.00	-2996.933	-3497.020	-1677.300	0.000	10.500
1.00	TH+4		3.00	SO4-2						
TH(SO4)4		-4.0	24.00	0.00	0.00	-3729.517	-4406.360	-2270.142	0.000	8.500
1.00	TH+4		4.00	SO4-2						
TH2OH2+6		6.0	0.00	0.00	0.00	-1849.462	-2047.737	-665.018	61.923	-6.100
2.00	TH+4		2.00	H2O	-2.00	H+				
TH4OH8+8		8.0	0.00	0.00	0.00	-4596.683	-5121.223	-1759.316	241.417	-21.100
4.00	TH+4		8.00	H2O	-8.00	H+				
THCl+3		3.0	0.00	0.00	0.00	-844.097	-936.080	-308.513	0.000	1.380
1.00	TH+4		1.00	CL-						
THCl2+2		2.0	0.00	0.00	0.00	-961.161	-1103.160	-476.266	0.000	-1.100
1.00	TH+4		2.00	CL-						
THCl3+		1.0	0.00	0.00	0.00	-1093.922	-1270.240	-591.372	0.000	-0.830
1.00	TH+4		3.00	CL-						
THCl4		0.0	0.00	0.00	0.00	-1219.948	-1437.320	-729.068	0.000	-1.740
1.00	TH+4		4.00	CL-						
THCO3+2		2.0	4.00	0.00	0.00	-1295.877	-1444.314	-497.859	0.000	11.030
1.00	TH+4		1.00	CO3-2						
THF4		0.0	0.00	0.00	0.00	-1958.366	-2125.881	-561.846	-15.481	22.300
1.00	TH+4		4.00	F-						
THH2P4+3		3.0	0.00	0.00	0.00	-1868.628	-2053.400	-619.727	0.000	24.200
1.00	TH+4		1.00	PO4-3	2.00	H+				
THH2P42+		2.0	0.00	0.00	0.00	-3029.973	-3337.800	-1032.455	0.000	48.000
1.00	TH+4		2.00	PO4-3	4.00	H+				
THH3P4+4		4.0	0.00	0.00	0.00	-1865.204	-2053.400	-631.214	0.000	23.600
1.00	TH+4		1.00	PO4-3	3.00	H+				
THHPO4+2		2.0	0.00	0.00	0.00	-1862.920	-1891.061	-94.383	162.339	23.200
1.00	TH+4		1.00	PO4-3	1.00	H+				

Table B.3: Selected aqueous species and minerals in HATCHES 3.0 data base. Page 20 of 50

		Charge	OPV	DH a	DH b	$\Delta_r G^\circ$	$\Delta_r H^\circ$	$\Delta_r S^\circ$	$\Delta_r H^\circ$	logK(25)
THHPO42		0.0	0.00	0.00	0.00	-3027.120	-3203.494	-591.561	134.306	47.500
1.00	TH+4		2.00	PO4-3	2.00	H+				
THHPO43-		-2.0	0.00	0.00	0.00	-4171.341	-4622.200	-1512.189	0.000	68.300
1.00	TH+4		3.00	PO4-3	3.00	H+				
THOH+3		3.0	0.00	0.00	0.00	-923.875	-1030.144	-356.430	24.686	-3.200
1.00	TH+4		1.00	H2O		-1.00	H+			
THOH2+		2.0	0.00	0.00	0.00	-1139.325	-1282.502	-480.221	58.158	-7.000
1.00	TH+4		2.00	H2O		-2.00	H+			
THOH3+		1.0	0.00	0.00	0.00	-1349.637	-1541.555	-643.694	84.935	-11.700
1.00	TH+4		3.00	H2O		-3.00	H+			
THOH4		0.0	0.00	0.00	0.00	-1562.804	-1834.079	-909.860	78.241	-15.900
1.00	TH+4		4.00	H2O		-4.00	H+			
THSO4+2		2.0	6.00	0.00	0.00	-1480.393	-1661.604	-607.783	16.736	5.500
1.00	TH+4		1.00	SO4-2						
U(CO3)5-		-6.0	24.00	0.00	0.00	-3393.776	-3894.550	-1679.605	73.220	39.300
1.00	U+4		5.00	CO3-2						
U(HPO4)2		0.0	4.00	0.00	0.00	-2847.413	-3152.845	-1024.424	7.155	46.700
1.00	U+4		2.00	H+		2.00	PO4-3			
U(HPO4)3		-2.0	4.00	0.00	0.00	-3994.489	-4479.378	-1626.328	-34.978	68.000
1.00	U+4		3.00	H+		3.00	PO4-3			
U(HPO4)4		-4.0	4.00	0.00	0.00	-5134.144	-5839.132	-2364.542	-110.332	88.000
1.00	U+4		4.00	H+		4.00	PO4-3			
U(SO4)2		0.0	16.00	0.00	0.00	-2074.939	-2386.868	-1046.215	23.012	10.000
1.00	U+4		2.00	SO4-2						
UBR+3		3.0	4.00	0.00	0.00	-639.304	-712.610	-245.870	0.000	0.980
1.00	U+4		1.00	BR-						
UCL+3		3.0	4.00	0.00	0.00	-661.251	-751.042	-301.159	7.238	0.030
1.00	U+4		1.00	CL-						
UCL2+2		2.0	4.00	0.00	0.00	-792.585	-925.360	-445.328	0.000	0.050
1.00	U+4		2.00	CL-						
UEDTA		0.0	4.00	0.00	0.00	-695.960	-591.200	351.367	0.000	29.100
1.00	EDTA4-		1.00	U+4						
UF+3		3.0	4.00	0.00	0.00	-850.080	-905.839	-187.019	20.711	6.780
1.00	U+4		1.00	F-						
UF2+2		2.0	4.00	0.00	0.00	-1159.340	-1232.026	-243.791	29.874	11.640
1.00	U+4		2.00	F-						
UF3+		1.0	4.00	0.00	0.00	-1461.751	-1566.707	-352.024	30.543	15.300
1.00	U+4		3.00	F-						
UF4		0.0	4.00	0.00	0.00	-1790.818	-1913.646	-411.969	18.954	23.630
1.00	U+4		4.00	F-						
UHPO4+2		2.0	4.00	0.00	0.00	-1692.347	-1844.513	-510.368	31.087	24.000
1.00	U+4		1.00	H+		1.00	PO4-3			
UL(HPO4)		-2.0	6.00	0.00	0.00	-3252.057	-3636.265	-1288.640	95.395	34.500
1.00	U+4		2.00	H2O		2.00	PO4-3	-2.00	H+	-2.00 E-
UL2CIT2-		-2.0	12.00	0.00	0.00	-2024.262	-2325.720	-1011.095	0.000	2.800
2.00	CIT3-		2.00	U+4		4.00	H2O	-8.00	H+	-4.00 E-

Table B.3: Selected aqueous species and minerals in HATCHES 3.0 data base. Page 21 of 50

		Charge	OPV	DH a	DH b	$\Delta_f G^\circ$	$\Delta_f H^\circ$	$\Delta_f S^\circ$	$\Delta_f H^\circ$	logK(25)
UL2EDTA		0.0	12.00	0.00	0.00	-2008.851	-2325.720	-1062.785	0.000	0.100
1.00	EDTA4-		2.00	U+4	4.00	H2O	-8.00	H+	-4.00	E-
UL2EDTA2		-4.0	12.00	0.00	0.00	-2059.651	-2325.720	-892.399	0.000	9.000
2.00	EDTA4-		2.00	U+4	4.00	H2O	-8.00	H+	-4.00	E-
UL2EDTAO		-1.0	12.00	0.00	0.00	-2217.451	-2611.550	-1321.814	0.000	-4.900
1.00	EDTA4-		2.00	U+4	5.00	H2O	-9.00	H+	-4.00	E-
UL2OH+2		2.0	12.00	0.00	0.00	-2344.999	-2565.589	-739.860	331.791	-24.100
2.00	U+4		6.00	H2O	-10.00	H+	-4.00	E-		
UL2OH+3		3.0	12.00	0.00	0.00	-2124.983	-2309.047	-617.352	302.503	-21.100
2.00	U+4		5.00	H2O	-9.00	H+	-4.00	E-		
UL3CO36-		-6.0	42.00	0.00	0.00	-6327.198	-7170.180	-2827.376	370.284	25.800
3.00	U+4		6.00	CO3-2	6.00	H2O	-12.00	H+	-6.00	E-
UL3OH3CO		1.0	22.00	0.00	0.00	-4109.632	-4518.049	-1369.836	503.335	-24.900
3.00	U+4		9.00	H2O	1.00	CO3-2	-15.00	H+	-6.00	E-
UL3OH4+2		2.0	18.00	0.00	0.00	-3734.947	-4115.176	-1275.295	516.724	-39.600
3.00	U+4		10.00	H2O	-16.00	H+	-6.00	E-		
UL3OH5+		1.0	18.00	0.00	0.00	-3951.538	-4380.086	-1437.356	537.644	-43.200
3.00	U+4		11.00	H2O	-17.00	H+	-6.00	E-		
UL3OH7-1		-1.0	18.00	0.00	0.00	-4313.373	-4826.226	-1720.118	663.164	-62.900
3.00	U+4		13.00	H2O	-19.00	H+	-6.00	E-		
UL4EDTA2		-4.0	24.00	0.00	0.00	-4858.382	-5794.760	-3140.627	0.000	-18.700
2.00	EDTA4-		4.00	U+4	12.00	H2O	-20.00	H+	-8.00	E-
UL4OH7+		1.0	24.00	0.00	0.00	-5341.486	-5917.540	-1932.094	734.710	-58.700
4.00	U+4		15.00	H2O	-23.00	H+	-8.00	E-		
ULCIT-		-1.0	6.00	0.00	0.00	-1001.286	-1162.860	-541.922	0.000	-0.500
1.00	CIT3-		1.00	U+4	2.00	H2O	-4.00	H+	-2.00	E-
ULCL+		1.0	6.00	0.00	0.00	-1082.276	-1329.940	-830.668	0.000	-9.300
1.00	U+4		2.00	H2O	1.00	CL-	-4.00	H+	-2.00	E-
ULCL2		0.0	6.00	0.00	0.00	-1210.072	-1497.020	-962.429	0.000	-9.900
1.00	U+4		2.00	H2O	2.00	CL-	-4.00	H+	-2.00	E-
ULCL3-		-1.0	6.00	0.00	0.00	-1331.588	-1664.100	-1115.250	0.000	-11.600
1.00	U+4		2.00	H2O	3.00	CL-	-4.00	H+	-2.00	E-
ULCO3		0.0	10.00	0.00	0.00	-1533.771	-1702.194	-564.892	135.980	0.300
1.00	U+4		1.00	CO3-2	2.00	H2O	-4.00	H+	-2.00	E-
ULCO32-2		-2.0	14.00	0.00	0.00	-2102.217	-2354.496	-846.150	158.992	7.400
1.00	U+4		2.00	CO3-2	2.00	H2O	-4.00	H+	-2.00	E-
ULCO33-4		-4.0	18.00	0.00	0.00	-2656.963	-3080.436	-1420.338	108.366	12.100
1.00	U+4		3.00	CO3-2	2.00	H2O	-4.00	H+	-2.00	E-
ULF+		1.0	6.00	0.00	0.00	-1261.116	-1498.210	-795.217	0.000	-4.300
1.00	U+4		2.00	H2O	-2.00	E-	-4.00	H+	1.00	F-
ULF2		0.0	6.00	0.00	0.00	-1563.755	-1833.560	-904.930	0.000	-0.600
1.00	U+4		2.00	H2O	-2.00	E-	-4.00	H+	2.00	F-
ULF3-		-1.0	6.00	0.00	0.00	-1860.116	-2168.910	-1035.701	0.000	2.000
1.00	U+4		2.00	H2O	-2.00	E-	-4.00	H+	3.00	F-
ULF4-2		-2.0	6.00	0.00	0.00	-2148.485	-2504.260	-1193.274	0.000	3.200
1.00	U+4		2.00	H2O	-2.00	E-	-4.00	H+	4.00	F-

Table B.3: Selected aqueous species and minerals in HATCHES 3.0 data base. Page 22 of 50

		Charge	OPV	DH a	DH b	$\Delta_f G^\circ$	$\Delta_f H^\circ$	$\Delta_f S^\circ$	$\Delta_f H^\circ$	logK(25)
ULH2P4+		1.0	6.00	0.00	0.00 -2106.123	-2317.974	-710.553	129.286	13.400	
1.00	U+4		2.00	H2O	1.00 PO4-3	-2.00	H+	-2.00	E-	
ULH2P42		0.0	6.00	0.00	0.00 -3257.194	-3656.766	-1340.173	74.894	35.400	
1.00	U+4		2.00	H2O	2.00 PO4-3	-2.00	E-			
ULH2P43-		-1.0	6.00	0.00	0.00 -4404.269	-4990.370	-1965.792	25.690	56.700	
1.00	U+4		2.00	H2O	3.00 PO4-3	-2.00	E-	2.00	H+	
ULHEDTA-		-1.0	6.00	0.00	0.00 -1056.082	-1162.860	-358.135	0.000	9.100	
1.00	EDTA4-		1.00	U+4	2.00 H2O	-3.00	H+	-2.00	E-	
ULHPO4		0.0	6.00	0.00	0.00 -2092.424	-2312.117	-736.853	135.143	11.000	
1.00	U+4		2.00	H2O	1.00 PO4-3	-3.00	H+	-2.00	E-	
ULNO3+		1.0	11.00	0.00	0.00 -1062.988	-1369.710	-1028.750	0.000	-9.100	
1.00	U+4		2.00	H2O	1.00 NO3-	-4.00	H+	-2.00	E-	
ULOH+		1.0	6.00	0.00	0.00 -1158.515	-1261.247	-344.563	187.443	-14.500	
1.00	U+4		3.00	H2O	-5.00 H+	-2.00	E-			
ULOH2		0.0	6.00	0.00	0.00 -1357.983	-1517.370	-534.587	217.150	-21.100	
1.00	U+4		4.00	H2O	-6.00 H+	-2.00	E-			
ULOH3-		-1.0	6.00	0.00	0.00 -1150.477	-2020.350	-2917.567	0.000	-99.000	
1.00	U+4		5.00	H2O	-7.00 H+	-2.00	E-			
ULOH4-2		-2.0	6.00	0.00	0.00 -1692.419	-2009.534	-1063.609	296.646	-45.600	
1.00	U+4		6.00	H2O	-8.00 H+	-2.00	E-			
ULOX		0.0	6.00	0.00	0.00 -992.724	-1162.860	-570.638	0.000	-2.000	
1.00	U+4		2.00	H2O	-2.00 E-	-4.00	H+	1.00	OX2-	
ULOX2-2		-2.0	6.00	0.00	0.00 -1016.697	-1162.860	-490.232	0.000	2.200	
1.00	U+4		2.00	H2O	-2.00 E-	-4.00	H+	2.00	OX2-	
ULSIOOH3		1.0	6.00	0.00	0.00 -2245.663	-2619.820	-1254.928	0.000	-11.600	
1.00	U+4		1.00	H4SiO4	-5.00 H+	2.00	H2O	-2.00	E-	
ULSO4		0.0	12.00	0.00	0.00 -1712.180	-1906.095	-650.394	166.105	-6.300	
1.00	U+4		1.00	SO4-2	2.00 H2O	-4.00	H+	-2.00	E-	
ULSO42-2		-2.0	18.00	0.00	0.00 -2464.171	-2981.540	-1735.263	0.000	-4.900	
1.00	U+4		2.00	SO4-2	2.00 H2O	-4.00	H+	-2.00	E-	
UNO3+3		3.0	9.00	0.00	0.00 -649.783	-798.050	-497.291	0.000	1.600	
1.00	U+4		1.00	NO3-						
UO2+		1.0	5.00	0.00	0.00 -967.609	-1032.319	-217.038	130.541	-6.400	
1.00	U+4		2.00	H2O	-4.00 H+	-1.00	E-			
UO2+2		2.0	6.00	0.00	0.00 -951.627	-1018.512	-224.333	144.348	-9.200	
1.00	U+4		2.00	H2O	-4.00 H+	-2.00	E-			
UO2CO33-		-5.0	17.00	0.00	0.00 -2636.414	-3188.802	-1852.718	0.000	8.500	
1.00	U+4		2.00	H2O	-4.00 H+	-1.00	E-	3.00	CO3-2	
UO2OH		0.0	5.00	0.00	0.00 -1147.670	-1448.690	-1009.625	0.000	-16.400	
1.00	U+4		3.00	H2O	-5.00 H+	-1.00	E-			
UO2OH2-		-1.0	5.00	0.00	0.00 -1330.014	-1734.520	-1356.718	0.000	-26.000	
1.00	U+4		4.00	H2O	-6.00 H+	-1.00	E-			
UOH+3		3.0	4.00	0.00	0.00 -761.292	-827.659	-222.595	49.371	-1.000	
1.00	U+4		1.00	H2O	-1.00 H+					
UOH2+2		2.0	4.00	0.00	0.00 -992.724	-1088.385	-320.847	74.475	-2.000	
1.00	U+4		2.00	H2O	-2.00 H+					

Table B.3: Selected aqueous species and minerals in HATCHES 3.0 data base. Page 23 of 50

		Charge	OPV	DH a	DH b	$\Delta_f G^\circ$	$\Delta_f H^\circ$	$\Delta_f S^\circ$	$\Delta_f H^\circ$	logK(25)
UOH3+		1.0	4.00	0.00	0.00	-1195.617	-1448.690	-848.812	0.000	-8.000
	1.00	U+4		3.00	H2O		-3.00	H+		
UOH4		0.0	4.00	0.00	0.00	-1409.925	-1734.520	-1088.697	0.000	-12.000
	1.00	U+4		4.00	H2O		-4.00	H+		
UOH5-		-1.0	4.00	0.00	0.00	-1567.154	-2020.350	-1520.025	0.000	-26.000
	1.00	U+4		5.00	H2O		-5.00	H+		
USO4+2		2.0	10.00	0.00	0.00	-1302.400	-1495.519	-647.727	5.021	5.000
	1.00	SO4-2		1.00	U+4					
ZR3OH4+8		8.0	0.00	0.00	0.00	-2518.635	-1143.320	4612.830	0.000	-0.600
	3.00	ZR+4		4.00	H2O		-4.00	H+		
ZR4OH8+8		8.0	0.00	0.00	0.00	-4029.367	-2286.640	5845.136	0.000	6.000
	4.00	ZR+4		8.00	H2O		-8.00	H+		
ZRCL+3		3.0	0.00	0.00	0.00	-656.862	-167.080	1642.735	0.000	0.200
	1.00	ZR+4		1.00	CL-					
ZROH3+		3.0	0.00	0.00	0.00	-763.352	-285.830	1601.618	0.000	0.300
	1.00	ZR+4		1.00	H2O		-1.00	H+		
ZROH4		0.0	0.00	0.00	0.00	-1417.693	-1143.320	920.253	0.000	-9.700
	1.00	ZR+4		4.00	H2O		-4.00	H+		
ZROH5-		-1.0	0.00	0.00	0.00	-1618.874	-1429.150	636.336	0.000	-16.000
	1.00	ZR+4		5.00	H2O		-5.00	H+		
ZRSO4+2		2.0	6.00	0.00	0.00	-1285.909	-909.340	1263.019	0.000	3.050
	1.00	ZR+4		1.00	SO4-2					

Table B.3: Selected aqueous species and minerals in HATCHES 3.0 data base. Page 24 of 50

	Charge	OPV	DH a	DH b	$\Delta_f G^\circ$	$\Delta_f H^\circ$	$\Delta_f S^\circ$	$\Delta_f H^\circ$	logK(25)
MINERALS									
AKERMANI		0.00			-3681.404	-4181.090	-1675.956	0.000	-45.190
	-1.00	H2O		2.00 CA+2		1.00 MG+2	2.00	H4SIO4	-6.00 H+
AL(ASO4)		5.00			-1229.379	-1426.833	-662.264	112.257	-15.130
	1.00	AL+3		1.00 ASOH4-		-4.00 H+	-2.00	E-	
AL2SO4.6		18.00			-4624.826	-5519.800	-3001.758	0.000	-2.280
	2.00	AL+3		3.00 SO4-2		6.00 H2O			
AL2SO43		18.00			-3102.440	-3804.820	-2355.794	0.000	-19.720
	2.00	AL+3		3.00 SO4-2					
ALABANDI		0.00			-217.780	-154.716	211.519	-167.946	34.030
	8.00	H+		1.00 MN+2		1.00 SO4-2	8.00	E-	-4.00 H2O
ALBITE-L		0.00			-3710.400	-4006.300	-992.452	0.000	-3.100
	-4.00	H2O		1.00 NA+		1.00 AL+3	3.00	H4SIO4	-4.00 H+
ALBITE		0.00			-3710.400	-4006.300	-992.452	0.000	-3.100
	-4.00	H2O		1.00 NA+		1.00 AL+3	3.00	H4SIO4	-4.00 H+
ALBITE-H		0.00			-3702.866	-4006.300	-1017.722	0.000	-4.420
	-4.00	H2O		1.00 NA+		1.00 AL+3	3.00	H4SIO4	-4.00 H+
ALSTONIT		8.00			-2267.261	-2426.128	-532.842	0.000	18.090
	1.00	BA+2		1.00 CA+2		2.00 CO3-2			
ALUNITE		12.00			-4664.026	-5401.000	-2471.824	0.000	-0.670
	1.00	K+		3.00 AL+3		6.00 H2O	2.00	SO4-2	-6.00 H+
AM		0.00			-0.341	0.022	1.215	616.722	-104.900
	1.00	AM+3		3.00 E-					
AM2CO33		18.00			-2996.574	-3215.410	-733.979	43.932	37.600
	2.00	AM+3		3.00 CO3-2					
AM2O3		6.00			-1614.521	-1692.155	-260.384	398.735	-51.700
	2.00	AM+3		3.00 H2O		-6.00 H+			
AMCL3(C)		3.00			-910.566	-977.358	-224.020	140.582	-14.400
	1.00	AM+3		3.00 CL-					
AMES-14		0.00			-4166.739	-4896.910	-2449.007	0.000	-38.630
	5.00	H2O		2.00 MG+2		2.00 AL+3	1.00	H4SIO4	-10.00 H+
AMF3(C)		3.00			-1529.906	-1622.750	-311.399	0.000	15.110
	1.00	AM+3		3.00 F-					
AMH2		-2.00			-143.038	-184.074	-137.636	432.626	-79.900
	1.00	AM+3		2.00 H+		5.00 E-			
AMO.SIO2		0.00			-848.923	-885.300	-122.008	0.000	2.710
	1.00	H4SIO4		-2.00 H2O					
AMO2		4.00			-879.882	-932.299	-175.808	256.061	-33.900
	1.00	AM+3		2.00 H2O		-1.00 E-	-4.00	H+	
AMOCL		3.00			-904.102	-953.295	-164.993	116.315	-11.100
	1.00	AM+3		1.00 H2O		-2.00 H+	1.00	CL-	
AMOH3(C)		3.00			-1210.632	-1272.103	-206.175	202.087	-17.500
	1.00	AM+3		3.00 H2O		-3.00 H+			
AMOHCO3(7.00			-1404.286	-1523.034	-398.283	54.810	7.030
	1.00	AM+3		1.00 H2O		-1.00 H+	1.00	CO3-2	

Table B.3: Selected aqueous species and minerals in HATCHES 3.0 data base. Page 25 of 50

	Charge	OPV	DH a	DH b	$\Delta_f G^\circ$	$\Delta_f H^\circ$	$\Delta_f S^\circ$	$\Delta_f H^\circ$	logK(25)
AMPO4(C)		3.00			-1755.879	-1901.100	-487.074	0.000	23.000
1.00 AM+3		1.00	PO4-3						
ANALC-DE		0.00			-2826.202	-3121.000	-988.757	0.000	-11.990
-2.00 H2O		1.00	NA+		1.00 AL+3	2.00	H4SiO4	-4.00 H+	
ANALCIME		0.00			-3090.226	-3406.830	-1061.894	0.000	-7.280
-1.00 H2O		1.00	NA+		1.00 AL+3	2.00	H4SiO4	-4.00 H+	
ANDALUSI		0.00			-2433.295	-2819.590	-1295.640	0.000	-16.570
1.00 H2O		2.00	AL+3		1.00 H4SiO4	-6.00	H+		
ANDRADIT		6.00			-5403.059	-6094.400	-2318.769	83.680	-58.930
-12.00 H+		2.00	FE+2		-2.00 E-	3.00	H4SiO4	3.00 CA+2	
ANHYDRIT		6.00			-1321.180	-1452.340	-439.914	0.000	4.270
1.00 CA+2		1.00	SO4-2						
ANNITE		6.00			-4764.105	-5428.720	-2229.130	0.000	-29.750
-10.00 H+		3.00	FE+2		3.00 H4SiO4	1.00	AL+3	1.00 K+	
ANORTHIT		0.00			-3996.821	-4533.720	-1800.768	0.000	-27.060
1.00 CA+2		2.00	AL+3		2.00 H4SiO4	-8.00	H+		
ANTARCTI		0.00			-2214.513	-2592.140	-1266.566	0.000	-4.130
1.00 CA+2		2.00	CL-		6.00 H2O				
ANTHOPHY		0.00			-11365.621-12638.040	-4267.714		0.000	-67.790
-8.00 H2O		7.00	MG+2		8.00 H4SiO4	-14.00	H+		
ANTIGORI		0.00			-33084.109-37548.385-14973.256			0.000	-241.990
5.50 H2O		24.00	MG+2		17.00 H4SiO4	-48.00	H+		
ARCANITE		6.00			-1318.666	-1413.620	-318.476	0.000	1.690
2.00 K+		1.00	SO4-2						
ARSENOLI		6.00			-576.367	-572.230	13.877	0.000	19.900
-5.00 H2O		2.00	ASOH4-		2.00 H+				
ARSENOCOPY		0.00			-37.584	-303.407	-891.573	-590.917	50.380
1.00 SO4-2		12.00	H+		11.00 E-	-8.00	H2O	1.00 FE+2	
1.00 ASOH4-									
ARTINITE		4.00			-2569.509	-3053.108	-1621.999	-14.644	-9.620
-2.00 H+		2.00	MG+2		1.00 CO3-2	5.00	H2O		
AS205(C)		10.00			-781.006	-919.377	-464.098	224.513	-27.340
-3.00 H2O		2.00	ASOH4-		-2.00 H+	-4.00	E-		
ASHCROFT		0.00			-10799.605-12188.860	-4659.584		0.000	-39.450
-16.00 H+		1.00	NA+		4.00 AL+3	5.00	H4SiO4	6.00 H2O	
1.00 K+		1.00	CA+2						
B2O3		0.00			-1258.802	-1288.110	-98.300	0.000	5.540
-3.00 H2O		2.00	H3BO3						
BA2Si3O8		0.00			-3952.314	-4292.560	-1141.192	0.000	-23.310
-4.00 H+		2.00	BA+2		3.00 H4SiO4	-4.00	H2O		
BA2SiO4		0.00			-2163.997	-2521.960	-1200.615	0.000	-44.580
-4.00 H+		2.00	BA+2		1.00 H4SiO4				
BA3ASO42		10.00			-3247.492	-3374.367	-425.539	224.513	-11.750
3.00 BA+2		2.00	ASOH4-		-8.00 H+	-4.00	E-		
BABR2.2H		0.00			-1224.554	-1346.980	-410.618	0.000	-2.240
1.00 BA+2		2.00	BR-		2.00 H2O				

Table B.3: Selected aqueous species and minerals in HATCHES 3.0 data base. Page 26 of 50

	Charge	OPV	DH a	DH b	$\Delta_f G^\circ$	$\Delta_f H^\circ$	$\Delta_f S^\circ$	$\Delta_f H^\circ$	logK(25)
BABR2(C)		0.00			-731.039	-775.320	-148.520	0.000	-5.610
1.00 BA+2		2.00	BR-						
BACL2.2H		0.00			-1290.710	-1438.320	-495.086	0.000	-0.240
1.00 BA+2		2.00	CL-		2.00 H2O				
BACL2.H2		0.00			-1050.031	-1152.490	-343.648	0.000	-0.860
1.00 BA+2		2.00	CL-		1.00 H2O				
BACL2(C)		0.00			-804.900	-866.660	-207.144	0.000	-2.260
1.00 BA+2		2.00	CL-						
BAF2(C)		0.00			-1151.278	-1203.200	-174.149	0.000	5.760
1.00 BA+2		2.00	F-						
BAHPO4(C)		0.00			-1692.903	-1831.670	-465.425	-14.770	19.630
1.00 BA+2		1.00	PO4-3		1.00 H+				
BAI2(C)		-2.00			-595.613	-646.060	-169.198	0.000	-11.070
1.00 BA+2		2.00	I-						
BAMNO4(C)		6.00			-1113.340	-1332.609	-735.430	563.961	-108.390
-8.00 H+		1.00	BA+2		4.00 H2O	-4.00 E-		1.00 MN+2	
BANO32(C)		10.00			-790.125	-946.200	-523.477	0.000	2.310
1.00 BA+2		2.00	NO3-						
BAO(C)		0.00			-519.662	-818.330	-1001.737	0.000	-47.800
-2.00 H+		1.00	BA+2		1.00 H2O				
BAOH2.10		0.00			-2786.973	-3390.800	-2025.244	0.000	-24.490
-2.00 H+		1.00	BA+2		10.00 H2O				
BARITE		6.00			-1356.325	-1468.116	-374.948	-26.276	9.980
1.00 BA+2		1.00	SO4-2						
BARYTOCA		8.00			-2266.348	-2426.128	-535.906	0.000	17.930
1.00 BA+2		1.00	CA+2		2.00 CO3-2				
BAS(C)		-2.00			-450.175	-466.466	-54.641	-167.946	17.410
1.00 BA+2		1.00	SO4-2		8.00 H+	8.00 E-		-4.00 H2O	
BASEO3(C)		4.00			-962.721	-1035.305	-243.447	-189.535	35.600
1.00 SEO4-2		2.00	H+		2.00 E-	-1.00 H2O		1.00 BA+2	
BASEO4(C)		6.00			-1039.469	-1141.223	-341.284	-9.623	7.500
1.00 SEO4-2		1.00	BA+2						
BASI2O5		0.00			-2405.356	-2588.930	-615.710	0.000	-9.470
-2.00 H+		1.00	BA+2		2.00 H4SiO4	-3.00 H2O			
BASIF6(C)		0.00			-2787.792	-2858.240	-236.284	0.000	32.260
-4.00 H2O		1.00	BA+2		1.00 H4SiO4	6.00 F-		4.00 H+	
BASIO3		0.00			-1534.857	-1703.630	-566.068	0.000	-15.960
-2.00 H+		1.00	BA+2		1.00 H4SiO4	-1.00 H2O			
BASSANIT		6.00			-1436.154	-1595.255	-533.628	0.000	3.640
1.00 CA+2		1.00	SO4-2		0.50 H2O				
BASSETIT		14.00			-4274.935	-4724.463	-1507.723	259.157	23.960
2.00 U+4		4.00	H2O		-8.00 H+	-4.00 E-		2.00 PO4-3	
1.00 FE+2									
BEID-NA		0.00			-5359.074	-5914.803	-1863.923	0.000	-6.380
-2.68 H2O		0.33	NA+		2.33 AL+3	3.67 H4SiO4		-7.32 H+	
BEID-CA		0.00			-5364.186	-5925.086	-1881.266	0.000	-6.320

Table B.3: Selected aqueous species and minerals in HATCHES 3.0 data base. Page 27 of 50

		Charge	OPV	DH a	DH b	$\Delta_f G^\circ$	$\Delta_f H^\circ$	$\Delta_f S^\circ$	$\Delta_f H^\circ$	logK(25)
-2.68	H2O		0.17	CA+2		2.33 AL+3	3.67	H4SiO4	-7.32	H+
BEID-MG			0.00			-5348.228	-5912.546	-1892.730	0.000	-6.300
-2.68	H2O		0.17	MG+2		2.33 AL+3	3.67	H4SiO4	-7.32	H+
BEID-K			0.00			-5367.743	-5918.697	-1847.910	0.000	-6.050
-2.68	H2O		0.33	K+		2.33 AL+3	3.67	H4SiO4	-7.32	H+
BERLINIT			0.00			-1626.760	-1837.570	-707.058	-14.770	19.230
1.00	AL+3		1.00	PO4-3						
BIRNESSI			28.00			-4789.611	-5504.886	-2399.045	1691.884	-269.950
-28.00	H+		8.00	MN+2		19.00 H2O	-12.00	E-		
BISCHOFI			0.00			-2114.766	-2516.140	-1346.215	0.000	-4.540
1.00	MG+2		2.00	CL-		6.00 H2O				
BIXBYITE			6.00			-880.855	-1017.009	-456.665	281.981	-50.240
-6.00	H+		2.00	MN+2		3.00 H2O	-2.00	E-		
BLOCKITE			-2.00			-106.221	-767.086	-2216.551	-1801.526	188.360
2.00	SEO4-2		16.00	H+		14.00 E-	-8.00	H2O	1.00	NI+2
BLOEDITE			12.00			-3428.703	-3909.680	-1613.205	0.000	2.250
2.00	NA+		1.00	MG+2		2.00 SO4-2	4.00	H2O		
BOEHMITE			0.00			-910.984	-1110.060	-667.704	0.000	-9.600
2.00	H2O		1.00	AL+3		-3.00 H+				
BOLT-NA			6.00			-2918.197	-3291.012	-1250.429	144.348	-23.840
-7.00	H+		1.00	U+4		4.00 H2O	-2.00	E-	0.70	NA+
0.30	K+		1.00	H4SiO4						
BOLT'ITE			6.00			-2693.622	-3013.442	-1072.682	144.348	-24.160
-7.00	H+		1.00	U+4		3.00 H2O	-2.00	E-	1.00	K+
1.00	H4SiO4									
BORAX			0.00			-5517.791	-6201.030	-2291.593	0.000	-12.090
-2.00	H+		2.00	NA+		4.00 H3BO3	5.00	H2O		
BORIC			0.00			-969.471	-1072.800	-346.566	0.000	0.030
1.00	H3BO3									
BREWS-SR			0.00			-8639.239	-9511.970	-2927.154	0.000	-7.460
-8.00	H+		1.00	SR+2		2.00 AL+3	6.00	H4SiO4	-3.00	H2O
BREWS-BA			0.00			-8637.048	-9493.570	-2872.790	0.000	-6.360
-8.00	H+		1.00	BA+2		2.00 AL+3	6.00	H4SiO4	-3.00	H2O
BREWS-CA			0.00			-8638.091	-9504.070	-2904.509	0.000	-5.730
-8.00	H+		1.00	CA+2		2.00 AL+3	6.00	H4SiO4	-3.00	H2O
BUNSENIT			0.00			-211.677	-339.830	-429.829	0.000	-12.450
1.00	NI+2		-2.00	H+		1.00 H2O				
BURKEITE			16.00			-3591.500	-3950.678	-1204.688	-14.644	0.680
6.00	NA+		1.00	CO3-2		2.00 SO4-2				
C'PTL-NA			0.00			-12732.165-13840.440	-3717.171		0.000	7.890
-8.00	H2O		2.00	NA+		2.00 AL+3	10.00	H4SiO4	-8.00	H+
C'PTL-MG			0.00			-12646.599-13826.760	-3958.280		0.000	4.900
-8.00	H2O		1.00	MG+2		2.00 AL+3	10.00	H4SiO4	-8.00	H+
C'PTL-K			0.00			-12813.355-13864.040	-3524.015		0.000	14.910
-8.00	H2O		2.00	K+		2.00 AL+3	10.00	H4SiO4	-8.00	H+
C'PTL-CA			0.00			-12768.093-13902.760	-3805.691		0.000	9.120

Table B.3: Selected aqueous species and minerals in HATCHES 3.0 data base. Page 28 of 50

		Charge	OPV	DH a	DH b	$\Delta_f G^\circ$	$\Delta_f H^\circ$	$\Delta_f S^\circ$	$\Delta_r H^\circ$	logK(25)
-8.00	H2O		1.00	CA+2	2.00	AL+3	10.00	H4SiO4	-8.00	H+
C4S3.1.5			0.00			-5645.648	-6399.965	-2529.991	0.000	-64.860
-8.00	H+		4.00	CA+2	3.00	H4SiO4	-0.50	H2O		
C5S6.3.5			0.00			-9414.521	-10456.355	-3494.328	0.000	-64.110
-10.00	H+		5.00	CA+2	6.00	H4SiO4	-3.50	H2O		
C5S6.3H			0.00			-9264.272	-10313.440	-3518.926	0.000	-69.660
-10.00	H+		5.00	CA+2	6.00	H4SiO4	-4.00	H2O		
C5S6.5.5			0.00			-9878.242	-11028.015	-3856.359	0.000	-65.960
-10.00	H+		5.00	CA+2	6.00	H4SiO4	-1.50	H2O		
C6S6.H2			0.00			-9449.285	-10570.610	-3760.942	0.000	-92.550
-12.00	H+		6.00	CA+2	6.00	H4SiO4	-5.00	H2O		
CA-AL			0.00			-3109.712	-3648.420	-1806.836	0.000	-36.460
2.00	H2O		1.00	CA+2	2.00	AL+3	1.00	H4SiO4	-8.00	H+
CA(IO3)2			10.00			-838.188	-1005.882	-562.449	1365.658	-217.400
1.00	CA+2		2.00	I-	6.00	H2O	-12.00	H+	-12.00	E-
CA2CL2(O			0.00			-1929.071	-2277.650	-1169.141	0.000	-26.350
2.00	CA+2		-2.00	H+	2.00	CL-	3.00	H2O		
CA2Si3O8			0.00			-4539.886	-5028.135	-1637.594	0.000	-23.340
-4.00	H+		2.00	CA+2	3.00	H4SiO4	-1.50	H2O		
CA2SiO4.			0.00			-2479.413	-2876.524	-1331.917	0.000	-36.910
-4.00	H+		2.00	CA+2	1.00	H4SiO4	1.17	H2O		
CA2SiO4(0.00			-2199.245	-2542.960	-1152.824	0.000	-37.510
-4.00	H+		2.00	CA+2	1.00	H4SiO4				
CA3ASO42			10.00			-3061.233	-3405.867	-1155.908	224.513	-43.040
3.00	CA+2		2.00	ASOH4-	-8.00	H+	-4.00	E-		
CA3Si2O7			0.00			-4404.384	-5114.580	-2382.010	0.000	-60.230
-6.00	H+		3.00	CA+2	2.00	H4SiO4	2.00	H2O		
CA3SiO5			0.00			-2780.854	-3371.790	-1982.009	0.000	-74.010
-6.00	H+		3.00	CA+2	1.00	H4SiO4	1.00	H2O		
CA4CL2(O			0.00			-6588.622	-7936.930	-4522.248	0.000	-68.450
4.00	CA+2		-6.00	H+	2.00	CL-	19.00	H2O		
CAACL2.2H			0.00			-1243.293	-1448.820	-689.341	0.000	-8.100
1.00	CA+2		2.00	CL-	2.00	H2O				
CAACL2.4H			0.00			-1735.895	-2020.480	-954.502	0.000	-4.890
1.00	CA+2		2.00	CL-	4.00	H2O				
CAACL2.H2			0.00			-1005.411	-1162.990	-528.523	0.000	-8.230
1.00	CA+2		2.00	CL-	1.00	H2O				
CAHPO4(C			0.00			-1687.040	-1821.542	-451.125	5.858	19.050
1.00	CA+2		1.00	PO4-3	1.00	H+				
CAI2(C)			-2.00			-528.390	-536.856	-28.395	119.704	-22.400
1.00	CA+2		2.00	I-						
CALCITE			4.00			-1129.072	-1207.519	-263.114	10.795	8.470
1.00	CO3-2		1.00	CA+2						
CALCIUM			0.00			-1735.838	-2020.480	-954.693	0.000	-4.900
1.00	CA+2		2.00	CL-	4.00	H2O				

Table B.3: Selected aqueous species and minerals in HATCHES 3.0 data base. Page 29 of 50

	Charge	OPV	DH a	DH b	$\Delta_f G^\circ$	$\Delta_f H^\circ$	$\Delta_f S^\circ$	$\Delta_f H^\circ$	logK(25)
CAO		0.00			-603.698	-635.278	-105.920	193.552	-32.630
1.00 CA+2		-2.00 H+		1.00 H2O					
CAOH2(C)		0.00			-896.890	-985.040	-295.657	129.620	-22.810
1.00 CA+2		-2.00 H+		2.00 H2O					
CARNALLI		0.00			-2528.896	-2935.360	-1363.288	0.000	-4.470
1.00 K+		1.00 MG+2		3.00 CL-	6.00 H2O				
CASEO3		4.00			-1428.741	-1623.741	-654.035	-195.811	34.600
1.00 SEO4-2		2.00 H+		2.00 E-	1.00 H2O	1.00 CA+2			
CASEO3.2		4.00			-1423.090	-1623.741	-672.988	-195.811	33.610
1.00 CA+2		1.00 SEO4-2		2.00 H+	2.00 E-	1.00 H2O			
CASEO4		6.00			-1011.744	-1142.100	-437.215	0.000	3.090
1.00 CA+2		1.00 SEO4-2							
CASEO4.H		6.00			-1486.652	-1706.647	-737.867	7.113	3.200
1.00 SEO4-2		2.00 H2O		1.00 CA+2					
CASI205.		0.00			-2874.229	-3171.090	-995.676	0.000	-9.970
-2.00 H+		1.00 CA+2		2.00 H4SIO4	1.00 H2O				
CASO4.HY		6.00			-1435.183	-1595.255	-536.883	0.000	3.470
1.00 CA+2		1.00 SO4-2		0.50 H2O					
CAU(PO4)		4.00			-3916.739	-4274.660	-1200.474	0.000	54.100
1.00 U+4		1.00 CA+2		2.00 H2O	2.00 PO4-3				
CAUL2SI3		12.00			-4974.497	-5328.341	-1186.799	454.299	-35.400
1.00 CA+2		2.00 H4SIO4		2.00 U+4	4.00 H2O	1.00 H+			
-4.00 E-									
CAUO4		6.00			-1893.096	-2001.460	-363.455	276.060	-24.200
1.00 U+4		4.00 H2O		2.00 H+	2.00 E-	1.00 CA+2			
CCHL-7A		0.00			-8195.418	-9497.660	-4367.740	0.000	-71.940
6.00 H2O		5.00 MG+2		2.00 AL+3	3.00 H4SIO4	1.00 H+			
CCHL-14A		0.00			-8214.654	-9497.660	-4303.224	0.000	-68.570
6.00 H2O		5.00 MG+2		2.00 AL+3	3.00 H4SIO4	1.00 H+			
CELESTIT		6.00			-1344.760	-1458.274	-380.726	1.966	6.470
1.00 SR+2		1.00 SO4-2							
CHABAZIT		0.00			-7163.228	-8019.300	-2871.279	0.000	-13.630
-8.00 H+		1.00 CA+2		2.00 AL+3	4.00 H4SIO4	2.00 H2O			
CHALCEDY		0.00			-853.547	-904.630	-171.334	-19.330	3.520
1.00 H4SIO4		-2.00 H2O							
CHAMOSIT		4.00			-3443.534	-4141.110	-2339.682	0.000	-33.410
-10.00 H+		2.00 FE+2		1.00 H4SIO4	2.00 AL+3	5.00 H2O			
CHLOROMA		0.00			-592.266	-801.160	-700.634	0.000	-22.000
1.00 MG+2		2.00 CL-							
CHRYSOTI		0.00			-4038.726	-4600.750	-1885.039	0.000	-31.550
1.00 H2O		3.00 MG+2		2.00 H4SIO4	6.00 H+				
CL'ZOISI		0.00			-6489.768	-7357.910	-2911.763	0.000	-43.920
1.00 H2O		2.00 CA+2		3.00 AL+3	3.00 H4SIO4	1.00 H+			
CLAUDETI		6.00			-577.109	-572.230	16.365	0.000	20.030
-5.00 H2O		2.00 ASOH4-		2.00 H+					
COFFINIT		4.00			-1884.856	-2048.160	-547.723	0.000	8.280

Table B.3: Selected aqueous species and minerals in HATCHES 3.0 data base. Page 30 of 50

	Charge	OPV	DH a	DH b	$\Delta_f G^\circ$	$\Delta_f H^\circ$	$\Delta_f S^\circ$	$\Delta_f H^\circ$	logK(25)
-4.00	H+		1.00	U+4		1.00	H4SiO4		
COLEMANI		0.00			-6324.014	-6951.140	-2103.389	0.000	-21.570
-2.00	H2O		-4.00	H+		2.00	CA+2	6.00	H3BO3
CORD-HYD		0.00			-8885.234	-10086.570	-4029.301	0.000	-51.350
-1.00	H2O		2.00	MG+2		4.00	AL+3	5.00	H4SiO4
CORD-ANH		0.00			-8633.938	-9800.740	-3913.472	0.000	-53.830
-2.00	H2O		2.00	MG+2		4.00	AL+3	5.00	H4SiO4
CORUNDUM		0.00			-1572.385	-1934.290	-1213.835	0.000	-21.380
3.00	H2O		2.00	AL+3		-6.00	H+		
CRIST		0.00			-853.147	-885.300	-107.841	0.000	3.450
1.00	H4SiO4		-2.00	H2O					
CRIST.BE		0.00			-850.636	-885.300	-116.264	0.000	3.010
1.00	H4SiO4		-2.00	H2O					
CRONSTED		10.00			-2568.104	-3158.830	-1981.304	83.680	-42.210
-10.00	H+		4.00	FE+2		-2.00	E-	1.00	H4SiO4
DACH-NA		0.00			-24801.538	-27002.660	-7382.598	0.000	-3.230
-20.00	H+		5.00	NA+		5.00	AL+3	19.00	H4SiO4
DACH-CA		0.00			-24900.576	-27158.460	-7572.980	0.000	1.460
-20.00	H+		2.50	CA+2		5.00	AL+3	19.00	H4SiO4
DACH-K		0.00			-24941.896	-27061.660	-7109.722	0.000	3.350
-20.00	H+		5.00	K+		5.00	AL+3	19.00	H4SiO4
DAPH-7A		10.00			-6403.103	-7608.160	-4041.780	0.000	-56.140
-16.00	H+		5.00	FE+2		3.00	H4SiO4	2.00	AL+3
DAPH-14A		10.00			-6422.339	-7608.160	-3977.264	0.000	-52.770
-16.00	H+		5.00	FE+2		3.00	H4SiO4	2.00	AL+3
DAWSONIT		4.00			-1787.899	-2040.358	-846.753	-14.644	5.650
-2.00	H+		1.00	NA+		1.00	AL+3	1.00	CO3-2
DIASPORE		0.00			-915.836	-1110.060	-651.431	0.000	-8.750
2.00	H2O		1.00	AL+3		-3.00	H+		
DIOPSIDE		0.00			-3029.702	-3352.260	-1081.864	0.000	-20.970
-2.00	H2O		1.00	CA+2		1.00	MG+2	2.00	H4SiO4
DOL-DIS		8.00			-2158.796	-2389.916	-775.179	-29.288	16.600
1.00	CA+2		1.00	MG+2		2.00	CO3-2		
DOLOMITE		8.00			-2161.194	-2325.943	-552.571	34.685	17.020
1.00	CA+2		1.00	MG+2		2.00	CO3-2		
EDINGTON		0.00			-5831.961	-6551.840	-2414.486	0.000	-18.200
-8.00	H+		1.00	BA+2		2.00	AL+3	3.00	H4SiO4
ENSTATIT		0.00			-1460.525	-1638.130	-595.689	0.000	-11.470
-1.00	H2O		1.00	MG+2		1.00	H4SiO4	-2.00	H+
EPID-ORD		3.00			-6063.640	-6866.770	-2693.711	41.840	-46.290
-13.00	H+		1.00	FE+2		-1.00	E-	3.00	H4SiO4
1.00	H2O		2.00	CA+2				2.00	AL+3
EPIDOTE		3.00			-6063.640	-6866.770	-2693.711	41.840	-46.290
-13.00	H+		1.00	FE+2		-1.00	E-	3.00	H4SiO4
1.00	H2O		2.00	CA+2				2.00	AL+3
EPISTILB		0.00			-8638.091	-9504.070	-2904.509	0.000	-5.730

Table B.3: Selected aqueous species and minerals in HATCHES 3.0 data base. Page 31 of 50

	Charge	OPV	DH a	DH b	$\Delta_f G^\circ$	$\Delta_f H^\circ$	$\Delta_f S^\circ$	$\Delta_f H^\circ$	logK(25)
-8.00	H+		1.00	CA+2	2.00 AL+3	6.00	H4SIO4	-3.00	H2O
EPSOMITE			6.00		-2869.654	-3377.150	-1702.149	0.000	1.800
1.00	MG+2		1.00	SO4-2	7.00 H2O				
ERION-NA			0.00		-39760.139	-43774.110	-13462.924	0.000	-34.250
-36.00	H+		9.00	NA+	9.00 AL+3	27.00	H4SIO4	-9.00	H2O
ERION-CA			0.00		-39938.395	-44054.550	-13805.650	0.000	-25.810
-36.00	H+		4.50	CA+2	9.00 AL+3	27.00	H4SIO4	-9.00	H2O
ERION-K			0.00		-40023.092	-43880.310	-12937.172	0.000	-20.600
-36.00	H+		9.00	K+	9.00 AL+3	27.00	H4SIO4	-9.00	H2O
EUCRYPTI			0.00		-2012.587	-2273.830	-876.214	0.000	-13.940
-4.00	H+		1.00	LI+	1.00 AL+3	1.00	H4SIO4		
FAUJ-NA			0.00		-7597.756	-8528.640	-3122.200	0.000	-15.530
-8.00	H+		2.00	NA+	2.00 AL+3	4.00	H4SIO4	4.00	H2O
FAUJ-CA			0.00		-7637.451	-8590.960	-3198.084	0.000	-13.640
-8.00	H+		1.00	CA+2	2.00 AL+3	4.00	H4SIO4	4.00	H2O
FAYALITE			4.00		-1356.799	-1635.160	-933.626	0.000	-19.050
-4.00	H+		2.00	FE+2	1.00 H4SIO4				
FE2SO43			24.00		-2236.429	-2822.540	-1965.827	83.680	-26.870
3.00	SO4-2		2.00	FE+2	-2.00 E-				
FE3PO42			6.00		-4390.299	-5122.740	-2456.620	0.000	36.000
3.00	FE+2		2.00	PO4-3	8.00 H2O				
FE3SE4			0.00		-219.697	-206.269	45.038	-2115.849	352.500
4.00	SEO4-2		-16.00	H2O	30.00 E-	32.00	H+	3.00	FE+2
FEF2(C)			2.00		-655.867	-759.800	-348.592	0.000	2.440
2.00	F-		1.00	FE+2					
FEF3(C)			3.00		-959.363	-1053.310	-315.101	41.840	6.290
3.00	F-		1.00	FE+2	-1.00 E-				
FEO(C)			2.00		-251.198	-374.930	-414.999	0.000	-11.360
-2.00	H+		1.00	FE+2	1.00 H2O				
FEOH2(S)			2.00		-475.495	-569.047	-313.773	91.713	-13.610
1.00	FE+2		2.00	H2O	-2.00 H+				
FEOH3A			3.00		-688.034	-904.750	-726.868	41.840	-17.920
1.00	FE+2		-1.00	E-	3.00 H2O	-3.00	H+		
FEPO4(S)			3.00		-1655.163	-1895.203	-805.098	49.957	13.400
1.00	FE+2		1.00	PO4-3	-1.00 E-	2.00	H2O		
FERR-MG			6.00		-1292.461	-1704.840	-1383.126	83.680	-47.180
-8.00	H+		2.00	FE+2	-2.00 E-	4.00	H2O	1.00	MG+2
FERR-2-C			6.00		-1976.157	-2609.670	-2124.813	83.680	-82.860
-10.00	H+		2.00	FE+2	-2.00 E-	5.00	H2O	2.00	CA+2
FERR-CA			6.00		-1387.357	-1780.840	-1319.750	83.680	-47.620
-8.00	H+		2.00	FE+2	-2.00 E-	4.00	H2O	1.00	CA+2
FERROSIL			2.00		-1107.142	-1260.230	-513.459	0.000	-7.420
-2.00	H+		1.00	FE+2	1.00 H4SIO4	-1.00	H2O		
FESE			0.00		-87.064	-64.951	74.166	-520.071	90.300
1.00	FE+2		1.00	SEO4-2	8.00 H+	8.00	E-	-4.00	H2O

Table B.3: Selected aqueous species and minerals in HATCHES 3.0 data base. Page 32 of 50

		Charge	OPV	DH a	DH b	$\Delta_r G^\circ$	$\Delta_r H^\circ$	$\Delta_r S^\circ$	$\Delta_r H^\circ$	logK(25)
FESE2			0.00			-96.369	-102.726	-21.319	-1102.066	180.800
2.00	SEO4-2		-8.00	H2O	14.00	E-	16.00	H+	1.00	FE+2
FESO4(C)			8.00			-807.831	-998.440	-639.305	0.000	-2.640
1.00	SO4-2		1.00	FE+2						
FLUORAPA			0.00			-6524.453	-6947.859	-1420.108	-44.309	70.500
5.00	CA+2		3.00	PO4-3	1.00	F-				
FLUORITE			0.00			-1178.406	-1233.407	-184.474	-19.707	10.960
1.00	CA+2		2.00	F-						
FORSTERI			0.00			-2057.857	-2390.960	-1117.231	0.000	-28.150
2.00	MG+2		1.00	H4SiO4	-4.00	H+				
GARRONIT			0.00			-18690.905	-20969.905	-7643.805	0.000	-49.700
6.00	AL+3		10.00	H4SiO4	5.50	H2O	2.50	CA+2	-24.00	H+
1.00	NA+									
GAYLUSSI			8.00			-3372.013	-3832.746	-1545.304	-29.288	9.420
1.00	CA+2		2.00	NA+	2.00	CO3-2	5.00	H2O		
GEHENIT			0.00			-3784.416	-4477.250	-2323.776	0.000	-56.650
3.00	H2O		2.00	CA+2	2.00	AL+3	1.00	H4SiO4	-10.00	H+
GIBBSITE			0.00			-1152.862	-1300.495	-495.164	95.395	-8.770
1.00	AL+3		3.00	H2O	-3.00	H+				
GISMONDI			0.00			-4977.003	-5677.040	-2347.936	0.000	-21.520
-8.00	H+		1.00	CA+2	2.00	AL+3	2.00	H4SiO4	4.00	H2O
GLASERIT			24.00			-5236.571	-5630.880	-1322.520	0.000	7.290
2.00	NA+		6.00	K+	4.00	SO4-2				
GLAUBERI			12.00			-2595.358	-2842.360	-828.447	0.000	5.370
2.00	NA+		1.00	CA+2	2.00	SO4-2				
GMEL-NA			0.00			-7123.590	-7956.980	-2795.202	0.000	-15.510
-8.00	H+		2.00	NA+	2.00	AL+3	4.00	H4SiO4	2.00	H2O
GMEL-CA			0.00			-7163.228	-8019.300	-2871.279	0.000	-13.630
-8.00	H+		1.00	CA+2	2.00	AL+3	4.00	H4SiO4	2.00	H2O
GOETHITE			3.00			-475.952	-558.336	-276.316	102.424	-13.530
1.00	FE+2		-1.00	E-	2.00	H2O	-3.00	H+		
GRAPHITE			0.00			-103.738	750.541	2865.265	711.280	29.550
-2.50	H2O		1.00	CO3-2	6.00	H+	4.00	E-		
GREENALI			6.00			-2960.368	-3467.050	-1699.418	0.000	-22.590
-6.00	H+		3.00	FE+2	2.00	H4SiO4	1.00	H2O		
GROSSULA			0.00			-6267.073	-7076.680	-2715.436	0.000	-52.130
3.00	CA+2		2.00	AL+3	3.00	H4SiO4	-12.00	H+		
GUMMITE			6.00			-1129.348	-1304.342	-586.933	144.348	-19.610
-6.00	H+		1.00	U+4	3.00	H2O	-2.00	E-		
GYPSUM			6.00			-1797.343	-2023.874	-759.789	0.126	4.600
1.00	CA+2		1.00	SO4-2	2.00	H2O				
H2-GAS			-2.00			0.000	0.004	0.014	0.004	0.000
2.00	H+		2.00	E-						
H2SNOH6			4.00			-1433.430	-1723.880	-974.173	0.000	-2.980
1.00	SN+2		6.00	H2O	-2.00	E-	-4.00	H+		
HAIWEEIT			12.00			-9393.639	-10178.464	-2632.317	288.696	-11.440

Table B.3: Selected aqueous species and minerals in HATCHES 3.0 data base. Page 33 of 50

Table B.3: Selected aqueous species and minerals in HATCHES 3.0 data base. Page 34 of 50

	Charge	OPV	DH a	DH b	$\Delta_f G^\circ$	$\Delta_f H^\circ$	$\Delta_f S^\circ$	$\Delta_f H^\circ$	logK(25)
K-SODIUM		4.00			-2495.162	-2897.418	-1349.174	-14.644	-0.010
1.00 K+		1.00 NA+		1.00 CO3-2	6.00	H2O			
K-FELD		0.00			-3748.198	-4018.100	-905.255	0.000	-0.080
-4.00 H2O		1.00 K+		1.00 AL+3	3.00	H4SIO4	-4.00	H+	
K-SEQUI		24.00			-6332.398	-7014.358	-2287.306	-87.864	33.880
8.00 K+		6.00 CO3-2		4.00 H+	3.00	H2O			
K-CARBON		4.00			-1430.669	-1622.983	-645.024	-14.644	-3.150
2.00 K+		1.00 CO3-2		1.50 H2O					
K(UO2)(A		11.00			-2009.974	-2159.085	-500.121	256.605	-17.680
1.00 U+4		2.00 H2O		-8.00 H+	-4.00	E-	1.00	ASOH4-	
1.00 K+									
K2CO3.3/		4.00			-1430.726	-1622.983	-644.833	-14.644	-3.140
2.00 K+		1.00 CO3-2		1.50 H2O					
K2SE		-2.00			-371.409	-1001.813	-2114.385	-1041.753	54.950
1.00 SEO4-2		8.00 H+		8.00 E-	-4.00	H2O	2.00	K+	
K8H4(CO3		24.00			-6332.455	-7014.358	-2287.114	-87.864	33.890
8.00 K+		6.00 CO3-2		4.00 H+	3.00	H2O			
KAINITE		6.00			-2325.121	-2653.050	-1099.880	0.000	0.100
1.00 K+		1.00 MG+2		1.00 CL-	1.00	SO4-2	3.00	H2O	
KALICINI		4.00			-867.508	-942.098	-250.176	-14.644	10.000
1.00 K+		1.00 CO3-2		1.00 H+					
KALSILIT		0.00			-2017.474	-2247.500	-771.511	0.000	-11.260
1.00 K+		1.00 AL+3		1.00 H4SIO4	-4.00	H+			
KALSO42		12.00			-2240.548	-2609.220	-1236.531	0.000	-3.760
1.00 K+		1.00 AL+3		2.00 SO4-2					
KALSO42.		12.00			-187.361	-6039.180-19627.098		0.000	-862.020
1.00 K+		1.00 AL+3		2.00 SO4-2	12.00	H2O			
KAOLINIT		0.00			-3783.782	-4113.500	-1105.877	163.050	-9.080
1.00 H2O		-6.00 H+		2.00 H4SIO4	2.00	AL+3			
KBR		0.00			-380.024	-373.550	21.715	0.000	-1.110
1.00 K+		1.00 BR-							
KIESERIT		6.00			-1437.168	-1662.170	-754.661	0.000	0.110
1.00 MG+2		1.00 SO4-2		1.00 H2O					
KMGCL3		0.00			-1009.135	-1220.380	-708.518	0.000	-21.450
1.00 K+		1.00 MG+2		3.00 CL-					
KMGCL3.2		0.00			-1525.083	-1792.040	-895.378	0.000	-14.150
1.00 K+		1.00 MG+2		2.00 H2O	3.00	CL-			
KNACO3.6		4.00			-2495.276	-2897.418	-1348.791	-14.644	0.010
1.00 K+		1.00 NA+		1.00 CO3-2	6.00	H2O			
KTCO4		7.00			-918.841	-1109.630	-639.911	0.000	-30.780
1.00 K+		1.00 TCO+2		-6.00 H+	3.00	H2O	-3.00	E-	
KYANITE		0.00			-2434.836	-2819.590	-1290.471	0.000	-16.300
1.00 H2O		2.00 AL+3		1.00 H4SIO4	-6.00	H+			
LAB.SALT		18.00			-4339.593	-4804.040	-1557.762	0.000	5.730
4.00 NA+		1.00 CA+2		3.00 SO4-2	2.00	H2O			
LANSFORD		4.00			-2199.842	-2586.108	-1295.544	-14.644	5.400

Table B.3: Selected aqueous species and minerals in HATCHES 3.0 data base. Page 35 of 50

	Charge	OPV	DH a	DH b	$\Delta_f G^\circ$	$\Delta_f H^\circ$	$\Delta_f S^\circ$	$\Delta_f H^\circ$	logK(25)
1.00	MG+2	1.00	CO3-2	5.00	H2O				
LARNITE		0.00		-2190.855	-2542.960	-1180.967	0.000	-38.980	
-4.00	H+	2.00	CA+2	1.00	H4SiO4				
LAUMONTI		0.00		-6685.980	-7447.640	-2554.620	0.000	-14.150	
1.00	CA+2	2.00	AL+3	4.00	H4SiO4	-8.00	H+		
LAWRENCI		2.00		-289.741	-423.260	-447.827	0.000	-9.040	
2.00	CL-	1.00	FE+2						
LAWSONIT		0.00		-4495.930	-5105.380	-2044.104	0.000	-22.710	
-8.00	H+	1.00	CA+2	2.00	AL+3	2.00	H4SiO4	2.00	H2O
LEONHARD		6.00		-2152.755	-2519.660	-1230.607	0.000	0.840	
1.00	MG+2	1.00	SO4-2	4.00	H2O				
LEONITE		12.00		-3478.898	-3933.280	-1524.003	0.000	3.840	
2.00	K+	1.00	MG+2	2.00	SO4-2	4.00	H2O		
LEVYNE		0.00		-7163.228	-8019.300	-2871.279	0.000	-13.630	
-8.00	H+	1.00	CA+2	2.00	AL+3	4.00	H4SiO4	2.00	H2O
LI(UO2)(11.00		-2001.263	-2185.415	-617.651	256.605	-21.030	
1.00	U+4	2.00	H2O	-8.00	H+	-4.00	E-	1.00	ASOH4-
1.00	LI+								
LI2SE		-2.00		-394.056	-1054.473	-2215.050	-1041.753	55.270	
1.00	SEO4-2	8.00	H+	8.00	E-	-4.00	H2O	2.00	LI+
MAGNESIU		0.00		-2552.852	-3101.890	-1841.481	0.000	-26.130	
2.00	MG+2	-3.00	H+	1.00	CL-	7.00	H2O		
MAGNETIT		8.00		-977.721	-1326.940	-1171.288	83.680	-36.360	
-8.00	H+	3.00	FE+2	4.00	H2O	-2.00	E-		
MANGANIT		3.00		-477.660	-651.420	-582.794	140.990	-39.370	
-3.00	H+	1.00	MN+2	2.00	H2O	-1.00	E-		
MANGANOS		2.00		-362.897	-506.580	-481.914	0.000	-17.930	
-2.00	H+	1.00	MN+2	1.00	H2O				
MARGARIT		0.00		-5842.135	-6753.840	-3057.875	0.000	-42.170	
4.00	H2O	1.00	CA+2	4.00	AL+3	2.00	H4SiO4	-14.00	H+
MAX.MICR		0.00		-3748.198	-4018.100	-905.255	0.000	-0.080	
-4.00	H2O	1.00	K+	1.00	AL+3	3.00	H4SiO4	-4.00	H+
MELANTER		8.00		-2496.351	-2999.250	-1686.733	0.000	2.360	
1.00	SO4-2	1.00	FE+2	7.00	H2O				
MERCALLI		6.00		-1034.387	-1161.480	-426.272	0.000	1.380	
1.00	K+	1.00	H+	1.00	SO4-2				
MERWINIT		0.00		-4339.726	-5009.920	-2247.840	0.000	-68.250	
3.00	CA+2	1.00	MG+2	2.00	H4SiO4	-8.00	H+		
MESOL-S		0.00		-16510.929	-18481.380	-6608.926	0.000	-54.570	
2.00	CA+2	6.00	AL+3	9.00	H4SiO4	2.00	H2O	2.00	NA+
-24.00	H+								
MESOLITE		0.00		-5517.417	-6149.585	-2120.302	0.000	-14.220	
-7.96	H+	0.68	NA+	0.66	CA+2	1.99	AL+3	3.01	H4SiO4
0.61	H2O								
MG2CL(OH		0.00		-2552.967	-3101.890	-1841.098	0.000	-26.110	
2.00	MG+2	-3.00	H+	1.00	CL-	7.00	H2O		

Table B.3: Selected aqueous species and minerals in HATCHES 3.0 data base. Page 36 of 50

	Charge	OPV	DH a	DH b	$\Delta_f G^\circ$	$\Delta_f H^\circ$	$\Delta_f S^\circ$	$\Delta_f H^\circ$	logK(25)
MG3ASO42		10.00			-2773.921	-3177.867	-1354.842	224.513	-42.180
3.00	MG+2	2.00	ASOH4-		-8.00 H+	-4.00 E-			
MGBR2.6H		0.00			-2055.973	-2424.800	-1237.050	0.000	-5.250
1.00	MG+2	2.00	BR-		6.00 H2O				
MGBR2(S)		0.00			-499.454	-709.820	-705.570	0.000	-28.670
1.00	MG+2	2.00	BR-						
MGCL2.2H		0.00			-1118.488	-1372.820	-853.034	0.000	-12.900
1.00	MG+2	2.00	CL-		2.00 H2O				
MGCL2.4H		0.00			-1623.762	-1944.480	-1075.694	0.000	-7.470
1.00	MG+2	2.00	CL-		4.00 H2O				
MGCL2.H2		0.00			-862.227	-1086.990	-753.860	0.000	-16.250
1.00	MG+2	2.00	CL-		1.00 H2O				
MGCO3(S)		4.00			-1025.900	-1163.234	-460.621	-20.920	7.460
1.00	MG+2	1.00	CO3-2						
MGF2(C)		0.00			-1065.131	-1137.700	-243.399	0.000	8.180
1.00	MG+2	2.00	F-						
MGHPO4(S)		0.00			-2296.030	-2608.890	-1049.339	0.000	18.170
1.00	MG+2	1.00	PO4-3		1.00 H+	3.00 H2O			
MGI2(S)		-2.00			-359.063	-367.343	-27.772	213.217	-35.000
1.00	MG+2	2.00	I-						
MGOH2(S)		0.00			-833.502	-924.730	-305.980	113.930	-16.850
1.00	MG+2	-2.00	H+		2.00 H2O				
MGOHCL		0.00			-732.148	-919.910	-629.756	0.000	-16.050
-1.00	H+	1.00	MG+2		1.00 CL-	1.00 H2O			
MGSEO3(S)		4.00			-863.218	-976.081	-378.545	-195.811	35.680
1.00	MG+2	1.00	SEO4-2		2.00 H+	2.00 E-		-1.00 H2O	
MGSO4(C)		6.00			-1170.746	-1376.340	-689.565	0.000	-5.020
1.00	MG+2	1.00	SO4-2						
MGUO4		6.00			-1747.742	-1856.382	-364.379	345.138	-32.600
1.00	U+4	4.00	H2O		-8.00 H+	-2.00 E-		1.00 MG+2	
MHSH(MG1		6.00			-1520.081	-1778.920	-868.150	0.000	-5.310
-0.50	H+	1.00	SO4-2		1.25 MG+2	1.00 H2O			
MHSM(MG1		6.00			-1611.899	-1895.670	-951.774	0.000	-9.170
-1.00	H+	1.50	MG+2		1.00 SO4-2	1.00 H2O			
MILLERIT		-2.00			-79.060	12.034	305.531	-167.946	41.700
1.00	NI+2	1.00	SO4-2		8.00 H+	8.00 E-		-4.00 H2O	
MINNESOT		6.00			-4439.740	-4951.820	-1717.524	0.000	-13.900
-6.00	H+	3.00	FE+2		4.00 H4SiO4	-4.00 H2O			
MIRABILI		6.00			-3645.407	-4248.320	-2022.179	0.000	1.070
2.00	NA+	1.00	SO4-2		10.00 H2O				
MISENITE		42.00			-7528.470	-8382.500	-2864.432	0.000	10.580
8.00	K+	6.00	H+		7.00 SO4-2				
MN(OH)3(-3.00	H+	3.00			-566.052	-937.250	-1245.004	140.990	-65.430
MN3(PO4)		6.00			3.00 H2O	-1.00 E-			
3.00	MN+2	2.00	PO4-3		-2871.770	-3260.589	-1304.105	-29.539	23.910

Table B.3: Selected aqueous species and minerals in HATCHES 3.0 data base. Page 37 of 50

	Charge	OPV	DH a	DH b	$\Delta_f G^\circ$	$\Delta_f H^\circ$	$\Delta_f S^\circ$	$\Delta_f H^\circ$	logK(25)
MN3ASO42		16.00			-2143.620	-2439.117	-991.100	224.513	-33.140
3.00 MN+2		2.00	ASOH4-		-8.00 H+	-4.00 E-			
MNCL2.2		2.00			-942.045	-1126.570	-618.898	0.000	-3.990
1.00 MN+2		2.00	CL-		2.00 H2O				
MNCL2.4		2.00			-1423.574	-1698.230	-921.199	0.000	-2.720
1.00 MN+2		2.00	CL-		4.00 H2O				
MNCL2.H2		2.00			-696.115	-840.740	-485.074	0.000	-5.530
1.00 MN+2		2.00	CL-		1.00 H2O				
MNHPO4(C)		2.00			-1398.007	-1519.920	-408.897	-14.770	25.300
1.00 MN+2		1.00	PO4-3		1.00 H+				
MNOH2(S)		2.00			-615.620	-792.410	-592.957	0.000	-15.200
1.00 MN+2		2.00	H2O		-2.00 H+				
MNOH3(S)		3.00			-757.780	-1078.240	-1074.827	0.000	-31.840
1.00 MN+2		3.00	H2O		-3.00 H+	-1.00 E-			
MNSE		0.00			-106.295	-718.283	-2052.619	-1041.753	67.530
1.00 SEO4-2		8.00	H+		8.00 E-	-4.00 H2O		1.00 MN+2	
MNSEO3		6.00			-639.286	-729.831	-303.691	-195.811	36.270
1.00 MN+2		1.00	SEO4-2		2.00 H+	2.00 E-		-1.00 H2O	
MNSEO3.2		6.00			-1108.200	-1301.491	-648.301	-195.811	35.330
1.00 MN+2		1.00	SEO4-2		2.00 H+	2.00 E-		1.00 H2O	
MNSO4(C)		8.00			-956.860	-1130.090	-581.017	0.000	-2.670
1.00 MN+2		1.00	SO4-2						
MOLYSITE		3.00			-321.243	-548.500	-762.222	41.840	-26.510
3.00 CL-		1.00	FE+2		-1.00 E-				
MONOHYDR		4.00			-1361.360	-1518.788	-528.015	-14.644	7.620
1.00 CA+2		1.00	CO3-2		1.00 H2O				
MONT-NA		0.00			-5322.444	-5817.070	-1658.983	0.000	-3.060
-6.00 H+		0.33	NA+		4.00 H4SiO4	1.67 AL+3		-4.00 H2O	
0.33 MG+2									
MONT-MG		0.00			-5311.598	-5814.813	-1687.790	0.000	-2.980
-6.00 H+		0.49	MG+2		4.00 H4SiO4	1.67 AL+3		-4.00 H2O	
MONT-K		0.00			-5331.170	-5820.964	-1642.778	0.000	-2.720
-6.00 H+		0.33	K+		4.00 H4SiO4	1.67 AL+3		-4.00 H2O	
0.33 MG+2									
MONT-CA		0.00			-5327.214	-5827.353	-1677.475	0.000	-3.060
-6.00 H+		0.17	CA+2		4.00 H4SiO4	1.67 AL+3		-4.00 H2O	
0.33 MG+2									
MONTICEL		0.00			-2146.132	-2466.960	-1076.063	0.000	-29.750
1.00 CA+2		1.00	MG+2		1.00 H4SiO4	-4.00 H+			
MORD-K		0.00			-6169.509	-6646.190	-1598.796	0.000	7.450
-5.00 H2O		1.00	K+		1.00 AL+3	5.00 H4SiO4		-4.00 H+	
MORD-NA		0.00			-6128.914	-6634.390	-1695.374	0.000	3.940
-5.00 H2O		1.00	NA+		1.00 AL+3	5.00 H4SiO4		-4.00 H+	
MUSCOVIT		0.00			-5597.108	-6238.220	-2150.301	0.000	-14.560
1.00 K+		3.00	AL+3		3.00 H4SiO4	-10.00 H+			
NA2CO3		4.00			-1047.995	-1170.638	-411.348	-14.644	-0.670
2.00 NA+		1.00	CO3-2						

Table B.3: Selected aqueous species and minerals in HATCHES 3.0 data base. Page 38 of 50

		Charge	OPV	DH a	DH b	$\Delta_f G^\circ$	$\Delta_f H^\circ$	$\Delta_f S^\circ$	$\Delta_f H^\circ$	logK(25)
NA2SE		-2.00				-327.435	-978.213	-2182.719	-1041.753	54.450
1.00	SEO4-2	8.00	H+		8.00	E-	-4.00	H2O	2.00	NA+
NA2SE2		-2.00				-370.817	-1193.766	-2760.183	-1801.526	150.920
2.00	SEO4-2	16.00	H+		14.00	E-	-8.00	H2O	2.00	NA+
NA2SEO4		6.00				-962.346	-1080.198	-395.279	-0.418	-0.500
2.00	NA+	1.00	SEO4-2							
NA2SI2O5		0.00				-2324.294	-2537.110	-713.787	0.000	-18.160
-2.00	H+	2.00	NA+		2.00	H4SiO4	-3.00	H2O		
NA2U2O7		12.00				-2995.877	-3194.613	-666.563	469.277	-43.400
2.00	U+4	7.00	H2O		-14.00	H+	-4.00	E-	2.00	NA+
NA2UO4		6.00				-1769.666	-1889.183	-400.862	326.017	-40.760
1.00	U+4	4.00	H2O		-8.00	H+	-2.00	E-	2.00	NA+
NA3H(SO4		12.00				-2278.359	-2539.700	-876.541	0.000	0.790
1.00	H+	3.00	NA+		2.00	SO4-2				
NA3UO4		5.00				-1897.252	-2022.078	-418.668	433.462	-64.300
1.00	U+4	4.00	H2O		-8.00	H+	-1.00	E-	3.00	NA+
NA4SiO4		0.00				-1975.674	-2418.320	-1484.642	0.000	-66.550
-4.00	H+	4.00	NA+		1.00	H4SiO4				
NA6Si2O7		0.00				-3369.365	-4070.130	-2350.378	0.000	-101.730
-6.00	H+	6.00	NA+		2.00	H4SiO4	-1.00	H2O		
NABR		0.00				-349.076	-361.750	-42.509	0.000	-2.930
1.00	NA+	1.00	BR-							
NABR.2H2		0.00				-828.036	-933.410	-353.425	0.000	-2.110
1.00	NA+	1.00	BR-		2.00	H2O				
NAFeO2(C		3.00				-627.283	-859.260	-778.055	41.840	-32.910
-4.00	H+	1.00	FE+2		-1.00	E-	2.00	H2O	1.00	NA+
NAHCOLIT		4.00				-849.402	-930.298	-271.325	-14.644	10.430
1.00	CO3-2	1.00	H+		1.00	NA+				
NANPO2CO		9.00				-2600.578	-2902.829	-1013.754	140.990	0.620
1.00	NP+4	-4.00	H+		5.50	H2O	-1.00	E-	1.00	CO3-2
1.00	NA+									
NATCO4(S		7.00				-876.705	-1097.830	-741.658	0.000	-34.560
1.00	NA+	1.00	TCO+2		-6.00	H+	3.00	H2O	-3.00	E-
NATROLIT		0.00				-5320.913	-5928.360	-2037.388	0.000	-19.130
-8.00	H+	2.00	NA+		2.00	AL+3	3.00	H4SiO4		
NATRON		4.00				-3427.557	-4028.938	-2017.042	-14.644	0.760
2.00	NA+	1.00	CO3-2		10.00	H2O				
NAUO3		5.00				-1411.047	-1494.139	-278.692	194.891	-16.150
1.00	U+4	3.00	H2O		-6.00	H+	-1.00	E-	1.00	NA+
NEPHELIN		0.00				-1980.532	-2235.700	-855.837	0.000	-14.130
1.00	NA+	1.00	AL+3		1.00	H4SiO4	-4.00	H+		
NESQUEHO		4.00				-1724.363	-2014.448	-972.950	-14.644	5.190
1.00	MG+2	1.00	CO3-2		3.00	H2O				
NH4HSE		-5.00				-23.531	-629.531	-2032.535	-1824.391	198.220
1.00	NO3-	19.00	H+		16.00	E-	-7.00	H2O	1.00	SEO4-2
NI2P2O7		0.00				-2096.611	-2420.509	-1086.358	-29.539	33.560

Table B.3: Selected aqueous species and minerals in HATCHES 3.0 data base. Page 39 of 50

	Charge	OPV	DH a	DH b	$\Delta_f G^\circ$	$\Delta_f H^\circ$	$\Delta_f S^\circ$	$\Delta_f H^\circ$	logK(25)
2.00	NI+2	2.00	PO4-3	2.00	H+	-1.00	H2O		
NI2SiO4		0.00			-1317.084	-1564.960	-831.381	0.000	-14.340
2.00	NI+2	-4.00	H+	1.00	H4SiO4				
NI3PO4.2		0.00			-2366.451	-2760.339	-1321.105	-29.539	31.300
3.00	NI+2	2.00	PO4-3						
NI3S2		-6.00			-196.413	-311.912	-387.385	-617.872	82.120
16.00	H+	-8.00	H2O	18.00	E-	3.00	NI+2	2.00	SO4-2
NI3S4		-6.00			-310.537	384.118	2329.883	-389.802	173.790
3.00	NI+2	32.00	H+	-16.00	H2O	4.00	SO4-2	30.00	E-
NI3SE4		-6.00			-249.309	-1870.152	-5436.334	-3885.032	375.190
4.00	SEO4-2	32.00	H+	30.00	E-	-16.00	H2O	3.00	NI+2
NICl2.2H		0.00			-759.831	-959.820	-670.767	0.000	-3.940
1.00	NI+2	2.00	CL-	2.00	H2O				
NICl2.4H		0.00			-1234.567	-1531.480	-995.849	0.000	-3.860
1.00	NI+2	2.00	CL-	4.00	H2O				
NICl2.6H		0.00			-1712.729	-2103.140	-1309.445	0.000	-3.180
1.00	NI+2	2.00	CL-	6.00	H2O				
NICl2(S)		0.00			-258.952	-305.149	-154.947	83.011	-8.600
1.00	NI+2	2.00	CL-						
NiCO3(S)		4.00			-612.732	-729.314	-391.017	0.000	6.870
1.00	NI+2	1.00	CO3-2						
NiF2.4H2		0.00			-1580.488	-1901.492	-1076.652	-33.472	4.080
1.00	NI+2	2.00	F-	4.00	H2O				
NiF2(S)		0.00			-603.788	-724.700	-405.540	0.000	-0.850
1.00	NI+2	2.00	F-						
NiFe2O4		6.00			-947.731	-1291.840	-1154.147	83.680	-35.780
1.00	NI+2	-8.00	H+	4.00	H2O	2.00	FE+2	-2.00	E-
NINGYOIT		4.00			-3917.081	-4304.199	-1298.400	-29.539	54.160
1.00	CA+2	2.00	PO4-3	2.00	H2O	1.00	U+4		
NIO		0.00			-211.677	-339.830	-429.829	0.000	-12.450
1.00	NI+2	-2.00	H+	1.00	H2O				
NiOH2(S)		0.00			-458.235	-529.721	-239.766	95.939	-10.800
1.00	NI+2	2.00	H2O	-2.00	H+				
NIS		-2.00			-79.060	12.034	305.531	-167.946	41.700
1.00	NI+2	1.00	SO4-2	8.00	H+	8.00	E-	-4.00	H2O
NIS2		-2.00			-125.248	360.049	1627.695	-53.911	85.630
1.00	NI+2	-8.00	H2O	2.00	SO4-2	16.00	H+	14.00	E-
NISE2		-2.00			-106.564	-767.086	-2215.402	-1801.526	188.420
2.00	SEO4-2	16.00	H+	14.00	E-	-8.00	H2O	1.00	NI+2
NISEO3.2		4.00			-913.143	-1134.741	-743.244	-195.811	33.130
1.00	NI+2	1.00	SEO4-2	2.00	H+	2.00	E-	1.00	H2O
NISO4.6H		6.00			-2223.799	-2678.320	-1524.472	0.000	1.990
1.00	NI+2	1.00	SO4-2	6.00	H2O				
NISO4.7H		6.00			-2460.939	-2964.150	-1687.779	0.000	1.990
1.00	NI+2	1.00	SO4-2	7.00	H2O				

Table B.3: Selected aqueous species and minerals in HATCHES 3.0 data base. Page 40 of 50

	Charge	OPV	DH a	DH b	$\Delta_r G^\circ$	$\Delta_r H^\circ$	$\Delta_r S^\circ$	$\Delta_r H^\circ$	logK(25)
NISO4(S)		6.00			-759.177	-963.340	-684.767	0.000	-5.330
1.00	NI+2		1.00	SO4-2					
NITER		5.00			-393.814	-458.990	-218.602	0.000	0.090
1.00	K+		1.00	NO3-					
NITROBAR		10.00			-790.125	-946.200	-523.477	0.000	2.310
1.00	BA+2		2.00	NO3-					
NONT-NA		6.00			-4487.012	-4932.523	-1494.250	83.680	-14.590
-7.32	H+		2.00	FE+2	-2.00	E-	3.67	H4SiO4	
-2.68	H2O		0.33	NA+				0.33	AL+3
NONT-MG		6.00			-4476.167	-4930.266	-1523.056	83.680	-14.510
-7.32	H+		2.00	FE+2	-2.00	E-	3.67	H4SiO4	
-2.68	H2O		0.17	MG+2				0.33	AL+3
NONT-CA		6.00			-4492.125	-4942.806	-1511.592	83.680	-14.530
-7.32	H+		2.00	FE+2	-2.00	E-	3.67	H4SiO4	
-2.68	H2O		0.17	CA+2				0.33	AL+3
NONT-K		6.00			-4495.681	-4936.417	-1478.236	83.680	-14.260
-7.32	H+		2.00	FE+2	-2.00	E-	3.67	H4SiO4	
-2.68	H2O		0.33	K+				0.33	AL+3
NP(HPO4)		4.00			-2871.425	-3154.439	-949.234	-29.539	55.630
1.00	NP+4		2.00	PO4-3	2.00	H+			
NP(S)		0.00			-0.433	-1120.061	-3755.252	-563.961	-88.030
1.00	NP+4		4.00	E-					
NP2O5		10.00			-2012.500	-2259.369	-828.004	281.981	-31.360
2.00	NP+4		-10.00	H+	5.00	H2O	-2.00	E-	
NPO2		4.00			-992.477	-1127.760	-453.741	0.000	2.680
1.00	NP+4		-4.00	H+	2.00	H2O			
NPO2OH(S)		5.00			-1124.135	-1413.590	-970.837	0.000	-15.800
1.00	NP+4		3.00	H2O	-5.00	H+	-1.00	E-	
NPO2OH2(6.00			-1239.697	-1699.420	-1541.920	0.000	-37.100
1.00	NP+4		-6.00	H+	-2.00	E-	4.00	H2O	
NPOH3(S)		3.00			-1103.073	-1384.679	-944.510	28.911	-19.490
1.00	NP+4		1.00	E-	3.00	H2O	-3.00	H+	
NPOH4(S)		4.00			-1447.236	-1699.420	-845.829	0.000	-0.740
1.00	NP+4		-4.00	H+	4.00	H2O			
O2-GAS		4.00			0.161	-0.000	-0.541	571.660	-83.120
2.00	H2O		-4.00	H+	-4.00	E-			
ORPIMENT		0.00			-167.557	483.363	2183.197	-503.837	180.430
-20.00	H2O		2.00	ASO4-2	3.00	SO4-2	32.00	H+	
OXYCH-CA		0.00			-5706.636	-7936.930	-7480.442	0.000	-222.970
4.00	CA+2		2.00	CL-	19.00	H2O	-6.00	H+	
OXYCH-MG		0.00			-0.905	-3101.890	-10400.756	0.000	-473.220
2.00	MG+2		1.00	CL-	7.00	H2O	-3.00	H+	
PARAGONI		0.00			-5554.173	-6226.420	-2254.728	0.000	-18.480
1.00	NA+		3.00	AL+3	3.00	H4SiO4	-10.00	H+	
PARGASIT		0.00			-11920.790	-13551.300	-5468.758	0.000	-103.240
1.00	NA+		2.00	CA+2	4.00	MG+2	3.00	AL+3	
-22.00	H+							6.00	H4SiO4

Table B.3: Selected aqueous species and minerals in HATCHES 3.0 data base. Page 41 of 50

	Charge	OPV	DH a	DH b	$\Delta_f G^\circ$	$\Delta_f H^\circ$	$\Delta_f S^\circ$	$\Delta_f H^\circ$	logK(25)
PCO2		4.00			-394.377	-392.789	5.327	-3.305	18.150
1.00 CO3-2		2.00 H+		-1.00 H2O					
PD-OXYAN		9.00			-4713.133	-5303.200	-1979.094	125.520	-38.680
-13.00 H+		3.00 FE+2		-3.00 E-		3.00 H4SiO4	1.00 AL+3		
1.00 K+									
PENTAHYD		6.00			-2392.064	-2805.490	-1386.639	0.000	1.220
1.00 MG+2		1.00 SO4-2		5.00 H2O					
PETALITE		0.00			-9224.881	-9859.460	-2128.388	0.000	6.980
-8.00 H+		8.00 H4SiO4		2.00 Li+		2.00 AL+3	-12.00 H2O		
PHENGITE		0.00			-5466.355	-5942.060	-1595.522	0.000	-7.960
-4.00 H2O		1.00 K+		1.00 MG+2		1.00 AL+3	4.00 H4SiO4		
-6.00 H+									
PHILL-K		0.00			-9205.701-10228.080	-3429.076	0.000	-22.650	
-12.00 H+		3.00 K+		3.00 AL+3		5.00 H4SiO4	2.00 H2O		
PHILL-NA		0.00			-9118.050-10192.680	-3604.327	0.000	-27.200	
-12.00 H+		3.00 NA+		3.00 AL+3		5.00 H4SiO4	2.00 H2O		
PHILL-CA		0.00			-9177.507-10286.160	-3718.441	0.000	-24.380	
-12.00 H+		1.50 CA+2		3.00 AL+3		5.00 H4SiO4	2.00 H2O		
PHLOGOPI		0.00			-5845.259 -6562.420	-2405.370	0.000	-38.220	
1.00 K+		3.00 MG+2		1.00 AL+3		3.00 H4SiO4	-10.00 H+		
PICOMERI		12.00			-3955.005	-4504.940	-1844.491	0.000	4.160
2.00 K+		1.00 MG+2		2.00 SO4-2		6.00 H2O			
PIRSSONI		8.00			-2659.680	-2875.256	-1058.446	-29.288	9.260
2.00 NA+		1.00 CA+2		2.00 CO3-2		2.00 H2O			
POLYHALI		24.00			-5655.996	-6266.300	-2046.968	0.000	13.960
2.00 K+		1.00 MG+2		2.00 CA+2		4.00 SO4-2	2.00 H2O		
PREHNITE		0.00			-5821.860	-6533.680	-2387.456	0.000	-33.280
2.00 CA+2		2.00 AL+3		3.00 H4SiO4		-10.00 H+			
PSD		0.00			-1543.377	-1714.130	-572.708	0.000	-14.020
-2.00 H+		1.00 CA+2		1.00 H4SiO4		-1.00 H2O			
PU(OH)2C		8.00			-1626.497	-1783.374	-526.169	0.000	25.000
1.00 PU+4		2.00 H2O		-2.00 H+		1.00 CO3-2			
PU2O3		6.00			-1594.709	-1656.238	-206.368	274.052	-14.000
2.00 PU+4		2.00 E-		-6.00 H+		3.00 H2O			
PUCL3(S)		3.00			-1037.365	-1093.287	-187.566	-55.647	28.400
1.00 PU+4		1.00 E-		3.00 CL-					
PUF3(C)		3.00			-1483.356	-1598.097	-384.845	-55.647	27.540
1.00 PU+4		1.00 E-		3.00 F-					
PUF4(S)		4.00			-1683.024	-1846.002	-546.628	31.798	13.200
1.00 PU+4		4.00 F-							
PUHPO42C		4.00			-2831.802	-3085.368	-850.463	19.832	52.420
1.00 PU+4		2.00 PO4-3		2.00 H+					
PUK4(SO4)		28.00			-4690.382	-5182.320	-1649.967	0.000	18.000
1.00 PU+4		4.00 K+		4.00 SO4-2					
PUO2		4.00			-998.119	-1056.178	-194.734	51.882	7.400
1.00 PU+4		2.00 H2O		-4.00 H+					

Table B.3: Selected aqueous species and minerals in HATCHES 3.0 data base. Page 42 of 50

	Charge	OPV	DH a	DH b	$\Delta_f G^\circ$	$\Delta_f H^\circ$	$\Delta_f S^\circ$	$\Delta_f H^\circ$	logK(25)
PUO2CO3(10.00			-1363.362	-1497.439	-449.697	285.935	-21.100
1.00 PU+4		-4.00	H+		-2.00	E-	2.00	H2O	1.00 CO3-2
PUO2HP4(6.00			-1924.013	-2103.304	-601.346	289.156	-10.050
1.00 PU+4		-3.00	H+		-2.00	E-	2.00	H2O	1.00 PO4-3
PUO2OH(S		5.00			-1058.313	-1158.163	-334.899	235.727	-23.600
1.00 PU+4		3.00	H2O		-5.00	H+	-1.00	E-	
PUO2OH2(6.00			-1205.839	-1356.841	-506.461	322.879	-39.300
1.00 PU+4		-6.00	H+		-2.00	E-	4.00	H2O	
PUOH3(S)		3.00			-1164.480	-1296.821	-443.873	97.069	-5.000
1.00 PU+4		1.00	E-		-3.00	H+	3.00	H2O	
PUOH4(S)		4.00			-1427.877	-1615.286	-628.575	64.434	-0.400
1.00 PU+4		4.00	H2O		-4.00	H+			
PYRITE		0.00			-159.404	-4.311	520.186	-383.171	85.780
16.00 H+		14.00	E-		1.00 FE+2		2.00 SO4-2		-8.00 H2O
PYROLUSI		4.00			-464.817	-510.429	-152.985	281.981	-41.620
-4.00 H+		1.00	MN+2		2.00 H2O		-2.00 E-		
PYROPHYL		0.00			-5259.330	-5761.320	-1683.684	0.000	-1.060
-4.00 H2O		2.00	AL+3		4.00 H4SiO4		-6.00 H+		
PYRRHOTI		0.00			-82.191	-1.468	270.746	-157.486	38.142
8.00 H+		0.88	FE+2		1.00 SO4-2		7.75 E-		-4.00 H2O
QUARTZ		0.00			-856.344	-911.324	-184.406	-26.024	4.010
1.00 H4SiO4		-2.00	H2O						
RANKINIT		0.00			-3740.111	-4257.090	-1733.956	0.000	-51.970
-6.00 H+		3.00	CA+2		2.00 H4SiO4		-1.00 H2O		
REALGAR		0.00			-70.160	67.674	462.296	-308.936	69.910
-8.00 H2O		12.00	H+		9.00 E-		1.00 ASOH4-		1.00 SO4-2
RHODOCHR		6.00			-815.438	-887.361	-241.231	8.703	10.410
1.00 MN+2		1.00	CO3-2						
RHODONIT		2.00			-1243.157	-1391.880	-498.819	0.000	-9.730
-2.00 H+		1.00	MN+2		-1.00 H2O		1.00 H4SiO4		
RIPID-14		4.00			-7499.326	-8741.860	-4167.479	0.000	-61.970
-16.00 H+		2.00	FE+2		3.00 H4SiO4		2.00 AL+3		6.00 H2O
3.00 MG+2									
RIPID-7A		4.00			-7480.090	-8741.860	-4231.996	0.000	-65.340
-16.00 H+		2.00	FE+2		3.00 H4SiO4		2.00 AL+3		6.00 H2O
3.00 MG+2									
S(C)		0.00			0.674	348.015	1164.989	114.035	35.720
-4.00 H2O		1.00	SO4-2		8.00 H+		6.00 E-		
SALEEITE		12.00			-4660.340	-5102.363	-1482.553	259.157	25.520
2.00 U+4		4.00	H2O		-8.00 H+		-4.00 E-		2.00 PO4-3
1.00 MG+2									
SANID-HI		0.00			-3741.349	-4018.100	-928.228	0.000	-1.280
-4.00 H2O		1.00	K+		1.00 AL+3		3.00 H4SiO4		-4.00 H+
SAPON-MG		0.00			-5614.416	-6236.746	-2087.303	0.000	-26.800
-2.68 H2O		3.17	MG+2		0.33 AL+3		3.67 H4SiO4		-7.32 H+
SAPON-NA		0.00			-5625.262	-6239.003	-2058.497	0.000	-26.880

Table B.3: Selected aqueous species and minerals in HATCHES 3.0 data base. Page 43 of 50

	Charge	OPV	DH a	DH b	$\Delta_f G^\circ$	$\Delta_f H^\circ$	$\Delta_f S^\circ$	$\Delta_r H^\circ$	logK(25)
-2.68 H2O -7.32 H+		0.33 NA+		3.00 MG+2	0.33 AL+3	3.67	H4SiO4		
SAPON-K -2.68 H2O -7.32 H+		0.00 K+		-5633.931 3.00 MG+2	-6242.897 0.33 AL+3	-2042.483	0.000 3.67	-26.550 H4SiO4	
SAPON-H -2.68 H2O		0.00 3.00 MG+2		-5544.698 0.33 AL+3	-6159.691 3.67	-2062.696 H4SiO4	0.000 -6.99	-25.850 H+	
SAPON-CA -2.68 H2O -7.32 H+		0.00 0.17 CA+2		-5630.374 3.00 MG+2	-6249.286 0.33 AL+3	-2075.839	0.000 3.67	-26.820 H4SiO4	
SCACCHIT 1.00 MN+2		2.00 2.00 CL-		-440.482	-554.910	-383.795	0.000	-8.770	
SCHOEPIT -6.00 H+		6.00 5.00 H2O		-1633.594 1.00 U+4	-1876.002 -2.00 E-	-813.039	144.348	-14.360	
SCOLOCIT -8.00 H+		0.00 1.00 CA+2		-5601.972 2.00 AL+3	-6276.510 3.00	-2262.413 H4SiO4	0.000 1.00	-16.500 H2O	
SCORODIT 2.00 H2O		8.00 1.00 FE+2		-1241.971 -3.00 E-	-1507.353 1.00	-890.095 ASOH4-	154.097 -4.00	-23.730 H+	
SE 1.00 SEO4-2		0.00 -4.00 H2O		-0.173 6.00 E-	-0.118 8.00 H+	0.183	-544.338	88.900	
SE205 2.00 SEO4-2		10.00 -3.00 H2O		-282.484 2.00 E-	-413.512 6.00 H+	-439.468	-72.802	19.500	
SECL4(S) 1.00 SEO4-2		4.00 8.00 H+		-100.841 2.00 E-	-319.911 -4.00	-734.764 H2O	-195.811 4.00	14.580 CL-	
SEO2 1.00 SEO4-2		4.00 -2.00 H2O		-170.792 2.00 E-	-224.925 4.00 H+	-181.561	-197.485	35.700	
SEO3 1.00 SEO4-2		6.00 -1.00 H2O		-94.568 2.00 H+	-170.177	-253.594	143.093	-19.200	
SEPIOLIT 2.00 MG+2		0.00 3.00 H4SiO4		-4624.565 -0.50 H2O	-5049.625 -4.00 H+	-1425.656	112.340	-15.920	
SEQUIPO 3.00 K+		12.00 2.00 SO4-2		1.686 1.00 H+	-2575.100	-8642.584	0.000	-409.470	
SEQUISO 3.00 NA+		12.00 2.00 SO4-2		1.150 1.00 H+	-2539.700	-8522.053	0.000	-398.570	
SIDERITE 1.00 FE+2		6.00 1.00 CO3-2		-667.037	-742.113	-251.806	22.301	10.550	
SILL 1.00 H2O		0.00 2.00 AL+3		-2431.240 1.00 H4SiO4	-2819.590 -6.00 H+	-1302.532	0.000	-16.930	
SISE2 2.00 SEO4-2		-4.00 -12.00 H2O		-141.479 16.00 E-	-134.383 20.00 H+	23.798	-909.183 1.00	139.600 H4SiO4	
SKLODOWS -14.00 H+ 2.00 H4SiO4		12.00 2.00 U+4		-5825.089 10.00 H2O	-7132.924 -4.00 E-	-4386.499	288.696 1.00	-118.590 MG+2	
SMECT-LO -7.00 H+ 1.25 AL+3 MG+2		1.06 0.45 FE+2 0.15 NA+		-5281.294 3.75 H4SiO4	-5830.150 -0.16 E-	-1840.872	6.694 -3.00	-13.645 H2O	
				0.02 CA+2	0.20 K+	0.90			

Table B.3: Selected aqueous species and minerals in HATCHES 3.0 data base. Page 44 of 50

	Charge	OPV	DH a	DH b	$\Delta_f G^\circ$	$\Delta_f H^\circ$	$\Delta_f S^\circ$	$\Delta_f H^\circ$	logK(25)
SMECT-HI		1.60			-5275.179	-5879.789	-2027.873	8.368	-20.576
-8.00 H+		0.70	FE+2		3.50 H4SIO4	-0.20 E-		-2.00 H2O	
1.25 AL+3		0.10	NA+		0.03 CA+2	0.20 K+		1.15	
MG+2									
SN(G)		0.00			4.250	-8.900	-44.106	0.000	-5.580
1.00 SN+2		2.00	E-						
SN(SO4)2		16.00			-1394.535	-1788.250	-1320.527	39.330	-21.210
1.00 SN+2		-2.00	E-		2.00 SO4-2				
SN(W)		0.00			-0.373	-8.900	-28.599	0.000	-4.770
1.00 SN+2		2.00	E-						
SN2S3		0.00			-251.643	462.283	2394.521	-221.857	141.930
2.00 SN+2		24.00	H+		-12.00 H2O	3.00 SO4-2	22.00 E-		
SN3S4		0.00			-356.482	519.418	2937.783	-389.802	191.300
3.00 SN+2		4.00	SO4-2		32.00 H+	30.00 E-	-16.00 H2O		
SNBR2(S)		2.00			-243.519	-251.720	-27.505	0.000	1.440
1.00 SN+2		2.00	BR-						
SNBR4		4.00			-350.075	-455.210	-352.625	39.330	-16.280
1.00 SN+2		-2.00	E-		4.00 BR-				
SNCL2(S)		2.00			-288.213	-343.060	-183.956	0.000	-0.320
1.00 SN+2		2.00	CL-						
SNO		2.00			-257.320	268.102	1762.272	562.832	-1.300
1.00 SN+2		1.00	H2O		-2.00 H+				
SNO2		4.00			-520.202	-580.811	-203.282	-0.251	3.210
1.00 SN+2		2.00	H2O		-2.00 E-	-4.00 H+			
SNOH2(S)		2.00			-491.377	-580.560	-299.120	0.000	-1.840
1.00 SN+2		-2.00	H+		2.00 H2O				
SNOH4(S)		4.00			-952.073	-1152.220	-671.298	0.000	-4.220
1.00 SN+2		4.00	H2O		-2.00 E-	-4.00 H+			
SNS		0.00			-97.704	57.134	519.331	-167.946	48.120
1.00 SN+2		1.00	SO4-2		8.00 H+	8.00 E-	-4.00 H2O		
SNSE		0.00			-87.363	-592.603	-1694.581	-1127.923	99.340
1.00 SN+2		-4.00	H2O		8.00 H+	8.00 E-	1.00 SEO4-2		
SNSE2		0.00			-121.042	-894.325	-2593.604	-1973.865	194.110
1.00 SN+2		-8.00	H2O		16.00 H+	14.00 E-	2.00 SEO4-2		
SNSO4(S)		8.00			-908.190	-918.240	-33.707	0.000	23.930
1.00 SN+2		1.00	SO4-2						
SODDYITE		12.00			-3682.758	-4065.644	-1284.206	288.696	-18.840
-12.00 H+		2.00	U+4		6.00 H2O	-4.00 E-		1.00 H4SIO4	
SPINEL		0.00			-2167.833	-2687.120	-1741.696	0.000	-38.390
4.00 H2O		1.00	MG+2		2.00 AL+3	-8.00 H+			
SPODUMEN		0.00			-2883.828	-3159.130	-923.367	0.000	-7.320
-4.00 H+		1.00	LI+		1.00 AL+3	2.00 H4SIO4		-2.00 H2O	
SR-AUTUN		12.00			-4772.879	-5186.263	-1386.495	259.157	26.240
2.00 U+4		4.00	H2O		-8.00 H+	-4.00 E-		2.00 PO4-3	
1.00 SR+2									
SR2SIO4(0.00			-2199.887	-2558.760	-1203.667	0.000	-41.260
-4.00 H+		2.00	SR+2		1.00 H4SIO4				

Table B.3: Selected aqueous species and minerals in HATCHES 3.0 data base. Page 45 of 50

		Charge	OPV	DH a	DH b	$\Delta_f G^\circ$	$\Delta_f H^\circ$	$\Delta_f S^\circ$	$\Delta_f H^\circ$	logK(25)
SR3ASO42				10.00		-3091.847	-3429.567	-1132.716	224.513	-43.470
3.00	SR+2			2.00	ASOH4-	-8.00	H+	-4.00	E-	
SR3PO42				0.00		-3901.164	-4152.046	-841.462	69.454	27.800
3.00	SR+2			2.00	PO4-3					
SRBR2.6				0.00		-2178.160	-2508.700	-1108.638	0.000	-2.840
1.00	SR+2			2.00	BR-	6.00	H2O			
SRBR2.H2				0.00		-958.326	-1079.550	-406.586	0.000	-8.820
1.00	SR+2			2.00	BR-	1.00	H2O			
SRBR2(C)				0.00		-701.094	-793.720	-310.668	0.000	-12.340
1.00	SR+2			2.00	BR-					
SRCL2.2				0.00		-1286.109	-1456.720	-572.232	0.000	-2.530
1.00	SR+2			2.00	CL-	2.00	H2O			
SRCL2.6				0.00		-2245.172	-2600.040	-1190.235	0.000	-0.690
1.00	SR+2			2.00	CL-	6.00	H2O			
SRCL2.H2				0.00		-1040.578	-1170.890	-437.067	0.000	-4.000
1.00	SR+2			2.00	CL-	1.00	H2O			
SRCL2(C)				0.00		-785.401	-885.060	-334.257	0.000	-7.160
1.00	SR+2			2.00	CL-					
SRCO3(S)				4.00		-1143.291	-1223.369	-268.581	2.845	9.030
1.00	SR+2			1.00	CO3-2					
SRF2(C)				0.00		-1175.616	-1221.600	-154.233	0.000	8.540
1.00	SR+2			2.00	F-					
SRHPO4(S)				0.00		-1699.547	-1833.794	-450.267	1.506	19.310
1.00	SR+2			1.00	PO4-3	1.00	H+			
SRI2(C)				-2.00		-562.701	-664.460	-341.301	0.000	-18.320
1.00	SR+2			2.00	I-					
SRNO32.H				10.00		-1733.799	-2107.920	-1254.809	0.000	-0.030
1.00	SR+2			2.00	NO3-	4.00	H2O			
SRNO32(S)				10.00		-783.469	-964.600	-607.515	0.000	-0.340
1.00	SR+2			2.00	NO3-					
SRNO32A				10.00		-782.042	-987.026	-687.519	-22.426	-0.590
1.00	SR+2			2.00	NO3-					
SRO(C)				0.00		-566.261	-836.730	-907.158	0.000	-41.120
-2.00	H+			1.00	SR+2	1.00	H2O			
SROH2(S)				0.00		-898.951	-964.154	-218.690	158.406	-24.380
1.00	SR+2			2.00	H2O	-2.00	H+			
SRS(C)				-2.00		-452.480	-484.866	-108.622	-167.946	16.330
8.00	H+			1.00	SR+2	1.00	SO4-2	8.00	E-	
SRSE				-2.00		-397.503	-1048.433	-2183.230	-1041.753	59.730
1.00	SR+2			-4.00	H2O	8.00	H+	8.00	E-	
SRSEO3(S)				4.00		-968.338	-1059.981	-307.374	-195.811	35.100
1.00	SR+2			1.00	SEO4-2	2.00	H+	2.00	E-	
SRSEO4(S)				6.00		-1030.245	-1150.000	-401.661	0.000	4.400
1.00	SR+2			1.00	SEO4-2					
SRSIO3(C)				0.00		-1554.115	-1722.030	-563.190	0.000	-14.070
-2.00	H+			1.00	SR+2	1.00	H4SiO4	-1.00	H2O	

Table B.3: Selected aqueous species and minerals in HATCHES 3.0 data base. Page 46 of 50

	Charge	OPV	DH a	DH b	$\Delta_f G^\circ$	$\Delta_f H^\circ$	$\Delta_f S^\circ$	$\Delta_f H^\circ$	logK(25)
STILB-NA		0.00			-9928.677	-10898.710	-3253.507	0.000	-3.670
-8.00	H+	2.00	NA+		2.00 AL+3	7.00	H4SIO4	-3.00	H2O
STILB-K		0.00			-9987.149	-10922.310	-3136.545	0.000	-0.630
-8.00	H+	2.00	K+		2.00 AL+3	7.00	H4SIO4	-3.00	H2O
STILB-CA		0.00			-9968.315	-10961.030	-3329.583	0.000	-1.790
-8.00	H+	1.00	CA+2		2.00 AL+3	7.00	H4SIO4	-3.00	H2O
STRENGIT		3.00			-1655.334	-1918.090	-881.286	27.070	13.430
1.00	FE+2	-1.00	E-		1.00 PO4-3	2.00	H2O		
STRONTIT		4.00			-1144.547	-1223.327	-264.229	2.887	9.250
1.00	SR+2	1.00	CO3-2						
SULFUR-R		0.00			0.674	348.015	1164.989	114.035	35.720
-4.00	H2O	1.00	SO4-2		8.00 H+	6.00	E-		
SYLVITE		0.00			-408.250	-419.220	-36.792	0.000	-0.960
1.00	K+	1.00	CL-						
SYNGENIT		12.00			-2885.491	-3151.790	-893.172	0.000	7.450
2.00	K+	1.00	CA+2		2.00 SO4-2	1.00	H2O		
TACHYHYD		0.00			-4996.890	-5909.440	-3060.708	0.000	-17.470
2.00	MG+2	1.00	CA+2		6.00 CL-	12.00	H2O		
TALC		0.00			-5525.518	-6085.520	-1878.257	0.000	-21.560
-4.00	H2O	3.00	MG+2		4.00 H4SIO4	-6.00	H+		
TC(C)		0.00			-0.792	-701.102	-2348.852	-986.932	24.060
2.00	H+	-1.00	H2O		4.00 E-	1.00	TCO+2		
TC207		14.00			-935.405	-1402.372	-1566.218	26.778	-79.100
2.00	TCO+2	-10.00	H+		5.00 H2O	-6.00	E-		
TC2S7		0.00			2051.927	1033.900	-3414.479	-1175.620	-60.780
-30.00	H2O	60.00	H+		2.00 TCO+2	50.00	E-	7.00	SO4-2
TC304		8.00			-864.291	-426.820	1467.283	-140.990	57.000
3.00	TCO+2	-2.00	H+		1.00 H2O	4.00	E-		
TC4O7		14.00			-1323.871	-857.490	1564.249	0.000	36.800
4.00	TCO+2	-6.00	H+		3.00 H2O	2.00	E-		
TCO2AM		4.00			-835.993	-857.490	-72.101	0.000	4.200
1.00	TCO+2	-2.00	H+		3.00 H2O				
TCO3		6.00			-460.151	-571.660	-374.003	0.000	-20.100
1.00	TCO+2	-4.00	H+		2.00 H2O	-2.00	E-		
TCOH(S)		2.00			-234.964	-281.981	-157.694	-281.981	23.540
2.00	E-	1.00	TCO+2						
TCOH2(S)		2.00			-461.202	-426.820	115.317	-140.990	21.630
1.00	TCO+2	1.00	H2O		2.00 E-				
TCOH3(S)		3.00			-658.558	-571.660	291.457	0.000	14.660
1.00	TCO+2	-1.00	H+		2.00 H2O	1.00	E-		
TCS2		0.00			-215.147	417.898	2123.244	-335.892	133.290
-9.00	H2O	1.00	TCO+2		2.00 SO4-2	18.00	H+	16.00	E-
TCS3		0.00			1103.539	483.933	-2078.171	-503.837	-61.900
1.00	TCO+2	26.00	H+		-13.00 H2O	22.00	E-	3.00	SO4-2
TEFHITOIT		4.00			-1632.254	-1898.460	-892.861	0.000	-23.070
-4.00	H+	2.00	MN+2		1.00 H4SIO4				

Table B.3: Selected aqueous species and minerals in HATCHES 3.0 data base. Page 47 of 50

		Charge	OPV	DH a	DH b	$\Delta_f G^\circ$	$\Delta_f H^\circ$	$\Delta_f S^\circ$	$\Delta_f H^\circ$	logK(25)
TH2S3			-8.00			-1076.007	-1621.878	-1830.859	-785.818	49.000
2.00	TH+4		24.00	H+		-12.00	H2O	26.00	E-	3.00 SO4-2
TH2SE3			-8.00			-932.253	-3312.580	-7983.657	-3407.240	182.910
2.00	TH+4		24.00	H+		3.00	SEO4-2	26.00	E-	-12.00 H2O
TH7S12			-28.00			-4116.451	-5154.550	-3481.802	-2579.310	286.650
7.00	TH+4		96.00	H+		-48.00	H2O	100.00	E-	12.00 SO4-2
THBR4(C)			0.00			-926.502	-1254.640	-1100.579	0.000	-33.970
1.00	TH+4		4.00	BR-						
THCL4(C)			0.00			-1094.603	-1186.698	-308.891	250.622	-23.700
1.00	TH+4		4.00	CL-						
THENARDI			6.00			-1269.270	-1390.020	-404.998	0.000	0.240
2.00	NA+		1.00	SO4-2						
THERMONA			4.00			-1285.192	-1456.468	-574.463	-14.644	-0.660
2.00	NA+		1.00	CO3-2		1.00	H2O			
THF4.2.5			0.00			-2606.583	-2824.975	-732.490	0.000	32.000
1.00	TH+4		4.00	F-		2.50	H2O			
THF4(S)			0.00			-2003.459	-2097.848	-316.583	12.552	30.200
1.00	TH+4		4.00	F-						
THHPO42(0.00			-3050.522	-3347.423	-995.812	-9.623	51.600
1.00	TH+4		2.00	PO4-3		2.00	H+			
THI4(S)			-4.00			-654.396	-998.120	-1146.147	0.000	-45.110
1.00	TH+4		4.00	I-						
THNO34(S)			20.00			-2322.501	-3025.550	-2358.037	0.000	-1.990
1.00	TH+4		4.00	NO3-		5.00	H2O			
THO2			0.00			-1143.035	-1340.660	-662.838	0.000	-6.350
1.00	TH+4		-4.00	H+		2.00	H2O			
THO2(C)			0.00			-1169.006	-1226.437	-192.625	114.223	-1.800
1.00	TH+4		2.00	H2O		-4.00	H+			
THOCL2(S)			0.00			-1156.063	-1232.090	-254.996	156.900	-8.500
1.00	TH+4		1.00	H2O		2.00	CL-	-2.00	H+	
THOH4(A)			0.00			-1599.906	-1912.320	-1047.843	0.000	-9.400
1.00	TH+4		4.00	H2O		-4.00	H+			
THOH4(C)			0.00			-1589.061	-1912.320	-1084.217	0.000	-11.300
1.00	TH+4		4.00	H2O		-4.00	H+			
THORIANI			0.00			-1168.720	-1340.660	-576.688	0.000	-1.850
-4.00	H+		1.00	TH+4		2.00	H2O			
THS2			-4.00			-619.176	-636.932	-59.553	-335.892	56.640
1.00	TH+4		16.00	H+		2.00	SO4-2	16.00	E-	-8.00 H2O
THSO42(S)			12.00			-2308.870	-2542.911	-784.976	44.769	20.300
1.00	TH+4		2.00	SO4-2						
TODOROKI			24.00			-3862.158	-4422.797	-1880.391	1409.903	-226.290
-24.00	H+		7.00	MN+2		15.00	H2O	-10.00	E-	
TREMOLIT			0.00			-11595.367	-12790.040	-4006.951	0.000	-61.670
-8.00	H2O		2.00	CA+2		5.00	MG+2	8.00	H4SiO4	-14.00 H+
TREVORIT			6.00			-947.674	-1291.840	-1154.338	83.680	-35.790
1.00	NI+2		-8.00	H+		4.00	H2O	2.00	FE+2	-2.00 E-

Table B.3: Selected aqueous species and minerals in HATCHES 3.0 data base. Page 48 of 50

	Charge	OPV	DH a	DH b	$\Delta_f G^\circ$	$\Delta_f H^\circ$	$\Delta_f S^\circ$	$\Delta_f H^\circ$	logK(25)
TRIDYMIT		0.00			-855.316	-885.300	-100.566	0.000	3.830
	1.00	H4SiO4	-2.00	H2O					
TROILITE		0.00			-87.873	-23.066	217.364	-167.946	37.410
	8.00	H+	1.00	FE+2		1.00	SO4-2	8.00	E-
								-4.00	H2O
U-ALPH		0.00			0.633	-1155.161	-3876.553	-563.961	-92.940
	4.00	E-	1.00	U+4					
U(SO4)2(16.00			-2082.702	-2409.880	-1097.361	0.000	11.360
	1.00	U+4	2.00	SO4-2					
U3O8		16.00			-3366.663	-3574.394	-696.734	485.846	-21.030
	3.00	U+4	8.00	H2O	-16.00	H+	-4.00	E-	
U3SE4		0.00			-988.087	-4327.694	-11201.097	-4730.974	250.100
	4.00	SEO4-2	32.00	H+		36.00	E-	-16.00	H2O
								3.00	U+4
U4O9		18.00			-4273.107	-4509.833	-793.982	427.437	3.400
	4.00	U+4	9.00	H2O	-18.00	H+	-2.00	E-	
UCL4(S)		4.00			-928.595	-1259.520	-1109.927	0.000	-22.100
	1.00	U+4	4.00	CL-					
UF4.2.5		4.00			-2406.100	-2647.175	-808.570	0.000	27.560
	1.00	U+4	4.00	F-		2.50	H2O		
UF4(C)		4.00			-1790.304	-1932.600	-477.263	0.000	23.540
	1.00	U+4	4.00	F-					
UHPO42(S)		4.00			-3823.428	-4332.859	-1708.639	-29.539	51.510
	1.00	U+4	2.00	PO4-3		2.00	H+	4.00	H2O
ULCO3(S)		10.00			-1561.740	-1672.446	-371.309	165.728	5.200
	1.00	U+4	2.00	H2O	-4.00	H+	-2.00	E-	
UO2		4.00			-1030.396	-1084.745	-182.285	78.115	4.600
	1.00	U+4	2.00	H2O	-4.00	H+			
UO2(AM)		4.00			-981.308	-1162.860	-608.927	0.000	-4.000
	1.00	U+4	2.00	H2O	-4.00	H+			
UO22HPO4		12.00			-4226.516	-4592.854	-1228.704	301.666	29.300
	2.00	U+4	4.00	H2O	-6.00	H+	-4.00	E-	
								2.00	PO4-3
UO23PO42		18.00			-5186.134	-5564.630	-1269.483	492.750	21.500
	3.00	U+4	6.00	H2O	-12.00	H+	-6.00	E-	
								2.00	PO4-3
UO2CL2(S)		6.00			-1144.431	-1352.672	-698.444	144.348	-21.400
	1.00	U+4	2.00	H2O	-4.00	H+	-2.00	E-	
								2.00	CL-
UO2F2(C)		6.00			-1571.918	-1689.212	-393.407	144.348	0.830
	1.00	U+4	2.00	H2O	-4.00	H+	-2.00	E-	
								2.00	F-
UO2HPO4(6.00			-2111.260	-2447.260	-1126.949	0.000	14.300
	1.00	U+4	-3.00	H+	-2.00	E-	2.00	H2O	
								1.00	PO4-3
UO2NO3.6		16.00			-2583.262	-3147.192	-1891.432	144.348	-11.440
	1.00	U+4	8.00	H2O	-4.00	H+	-2.00	E-	
								2.00	NO3-
UO2NO3.H		16.00			-1863.337	-2289.702	-1430.036	144.348	-12.930
	1.00	U+4	5.00	H2O	-4.00	H+	-2.00	E-	
								2.00	NO3-
UO2NO32.		16.00			-1618.605	-2003.872	-1292.191	144.348	-14.260
	1.00	U+4	4.00	H2O	-4.00	H+	-2.00	E-	
								2.00	NO3-
UO2NO32(16.00			-1119.153	-1432.212	-1050.004	144.348	-18.670
	1.00	U+4	2.00	H2O	-4.00	H+	-2.00	E-	
								2.00	NO3-

Table B.3: Selected aqueous species and minerals in HATCHES 3.0 data base. Page 49 of 50

	Charge	OPV	DH a	DH b	$\Delta_f G^\circ$	$\Delta_f H^\circ$	$\Delta_f S^\circ$	$\Delta_f H^\circ$	logK(25)
UO2OH(S)		5.00			-1176.210	-1318.149	-476.067	130.541	-11.400
1.00 U+4		3.00	H2O		-5.00 H+	-1.00 E-			
UO2OH2(S)		6.00			-1393.372	-1533.270	-469.218	201.250	-14.900
1.00 U+4		4.00	H2O		-6.00 H+	-2.00 E-			
UO2SO4.		12.00			-1966.786	-2213.682	-828.092	144.348	-3.240
1.00 U+4		3.00	H2O		-4.00 H+	-2.00 E-		1.00 SO4-2	
UO2SO4(C)		12.00			-1724.167	-1927.852	-683.164	144.348	-4.200
1.00 U+4		2.00	H2O		-4.00 H+	-2.00 E-		1.00 SO4-2	
UO2SO425		12.00			-2297.382	-2642.427	-1157.288	144.348	-7.640
1.00 U+4		4.50	H2O		-4.00 H+	-2.00 E-		1.00 SO4-2	
UO2SO430		12.00			-2449.971	-2785.342	-1124.841	144.348	-1.680
1.00 U+4		5.00	H2O		-4.00 H+	-2.00 E-		1.00 SO4-2	
UO2SO435		12.00			-2534.579	-2928.257	-1320.404	144.348	-7.630
1.00 U+4		5.50	H2O		-4.00 H+	-2.00 E-		1.00 SO4-2	
UO3		6.00			-1144.816	-1223.800	-264.912	224.890	-16.900
1.00 U+4		3.00	H2O		-6.00 H+	-2.00 E-			
UO32H2O		6.00			-1631.083	-1826.463	-655.309	193.887	-14.800
1.00 U+4		5.00	H2O		-6.00 H+	-2.00 E-			
UOF2.H2O		4.00			-1667.468	-1833.560	-557.076	0.000	17.570
-2.00 H+		1.00	U+4		2.00 F-	2.00 H2O			
URANINIT		4.00			-1030.568	-1162.860	-443.711	0.000	4.630
-4.00 H+		2.00	H2O		1.00 U+4				
URANOCIR		12.00			-4763.154	-5167.863	-1357.402	259.157	26.020
2.00 U+4		4.00	H2O		-8.00 H+	-4.00 E-		2.00 PO4-3	
1.00 BA+2									
URANOPHA		12.00			-4972.385	-5493.944	-1749.317	288.696	-35.770
-14.00 H+		2.00	U+4		4.00 H2O	-4.00 E-		1.00 CA+2	
2.00 H4SiO4									
USE2		0.00			-426.664	-1586.266	-3889.325	-2083.506	159.660
2.00 SEO4-2		16.00	H+		16.00 E-	-8.00 H2O		1.00 U+4	
USIO4(S)		4.00			-1881.546	-1990.295	-364.747	57.865	7.700
1.00 U+4		1.00	H4SiO4		-4.00 H+				
VIVIANIT		6.00			-4390.641	-5152.279	-2554.546	-29.539	36.060
3.00 FE+2		2.00	PO4-3		8.00 H2O				
WAIRAKIT		0.00			-6186.528	-6875.980	-2312.432	0.000	-18.560
-2.00 H2O		1.00	CA+2		2.00 AL+3	4.00 H4SiO4		-8.00 H+	
WEEKSITE		12.00			-9040.341	-9853.914	-2728.738	288.696	-33.930
-14.00 H+		2.00	U+4		-1.00 H2O	-4.00 E-		2.00 K+	
6.00 H4SiO4									
WHITLOCK		0.00			-3906.909	-4227.339	-1074.729	-29.539	34.600
3.00 CA+2		2.00	PO4-3						
WITHERIT		4.00			-1159.480	-1207.814	-162.115	0.000	13.350
1.00 BA+2		1.00	CO3-2						
WOLLAST		0.00			-1545.660	-1714.130	-565.050	0.000	-13.620
-1.00 H2O		1.00	CA+2		1.00 H4SiO4	-2.00 H+			
WUSTITE		2.00			-233.311	-365.773	-444.280	4.435	-13.761
-2.00 H+		0.95	FE+2		1.00 H2O	-0.11 E-			

Table B.3: Selected aqueous species and minerals in HATCHES 3.0 data base. Page 50 of 50

	Charge	OPV	DH a	DH b	$\Delta_r G^\circ$	$\Delta_r H^\circ$	$\Delta_r S^\circ$	$\Delta_r H^\circ$	logK(25)
YUGAWARA		0.00			-7545.007	-8332.940	-2642.742	0.000	-9.670
	-8.00 H+		1.00 CA+2		2.00 AL+3	5.00 H4SIO4		-2.00 H2O	
ZOISITE		0.00			-6489.539	-7357.910	-2912.529	0.000	-43.960
	1.00 H2O		2.00 CA+2		3.00 AL+3	3.00 H4SIO4		-13.00 H+	
ZRCL4(S)		0.00			-835.162	-668.320	559.592	0.000	-37.530
	1.00 ZR+4		4.00 CL-						
ZRO2		0.00			-1009.625	-571.660	1468.942	0.000	1.900
	1.00 ZR+4		2.00 H2O		-4.00 H+				

Table B.4: Selected aqueous species and minerals in 0391 MINEQL-PSI data base. Page 1 of 37

	Charge	OPV	DH a	DH b	$\Delta_f G^0$	$\Delta_f H^0$	$\Delta_f S^0$	$\Delta_f H^0$	logK(25)
MASTER SPECIES									
AL+3	3.0	0.00	6.65	0.19	-491.500	-538.400	-157.303		
AM+3	3.0	0.00	9.00	0.00	-599.100	-616.700	-59.031		
ASO2-	-1.0	3.00	4.50	0.00	-349.960	-429.030	-265.202		
ASO4-3	-3.0	5.00	4.00	0.00	-648.410	-888.140	-804.058		
B(OH)4-	1.0	0.00	0.00	0.00	-1153.727	-1344.577	-640.114		
BA+2	2.0	0.00	4.55	0.09	-555.360	-532.500	76.673		
BR-	-1.0	0.00	3.00	0.00	-103.850	-121.410	-58.897		
CA+2	2.0	0.00	4.86	0.15	-552.807	-543.000	32.893		
CH4(AQ)	0.0	-4.00	0.00	0.00	-34.416	-88.607	-181.758		
CIT-3	-3.0	0.00	0.00	0.00	0.000	0.000	0.000		
CL-	-1.0	0.00	3.71	0.01	-131.220	-167.080	-120.275		
CO3-2	-2.0	4.00	5.40	0.00	-527.919	-675.314	-494.365		
E-	-1.0	-1.00	0.00	0.00	0.000	0.000	0.000		
EDTA-4	-4.0	0.00	0.00	0.00	0.000	0.000	0.000		
F-	-1.0	0.00	3.46	0.08	-281.520	-335.350	-180.547		
FE+2	2.0	2.00	5.08	0.16	-78.900	-89.100	-34.211		
FE+3	3.0	3.00	9.00	0.00	-4.583	-48.600	-147.634		
H+	1.0	0.00	9.00	0.00	0.000	0.000	0.000		
H2(AQ)	0.0	2.00	0.00	0.00	17.726	-4.039	-73.000		
H2O	0.0	0.00	0.00	0.00	-237.140	-285.830	-163.307		
H2SIO4-2	-2.0	0.00	4.00	0.00	-1175.654	-1381.960	-691.954		
HS-	-1.0	-2.00	3.50	0.00	12.240	-16.300	-95.724		
HSE-	-1.0	-2.00	3.50	0.00	44.000	15.900	-94.248		
I-	-1.0	0.00	3.00	0.00	-51.720	-56.780	-16.971		
K+	1.0	0.00	3.71	0.01	-282.510	-252.140	101.861		
LI+	1.0	0.00	4.76	0.20	-292.920	-278.470	48.466		
MG+2	2.0	0.00	5.46	0.22	-455.400	-467.000	-38.907		
MN+2	2.0	2.00	7.04	0.22	-228.100	-220.750	24.652		
MOO4-2	-2.0	0.00	5.00	0.00	-836.300	-997.900	-542.009		
N2(AQ)	0.0	0.00	0.00	0.00	18.188	-10.437	-96.009		
NA+	1.0	0.00	4.32	0.06	-261.950	-240.340	72.480		
NH3	0.0	-3.00	0.00	0.00	-26.659	-81.148	-182.757		
NI+2	2.0	0.00	5.51	0.22	-45.600	-54.000	-28.174		
NO3-	-1.0	5.00	3.00	0.00	-110.790	-206.850	-322.187		
NP+3	3.0	3.00	11.00	0.00	-517.100	-527.200	-33.876		
NP+4	4.0	4.00	11.00	0.00	-502.900	-556.100	-178.434		
NPO2+	1.0	5.00	11.00	0.00	-915.000	-978.200	-211.974		
NPO2+2	2.0	6.00	11.00	0.00	-795.800	-860.600	-217.340		
NTA-3	-3.0	0.00	0.00	0.00	0.000	0.000	0.000		
O2(AQ)	0.0	4.00	0.00	0.00	16.521	-12.059	-95.858		
OX-2	-2.0	0.00	0.00	0.00	0.000	0.000	0.000		
PD+2	2.0	0.00	5.50	0.00	176.500	149.000	-92.235		
PO4-3	-3.0	0.00	4.00	0.00	-1025.490	-1284.400	-868.388		
PU+3	3.0	3.74	11.00	0.00	-578.600	-592.000	-44.944		
PU+4	4.0	4.00	11.00	0.00	-481.600	-536.400	-183.800		
PUO2+	1.0	5.00	11.00	0.00	-849.800	-914.600	-217.340		
PUO2+2	2.0	6.00	11.00	0.00	-756.900	-822.200	-219.017		
S2O3-2	-2.0	8.00	4.00	0.00	-519.290	-648.500	-433.372		
SEO3-2	-2.0	4.00	4.50	0.00	-369.800	-509.200	-467.550		
SEO4-2	-2.0	6.00	4.50	0.00	-441.300	-599.100	-529.264		
SN+2	2.0	2.00	6.00	0.00	-27.600	-8.900	62.720		
SN+4	4.0	4.00	11.00	0.00	2.367	0.500	-6.262		
SO3-2	-2.0	6.00	4.50	0.00	-487.470	-635.500	-496.495		
SO4-2	-2.0	6.00	5.31	-0.07	-744.000	-909.340	-554.553		
SR+2	2.0	0.00	5.48	0.11	-563.830	-550.900	43.367		
TC+2	2.0	2.00	11.00	0.00	77.200	0.000	-258.930		
TCO+	1.0	3.00	5.00	0.00	0.000	0.000	0.000		
TCO+2	2.0	4.00	5.00	0.00	-100.600	0.000	337.414		
TCO4-	-1.0	7.00	11.00	0.00	-623.659	-857.490	-784.273		
TH+4	4.0	0.00	11.00	0.00	-705.000	-769.000	-214.657		
U+3	3.0	3.00	11.00	0.00	-476.473	-489.100	-42.351		
U+4	4.0	4.00	11.00	0.00	-529.860	-591.200	-205.735		
UO2+	1.0	5.00	11.00	0.00	-961.021	-1025.127	-215.013		
UO2+2	2.0	6.00	11.00	0.00	-952.551	-1019.000	-222.871		
ZR+4	4.0	0.00	11.00	0.00	-524.500	0.000	1759.182		

Table B.4: Selected aqueous species and minerals in 0391 MINEQL-PSI data base. Page 2 of 37

	Charge	OPV	DH a	DH b	$\Delta_f G^0$	$\Delta_f H^0$	$\Delta_f S^0$	$\Delta_f H^0$	logK(25)	
PRODUCT SPECIES										
ALCIT		0.0	0.00	0.00	0.00	-545.725	-538.400	24.569	0.000	9.500
	1.00	AL+3		1.00	CIT-3					
ALEDTA-		-1.0	0.00	0.00	0.00	-604.517	-538.400	221.756	0.000	19.800
	1.00	AL+3		1.00	EDTA-4					
ALF+2		2.0	0.00	0.00	0.00	-812.975	-869.315	-188.964	4.435	7.000
	1.00	AL+3		1.00	F-					
ALF2+		1.0	0.00	0.00	0.00	-1127.030	-1200.899	-247.758	8.201	12.700
	1.00	AL+3		2.00	F-					
ALF3		0.0	0.00	0.00	0.00	-1431.953	-1535.413	-347.006	9.037	16.800
	1.00	AL+3		3.00	F-					
ALF4-		-1.0	0.00	0.00	0.00	-1728.313	-1870.595	-477.216	9.205	19.400
	1.00	AL+3		4.00	F-					
ALF5-2		-2.0	0.00	0.00	0.00	-2016.683	-2207.451	-639.841	7.699	20.600
	1.00	AL+3		5.00	F-					
ALF6-3		-3.0	0.00	0.00	0.00	-2298.203	-2557.487	-869.644	-6.987	20.600
	1.00	AL+3		6.00	F-					
ALHCIT+		1.0	0.00	0.00	0.00	-562.849	-538.400	82.002	0.000	12.500
	1.00	AL+3		1.00	CIT-3		1.00	H+		
ALHEDTA		0.0	0.00	0.00	0.00	-619.928	-538.400	273.446	0.000	22.500
	1.00	AL+3		1.00	EDTA-4		1.00	H+		
ALHSO4+2		2.0	6.00	0.00	0.00	-1249.484	-1431.632	-610.925	16.108	2.450
	1.00	AL+3		1.00	SO4-2		1.00	H+		
ALNTA		0.0	0.00	0.00	0.00	-575.977	-538.400	126.034	0.000	14.800
	1.00	AL+3		1.00	NTA-3					
ALNTA2-3		-3.0	0.00	0.00	0.00	-610.224	-538.400	240.900	0.000	20.800
	1.00	AL+3		2.00	NTA-3					
ALOH+2		2.0	0.00	0.00	0.00	-700.100	-776.156	-255.091	48.074	-5.000
	1.00	AL+3		-1.00	H+		1.00	H2O		
ALOH2+		1.0	0.00	0.00	0.00	-908.073	-997.510	-299.974	112.550	-10.110
	1.00	AL+3		-2.00	H+		2.00	H2O		
ALOH3		0.0	0.00	0.00	0.00	-1106.228	-1228.990	-411.746	166.900	-16.940
	1.00	AL+3		-3.00	H+		3.00	H2O		
ALOH4-		-1.0	0.00	0.00	0.00	-1310.662	-1504.737	-650.931	176.983	-22.670
	1.00	AL+3		-4.00	H+		4.00	H2O		
ALOHEDTA		-2.0	0.00	0.00	0.00	-806.268	-824.230	-60.246	0.000	13.600
	1.00	AL+3		1.00	EDTA-4		-1.00	H+		
ALOHNTA-		-1.0	0.00	0.00	0.00	-782.294	-824.230	-140.653	0.000	9.400
	1.00	AL+3		1.00	NTA-3		-1.00	H+		
ALOX2-		-1.0	0.00	0.00	0.00	-562.849	-538.400	82.002	0.000	12.500
	1.00	AL+3		2.00	OX-2					
ALOX2-3		-3.0	0.00	0.00	0.00	-585.110	-538.400	156.665	0.000	16.400
	1.00	AL+3		3.00	OX-2					
ALSO4+		1.0	6.00	0.00	0.00	-1252.738	-1438.744	-623.869	8.996	3.020
	1.00	AL+3		1.00	SO4-2					

Table B.4: Selected aqueous species and minerals in 0391 MINEQL-PSI data base. Page 3 of 37

		Charge	OPV	DH a	DH b	$\Delta_f G^0$	$\Delta_f H^0$	$\Delta_f S^0$	$\Delta_f H^0$	logK(25)
ALSO42-		-1.0	12.00	0.00	0.00	-2007.583	-2345.197	-1132.365	11.883	4.920
1.00	AL+3		2.00	SO4-2						
AM1836		0.0	7.00	0.00	0.00	-1368.155	-1577.844	-703.302	0.000	0.700
1.00	AM+3		1.00	CO3-2		-1.00	H+	1.00	H2O	
AM1837		-2.0	11.00	0.00	0.00	-1919.476	-2253.158	-1119.175	0.000	4.800
1.00	AM+3		2.00	CO3-2		-1.00	H+	1.00	H2O	
AM1838		-1.0	7.00	0.00	0.00	-1560.202	-1863.674	-1017.850	0.000	-7.200
1.00	AM+3		1.00	CO3-2		-2.00	H+	2.00	H2O	
AM1839		1.0	7.00	0.00	0.00	-1173.253	-1292.014	-398.326	0.000	8.100
1.00	AM+3		1.00	CO3-2						
AM1840		-1.0	11.00	0.00	0.00	-1726.858	-1967.328	-806.542	0.000	12.600
1.00	AM+3		2.00	CO3-2						
AM1841		-3.0	15.00	0.00	0.00	-2263.909	-2642.642	-1270.276	0.000	14.200
1.00	AM+3		3.00	CO3-2						
AMCL+2		2.0	2.00	0.00	0.00	-736.599	-783.780	-158.247	0.000	1.100
1.00	AM+3		1.00	CL-						
AMF+2		2.0	3.00	0.00	0.00	-906.306	-952.050	-153.428	0.000	4.500
1.00	AM+3		1.00	F-						
AMF2+		1.0	3.00	0.00	0.00	-1207.803	-1287.400	-266.969	0.000	8.000
1.00	AM+3		2.00	F-						
AMF3		0.0	3.00	0.00	0.00	-1507.589	-1622.750	-386.253	0.000	11.200
1.00	AM+3		3.00	F-						
AMH2PO4+		2.0	3.00	0.00	0.00	-1751.363	-1901.100	-502.222	0.000	22.210
1.00	AM+3		1.00	PO4-3		2.00	H+			
AMH4PO42		1.0	3.00	0.00	0.00	-2894.493	-3185.500	-976.044	0.000	42.820
1.00	AM+3		2.00	PO4-3		4.00	H+			
AMOH+2		2.0	3.00	0.00	0.00	-799.139	-902.530	-346.776	0.000	-6.500
1.00	AM+3		-1.00	H+		1.00	H2O			
AMOH2+		1.0	3.00	0.00	0.00	-994.611	-1188.360	-649.838	0.000	-13.800
1.00	AM+3		-2.00	H+		2.00	H2O			
AMOH3		0.0	3.00	0.00	0.00	-1166.681	-1474.190	-1031.391	0.000	-25.200
1.00	AM+3		-3.00	H+		3.00	H2O			
AMSO4+		1.0	9.00	0.00	0.00	-1365.932	-1526.040	-537.006	0.000	4.000
1.00	AM+3		1.00	SO4-2						
AMSO42-		-1.0	15.00	0.00	0.00	-2119.635	-2435.380	-1059.014	0.000	5.700
1.00	AM+3		2.00	SO4-2						
BACIT-		-1.0	0.00	0.00	0.00	-578.648	-532.500	154.782	0.000	4.080
1.00	BA+2		1.00	CIT-3						
BACL+		1.0	-1.00	0.00	0.00	-685.838	-699.580	-46.091	0.000	-0.130
1.00	BA+2		1.00	CL-						
BACO3		0.0	4.00	0.00	0.00	-1098.747	-1192.961	-315.993	14.853	2.710
1.00	BA+2		1.00	CO3-2						
BAEDTA-2		-2.0	0.00	0.00	0.00	-613.581	-532.500	271.946	0.000	10.200
1.00	BA+2		1.00	EDTA-4						
BAH2CIT+		1.0	0.00	0.00	0.00	-626.024	-532.500	313.681	0.000	12.380

Table B.4: Selected aqueous species and minerals in 0391 MINEQL-PSI data base. Page 4 of 37

	Charge	OPV	DH a	DH b	$\Delta_f G^0$	$\Delta_f H^0$	$\Delta_f S^0$	$\Delta_f H^0$	logK(25)
1.00	BA+2	1.00	CIT-3	2.00	H+				
BAHCIT		0.0	0.00	0.00	0.00	-606.788	-532.500	249.164	0.000
1.00	BA+2	1.00	CIT-3	1.00	H+				9.010
BAHCO3+		1.0	4.00	0.00	0.00	-1147.835	-1199.446	-173.103	8.368
1.00	BA+2	1.00	CO3-2	1.00	H+				11.310
BAHEDTA-		-1.0	0.00	0.00	0.00	-643.262	-532.500	371.497	0.000
1.00	BA+2	1.00	EDTA-4	1.00	H+				15.400
BANO3+		1.0	5.00	0.00	0.00	-671.287	-739.350	-228.284	0.000
1.00	BA+2	1.00	NO3-						0.900
BANO32		0.0	10.00	0.00	0.00	-782.648	-946.200	-548.556	0.000
1.00	BA+2	2.00	NO3-						1.000
BANTA-		-1.0	0.00	0.00	0.00	-592.461	-532.500	201.111	0.000
1.00	BA+2	1.00	NTA-3						6.500
BAOH+		1.0	0.00	0.00	0.00	-715.615	-818.330	-344.509	0.000
1.00	BA+2	-1.00	H+	1.00	H2O				-13.470
BAOX		0.0	0.00	0.00	0.00	-565.063	-532.500	109.218	0.000
1.00	BA+2	1.00	OX-2						1.700
BAS2O3		0.0	0.00	0.00	0.00	-1087.778	-1181.000	-312.668	0.000
1.00	BA+2	1.00	S2O3-2						2.300
BASO4		0.0	6.00	0.00	0.00	-1314.771	-1441.840	-426.190	0.000
1.00	BA+2	1.00	SO4-2						2.700
BASO42-2		-2.0	12.00	0.00	0.00	-2062.767	-2351.180	-967.342	0.000
1.00	BA+2	2.00	SO4-2						3.400
BOH3		0.0	0.00	0.00	0.00	-969.271	-1072.805	-347.256	-14.058
1.00	H+	1.00	B(OH)4-	-1.00	H2O				9.230
CACIT-		-1.0	0.00	0.00	0.00	-579.520	-543.000	122.489	0.000
1.00	CA+2	1.00	CIT-3						4.680
CACO3		0.0	4.00	0.00	0.00	-1099.105	-1203.503	-350.150	14.811
1.00	CA+2	1.00	CO3-2						3.220
CAEDTA-2		-2.0	0.00	0.00	0.00	-624.156	-543.000	272.198	0.000
1.00	CA+2	1.00	EDTA-4						12.500
CAF+		1.0	0.00	0.00	0.00	-839.692	-861.112	-71.841	17.238
1.00	CA+2	1.00	F-						0.940
CAH2CIT+		1.0	0.00	0.00	0.00	-622.786	-543.000	267.603	0.000
1.00	CA+2	1.00	CIT-3	2.00	H+				12.260
CAH2PO4+		1.0	0.00	0.00	0.00	-1697.935	-1832.839	-452.472	-5.439
1.00	CA+2	1.00	PO4-3	2.00	H+				20.960
CAHCIT		0.0	0.00	0.00	0.00	-606.975	-543.000	214.573	0.000
1.00	CA+2	1.00	CIT-3	1.00	H+				9.490
CAHCO3+		1.0	4.00	0.00	0.00	-1146.024	-1221.954	-254.669	-3.640
1.00	CA+2	1.00	CO3-2	1.00	H+				11.440
CAHEDTA-		-1.0	0.00	0.00	0.00	-644.133	-543.000	339.203	0.000
1.00	CA+2	1.00	EDTA-4	1.00	H+				16.000
CAHPO40		0.0	0.00	0.00	0.00	-1664.486	-1829.492	-553.432	-2.092
1.00	CA+2	1.00	PO4-3	1.00	H+				15.100

Table B.4: Selected aqueous species and minerals in 0391 MINEQL-PSI data base. Page 5 of 37

		Charge	OPV	DH a	DH b	$\Delta_f G^0$	$\Delta_f H^0$	$\Delta_f S^0$	$\Delta_r H^0$	logK(25)
CANH3+2 1.00	CA+2	2.0 1.00	-3.00 1.00	0.00 NH3	0.00	-578.895	-624.148	-151.779	0.000	-0.100
CANH32+2 1.00	CA+2	2.0 2.00	-6.00 NH3	0.00	0.00	-602.129	-705.296	-346.022	0.000	-0.700
CANH33+2 1.00	CA+2	2.0 3.00	-9.00 NH3	0.00	0.00	-624.222	-786.444	-544.095	0.000	-1.500
CANH34+2 1.00	CA+2	2.0 4.00	-12.00 NH3	0.00	0.00	-644.602	-867.592	-747.911	0.000	-2.600
CANO3+ 1.00	CA+2	1.0 1.00	5.00 NO3-	0.00	0.00	-667.593	-749.850	-275.893	0.000	0.700
CANO32 1.00	CA+2	0.0 2.00	10.00 NO3-	0.00	0.00	-777.812	-956.700	-599.994	0.000	0.600
CANTA- 1.00	CA+2	-1.0 1.00	0.00 NTA-3	0.00	0.00	-599.612	-543.000	189.877	0.000	8.200
CAOH+ 1.00	CA+2	1.0 -1.00	0.00 H+	0.00	0.00	-717.000	-762.304	-151.952	66.526	-12.780
CAOX 1.00	CA+2	0.0 1.00	0.00 OX-2	0.00	0.00	-573.355	-543.000	101.813	0.000	3.600
CAPO4- 1.00	CA+2	-1.0 1.00	0.00 PO4-3	0.00	0.00	-1615.170	-1814.848	-669.723	12.552	6.460
CAS2O3 1.00	CA+2	0.0 1.00	0.00 S2O3-2	0.00	0.00	-1082.942	-1191.500	-364.105	0.000	1.900
CASO4 1.00	CA+2	0.0 1.00	6.00 SO4-2	0.00	0.00	-1309.935	-1445.436	-454.473	6.904	2.300
FE2OH2+4 2.00	FE+3	4.0 -2.00	6.00 H+	0.00	0.00	-466.608	-612.376	-488.909	56.484	-2.950
FEBOH4+2 1.00	FE+3	2.0 1.00	3.00 B(OH)4-	0.00	0.00	-1209.110	-1393.177	-617.363	0.000	8.900
FEBOH42+ 1.00	FE+3	1.0 2.00	3.00 B(OH)4-	0.00	0.00	-2402.222	-2737.754	-1125.380	0.000	15.800
FEBR+2 1.00	FE+3	2.0 1.00	2.00 BR-	0.00	0.00	-112.429	-170.010	-193.129	0.000	0.700
FECIT- 1.00	FE+2	-1.0 1.00	2.00 CIT-3	0.00	0.00	-111.435	-89.100	74.912	0.000	5.700
FECIT 1.00	FE+3	0.0 1.00	3.00 CIT-3	0.00	0.00	-81.240	-48.600	109.476	0.000	13.430
FECL+ 1.00	FE+2	1.0 1.00	1.00 CL-	0.00	0.00	-210.919	-256.180	-151.806	0.000	0.140
FECL+2 1.00	FE+3	2.0 1.00	2.00 CL-	0.00	0.00	-144.251	-209.488	-218.806	6.192	1.480
FECL2+ 1.00	FE+3	1.0 2.00	1.00 CL-	0.00	0.00	-279.181	-382.760	-347.406	0.000	2.130
FECL3 1.00	FE+3	0.0 3.00	0.00 CL-	0.00	0.00	-404.693	-549.840	-486.826	0.000	1.130
FECO3 1.00	FE+2	0.0 1.00	6.00 CO3-2	0.00	0.00	-631.820	-764.414	-444.724	0.000	4.380

Table B.4: Selected aqueous species and minerals in 0391 MINEQL-PSI data base. Page 6 of 37

		Charge	OPV	DH a	DH b	$\Delta_f G^0$	$\Delta_f H^0$	$\Delta_f S^0$	$\Delta_f H^0$	logK(25)
FEEDTA-		-1.0	3.00	0.00	0.00	-163.263	-48.600	384.581	0.000	27.800
1.00	FE+3		1.00	EDTA-4						
FEEDTA-2		-2.0	2.00	0.00	0.00	-174.222	-89.100	285.501	0.000	16.700
1.00	FE+2		1.00	EDTA-4						
PEF+		1.0	2.00	0.00	0.00	-366.128	-424.450	-195.613	0.000	1.000
1.00	FE+2		1.00	F-						
PEF+2		2.0	3.00	0.00	0.00	-321.492	-372.653	-171.595	11.297	6.200
1.00	FE+3		1.00	F-						
PEF2+		1.0	3.00	0.00	0.00	-629.268	-699.217	-234.608	20.083	10.800
1.00	FE+3		2.00	F-						
PEF3		0.0	3.00	0.00	0.00	-929.054	-1032.056	-345.473	22.594	14.000
1.00	FE+3		3.00	F-						
FEH2PO4+		1.0	2.00	0.00	0.00	-1233.160	-1373.500	-470.701	0.000	22.560
1.00	FE+2		1.00	PO4-3		2.00	H+			
FEH3SIO4		2.0	3.00	0.00	0.00	-1315.686	-1430.560	-385.291	0.000	23.730
1.00	FE+3		1.00	H2SIO4-2		1.00	H+			
FEHCIT		0.0	2.00	0.00	0.00	-135.408	-89.100	155.319	0.000	9.900
1.00	FE+2		1.00	CIT-3		1.00	H+			
FEHCO3+		1.0	6.00	0.00	0.00	-677.197	-779.309	-342.484	-14.895	12.330
1.00	FE+2		1.00	CO3-2		1.00	H+			
FEHEDTA-		-1.0	2.00	0.00	0.00	-193.629	-89.100	350.592	0.000	20.100
1.00	FE+2		1.00	EDTA-4		1.00	H+			
FEHEDTA		0.0	3.00	0.00	0.00	-172.395	-48.600	415.212	0.000	29.400
1.00	FE+3		1.00	EDTA-4		1.00	H+			
FEHPO4		0.0	2.00	0.00	0.00	-1195.431	-1373.500	-597.246	0.000	15.950
1.00	FE+2		1.00	PO4-3		1.00	H+			
FEHPO4+		1.0	3.00	0.00	0.00	-1148.227	-1333.000	-619.733	0.000	20.700
1.00	FE+3		1.00	PO4-3		1.00	H+			
FEHSO4+		1.0	8.00	0.00	0.00	-840.423	-982.332	-475.963	16.108	3.070
1.00	FE+2		1.00	SO4-2		1.00	H+			
FEHSO4+2		2.0	9.00	0.00	0.00	-774.097	-941.832	-562.583	16.108	4.470
1.00	FE+3		1.00	SO4-2		1.00	H+			
FEI+2		2.0	2.00	0.00	0.00	-68.290	-105.380	-124.402	0.000	2.100
1.00	FE+3		1.00	I-						
FENH3+2		2.0	-1.00	0.00	0.00	-112.979	-170.248	-192.080	0.000	1.300
1.00	FE+2		1.00	NH3						
FENH32+2		2.0	-4.00	0.00	0.00	-144.205	-251.396	-359.522	0.000	2.100
1.00	FE+2		2.00	NH3						
FENH34+2		2.0	-10.00	0.00	0.00	-206.084	-413.692	-696.319	0.000	3.600
1.00	FE+2		4.00	NH3						
FENTA-		-1.0	2.00	0.00	0.00	-139.404	-89.100	168.720	0.000	10.600
1.00	FE+2		1.00	NTA-3						
FENTA		0.0	3.00	0.00	0.00	-110.750	-48.600	208.452	0.000	18.600
1.00	FE+3		1.00	NTA-3						
FENTA2-3		-3.0	3.00	0.00	0.00	-159.267	-48.600	371.180	0.000	27.100
1.00	FE+3		2.00	NTA-3						

Table B.4: Selected aqueous species and minerals in 0391 MINEQL-PSI data base. Page 7 of 37

		Charge	OPV	DH a	DH b	$\Delta_f G^0$	$\Delta_f H^0$	$\Delta_f S^0$	$\Delta_r H^0$	logK(25)	
FEOH+	1.00	FE+2	1.0 -1.00	2.00 H+	0.00	0.00 1.00	-261.815 H2O	-319.701	-194.152	55.229	-9.500
FEOH+2	1.00	FE+3	2.0 -1.00	3.00 H+	0.00	0.00 1.00	-229.223 H2O	-290.916	-206.922	43.514	-2.190
FEOH2+	1.00	FE+3	1.0 -2.00	3.00 H+	0.00	0.00 2.00	-446.499 H2O	-548.714	-342.829	71.546	-5.670
FEOH2EDT	1.00	FE+3	-3.0 1.00	3.00 EDTA-4	0.00	0.00 -2.00	-536.513 H+	-620.260 2.00	-280.889 H2O	0.000	10.100
FEOH2NTA	1.00	FE+3	-2.0 1.00	3.00 NTA-3	0.00	0.00 -2.00	-514.823 H+	-620.260 2.00	-353.638 H2O	0.000	6.300
FEOH3	1.00	FE+3	0.0 -3.00	3.00 H+	0.00	0.00 3.00	-644.312 H2O	-802.327	-529.985	103.763	-12.560
FEOH4-	1.00	FE+3	-1.0 -4.00	3.00 H+	0.00	0.00 4.00	-829.852 H2O	-1058.450	-766.722	133.470	-21.600
FEOHCIT	2.00	FE+3	-2.0 2.00	6.00 CIT-3	0.00	0.00 -2.00	-150.151 H+	-97.200	177.599	0.000	24.700
FEOHEDTA	1.00	FE+3	-2.0 1.00	3.00 EDTA-4	0.00	0.00 -1.00	-361.018 H+	-334.430 1.00	89.177 H2O	0.000	20.900
FEOX+	1.00	FE+3	1.0 1.00	3.00 OX-2	0.00	0.00	-55.383	-48.600	22.752	0.000	8.900
FEOX2-	1.00	FE+3	-1.0 2.00	3.00 OX-2	0.00	0.00	-94.197	-48.600	152.934	0.000	15.700
FEOX3-3	1.00	FE+3	-3.0 3.00	3.00 OX-2	0.00	0.00	-121.024	-48.600	242.912	0.000	20.400
FES2O3+	1.00	FE+3	1.0 1.00	3.00 S2O3-2	0.00	0.00	-546.134	-697.100	-506.343	0.000	3.900
FESO4	1.00	FE+2	0.0 1.00	8.00 SO4-2	0.00	0.00	-835.743	-984.926	-500.362	13.514	2.250
FESO4+	1.00	FE+3	1.0 1.00	9.00 SO4-2	0.00	0.00	-771.643	-941.581	-569.974	16.359	4.040
FESO42-	1.00	FE+3	-1.0 2.00	15.00 SO4-2	0.00	0.00	-1523.292	-1848.034	-1089.190	19.246	5.380
FOHNTA-1	1.00	FE+3	-1.0 1.00	3.00 NTA-3	0.00	0.00	-325.058	-334.430	-31.432	0.000	14.600
FOHNTA-2	1.00	FE+2	-2.0 1.00	2.00 NTA-3	0.00	0.00	-315.469	-374.930	-199.432	0.000	-0.100
H2ASO4-	2.00	H+	-1.0 1.00	5.00 ASO4-3	0.00	0.00	-753.150	-909.562	-524.608	-21.422	18.350
H2CIT-	2.00	H+	-1.0 1.00	0.00 CIT-3	0.00	0.00	-63.700	0.000	213.652	0.000	11.160
H2CO3	2.00	H+	0.0 1.00	4.00 CO3-2	0.00	0.00	-623.127	-699.322	-255.559	-24.008	16.680
H2EDTA-2	2.00	H+	-2.0 1.00	0.00 EDTA-4	0.00	0.00	-101.715	0.000	341.153	0.000	17.820
H2F+	1.00	H+	-1.0 2.00	0.00 F-	0.00	0.00	-583.703	-654.382	-237.061	16.318	3.620

Table B.4: Selected aqueous species and minerals in 0391 MINEQL-PSI data base. Page 8 of 37

		Charge	OPV	DH a	DH b	$\Delta_f G^0$	$\Delta_f H^0$	$\Delta_f S^0$	$\Delta_r H^0$	logK(25)
H2NTA-		-1.0	0.00	0.00	0.00	-78.198	0.000	262.278	0.000	13.700
2.00	H+		1.00	NTA-3						
H2OX		0.0	0.00	0.00	0.00	-29.110	0.000	97.636	0.000	5.100
2.00	H+		1.00	OX-2						
H2PO4-		-1.0	0.00	0.00	0.00	-1137.137	-1304.107	-560.020	-19.707	19.560
2.00	H+		1.00	PO4-3						
H2S		0.0	-2.00	0.00	0.00	-27.658	-38.601	-36.701	-22.301	6.990
1.00	H+		1.00	HS-						
H2S2O3		0.0	0.00	0.00	0.00	-531.847	-648.500	-391.255	0.000	2.200
2.00	H+		1.00	S2O3-2						
H2SE		0.0	-2.00	0.00	0.00	22.310	19.247	-10.273	3.347	3.800
1.00	H+		1.00	HSE-						
H2SEO3		0.0	4.00	0.00	0.00	-433.729	-497.108	-212.577	12.092	11.200
2.00	H+		1.00	SEO3-2						
H2SO3		0.0	4.00	0.00	0.00	-539.184	-553.494	-47.996	82.006	9.060
2.00	H+		1.00	SO3-2						
H3ASO4		0.0	5.00	0.00	0.00	-765.993	-902.491	-457.817	-14.351	20.600
3.00	H+		1.00	ASO4-3						
H3CIT		0.0	0.00	0.00	0.00	-81.566	0.000	273.574	0.000	14.290
3.00	H+		1.00	CIT-3						
H3EDTA-		-1.0	0.00	0.00	0.00	-119.524	0.000	400.884	0.000	20.940
3.00	H+		1.00	EDTA-4						
H3NTA		0.0	0.00	0.00	0.00	-90.756	0.000	304.396	0.000	15.900
3.00	H+		1.00	NTA-3						
H3PO4		0.0	0.00	0.00	0.00	-1149.352	-1295.613	-490.564	-11.213	21.700
3.00	H+		1.00	PO4-3						
H3Si3O9-		-3.0	0.00	0.00	0.00	-3759.959	-4145.880	-1294.386	0.000	40.820
3.00	H+		3.00	H2SiO4-2						
H3SiO4-		-1.0	0.00	0.00	0.00	-1251.740	-1431.373	-602.491	-49.413	13.330
1.00	H+		1.00	H2SiO4-2						
H4EDTA		0.0	0.00	0.00	0.00	-132.195	0.000	443.385	0.000	23.160
4.00	H+		1.00	EDTA-4						
H4Si4O12		-4.0	0.00	0.00	0.00	-5014.039	-5527.840	-1723.296	0.000	54.560
4.00	H+		4.00	H2SiO4-2						
H4SiO4		0.0	0.00	0.00	0.00	-1307.735	-1456.979	-500.567	-75.019	23.140
2.00	H+		1.00	H2SiO4-2						
H5EDTA+		1.0	0.00	0.00	0.00	-140.757	0.000	472.101	0.000	24.660
5.00	H+		1.00	EDTA-4						
H5Si3O10		-3.0	0.00	0.00	0.00	-3751.968	-4145.880	-1321.188	0.000	39.420
3.00	H+		3.00	H2SiO4-2						
H5Si4O12		-3.0	0.00	0.00	0.00	-5085.388	-5527.840	-1483.991	0.000	67.060
5.00	H+		4.00	H2SiO4-2						
H6EDTA+2		2.0	0.00	0.00	0.00	-139.045	0.000	466.358	0.000	24.360
6.00	H+		1.00	EDTA-4						
H6Si2O8-		-2.0	0.00	0.00	0.00	-2507.020	-2763.920	-861.648	0.000	27.280
2.00	H+		2.00	H2SiO4-2						

Table B.4: Selected aqueous species and minerals in 0391 MINEQL-PSI data base. Page 9 of 37

	Charge	OPV	DH a	DH b	$\Delta_f G^0$	$\Delta_f H^0$	$\Delta_f S^0$	$\Delta_r H^0$	logK(25)
H7Si2O8-	-1.0	0.00	0.00	0.00	-2569.236	-2763.920	-652.974	0.000	38.180
3.00 H+		2.00	H2SiO4-2						
HASO2	0.0	3.00	0.00	0.00	-639.784	-742.182	-343.443	-27.322	9.230
1.00 H+		1.00	ASO2-	1.00	H2O				
HASO4-2	-2.0	5.00	0.00	0.00	-714.622	-906.340	-643.028	-18.200	11.600
1.00 H+		1.00	ASO4-3						
HCIT-2	-2.0	0.00	0.00	0.00	-36.531	0.000	122.524	0.000	6.400
1.00 H+		1.00	CIT-3						
HCO3-	-1.0	4.00	0.00	0.00	-586.882	-690.213	-346.576	-14.899	10.330
1.00 H+		1.00	CO3-2						
HEDTA-3	-3.0	0.00	0.00	0.00	-63.072	0.000	211.546	0.000	11.050
1.00 H+		1.00	EDTA-4						
HF	0.0	0.00	0.00	0.00	-299.671	-322.045	-75.042	13.305	3.180
1.00 H+		1.00	F-						
HMOO4-	-1.0	0.00	0.00	0.00	-860.844	-997.900	-459.688	0.000	4.300
1.00 H+		1.00	MOO4-2						
HNTA-2	-2.0	0.00	0.00	0.00	-59.933	0.000	201.016	0.000	10.500
1.00 H+		1.00	NTA-3						
HOX-	-1.0	0.00	0.00	0.00	-23.973	0.000	80.407	0.000	4.200
1.00 H+		1.00	OX-2						
HPO4-2	-2.0	0.00	0.00	0.00	-1095.983	-1299.002	-680.931	-14.602	12.350
1.00 H+		1.00	PO4-3						
HS2O3-	-1.0	0.00	0.00	0.00	-528.366	-632.517	-349.326	15.983	1.590
1.00 H+		1.00	S2O3-2						
HSEO3-	-1.0	4.00	0.00	0.00	-417.746	-504.179	-289.897	5.021	8.400
1.00 H+		1.00	SEO3-2						
HSEO4-	-1.0	6.00	0.00	0.00	-451.574	-575.293	-414.955	23.807	1.800
1.00 H+		1.00	SEO4-2						
HSO3-	-1.0	4.00	0.00	0.00	-528.681	-569.518	-136.969	65.982	7.220
1.00 H+		1.00	SO3-2						
HSO4-	-1.0	6.00	0.00	0.00	-755.359	-893.232	-462.428	16.108	1.990
1.00 H+		1.00	SO4-2						
KCIT-2	-2.0	0.00	0.00	0.00	-289.531	-252.140	125.409	0.000	1.230
1.00 K+		1.00	CIT-3						
KOH	0.0	0.00	0.00	0.00	-437.114	-537.970	-338.274	0.000	-14.460
1.00 K+		-1.00	H+	1.00	H2O				
KS2O3-	-1.0	0.00	0.00	0.00	-806.937	-900.640	-314.281	0.000	0.900
1.00 K+		1.00	S2O3-2						
KSO4-	-1.0	6.00	0.00	0.00	-1031.362	-1152.066	-404.844	9.414	0.850
1.00 K+		1.00	SO4-2						
LICIT-2	-2.0	0.00	0.00	0.00	-301.311	-278.470	76.608	0.000	1.470
1.00 LI+		1.00	CIT-3						
LIEDTA-3	-3.0	0.00	0.00	0.00	-315.752	-278.470	125.043	0.000	4.000
1.00 LI+		1.00	EDTA-4						
LIOH	0.0	0.00	0.00	0.00	-452.204	-564.300	-375.971	0.000	-13.640
1.00 LI+		-1.00	H+	1.00	H2O				

Table B.4: Selected aqueous species and minerals in 0391 MINEQL-PSI data base. Page 10 of 37

		Charge	OPV	DH a	DH b	$\Delta_f G^0$	$\Delta_f H^0$	$\Delta_f S^0$	$\Delta_r H^0$	logK(25)
LISO4-		-1.0	6.00	0.00	0.00	-1040.573	-1187.810	-493.835	0.000	0.640
1.00	Li+		1.00	SO4-2						
MGCIT-		-1.0	0.00	0.00	0.00	-482.113	-467.000	50.689	0.000	4.680
1.00	MG+2		1.00	CIT-3						
MGCO3		0.0	4.00	0.00	0.00	-1000.329	-1130.975	-438.192	11.339	2.980
1.00	MG+2		1.00	CO3-2						
MGEDTA-2		-2.0	0.00	0.00	0.00	-515.333	-467.000	162.110	0.000	10.500
1.00	MG+2		1.00	EDTA-4						
MGF+		1.0	0.00	0.00	0.00	-747.308	-788.961	-139.704	13.389	1.820
1.00	MG+2		1.00	F-						
MGH2CIT+		1.0	0.00	0.00	0.00	-526.349	-467.000	199.058	0.000	12.430
1.00	MG+2		1.00	CIT-3		2.00	H+			
MGHClCIT		0.0	0.00	0.00	0.00	-506.942	-467.000	133.967	0.000	9.030
1.00	MG+2		1.00	CIT-3		1.00	H+			
MGHCO3+		1.0	4.00	0.00	0.00	-1048.389	-1153.946	-354.038	-11.632	11.400
1.00	MG+2		1.00	CO3-2		1.00	H+			
MGHEDTA-		-1.0	0.00	0.00	0.00	-539.877	-467.000	244.431	0.000	14.800
1.00	MG+2		1.00	EDTA-4		1.00	H+			
MGHPO4		0.0	0.00	0.00	0.00	-1567.993	-1753.492	-622.168	-2.092	15.260
1.00	MG+2		1.00	PO4-3		1.00	H+			
MGNH3+2		2.0	-3.00	0.00	0.00	-482.630	-548.148	-219.749	0.000	0.100
1.00	MG+2		1.00	NH3						
MGNH32+2		2.0	-6.00	0.00	0.00	-508.718	-629.296	-404.421	0.000	0.000
1.00	MG+2		2.00	NH3						
MGNH33+2		2.0	-9.00	0.00	0.00	-533.665	-710.444	-592.921	0.000	-0.300
1.00	MG+2		3.00	NH3						
MGNH34+2		2.0	-12.00	0.00	0.00	-556.328	-791.592	-789.079	0.000	-1.000
1.00	MG+2		4.00	NH3						
MGNTA-		-1.0	0.00	0.00	0.00	-496.497	-467.000	98.933	0.000	7.200
1.00	MG+2		1.00	NTA-3						
MGOH+		1.0	0.00	0.00	0.00	-627.242	-752.830	-421.226	0.000	-11.440
1.00	MG+2		-1.00	H+		1.00	H2O			
MGOX		0.0	0.00	0.00	0.00	-471.953	-467.000	16.612	0.000	2.900
1.00	MG+2		1.00	OX-2						
MGS2O3		0.0	0.00	0.00	0.00	-984.964	-1115.500	-437.819	0.000	1.800
1.00	MG+2		1.00	S2O3-2						
MGSO4		0.0	6.00	0.00	0.00	-1212.928	-1357.303	-484.236	19.037	2.370
1.00	MG+2		1.00	SO4-2						
MNCIT-		-1.0	2.00	0.00	0.00	-258.352	-220.750	126.117	0.000	5.300
1.00	MN+2		1.00	CIT-3						
MNCL+		1.0	1.00	0.00	0.00	-362.802	-387.830	-83.945	0.000	0.610
1.00	MN+2		1.00	CL-						
MNCL2		0.0	0.00	0.00	0.00	-491.967	-554.910	-211.112	0.000	0.250
1.00	MN+2		2.00	CL-						
MNCL3-		-1.0	-1.00	0.00	0.00	-619.991	-721.990	-342.108	0.000	-0.310
1.00	MN+2		3.00	CL-						

Table B.4: Selected aqueous species and minerals in 0391 MINEQL-PSI data base. Page 11 of 37

		Charge	OPV	DH a	DH b	$\Delta_f G^0$	$\Delta_f H^0$	$\Delta_f S^0$	$\Delta_r H^0$	logK(25)
MNCO3		0.0	6.00	0.00	0.00	-783.988	-896.064	-375.906	0.000	4.900
1.00	MN+2		1.00	CO3-2						
MNEDTA-2		-2.0	2.00	0.00	0.00	-318.285	-220.750	327.134	0.000	15.800
1.00	MN+2		1.00	EDTA-4						
MNF+		1.0	2.00	0.00	0.00	-514.415	-556.100	-139.813	0.000	0.840
1.00	MN+2		1.00	F-						
MNHClT		0.0	2.00	0.00	0.00	-281.983	-220.750	205.375	0.000	9.440
1.00	MN+2		1.00	CIT-3		1.00	H+			
MNHCO3+		1.0	6.00	0.00	0.00	-826.112	-910.959	-284.578	-14.895	12.280
1.00	MN+2		1.00	CO3-2		1.00	H+			
MNHEDTA-		-1.0	2.00	0.00	0.00	-338.263	-220.750	394.139	0.000	19.300
1.00	MN+2		1.00	EDTA-4		1.00	H+			
MNHPO4		0.0	2.00	0.00	0.00	-1346.058	-1505.150	-533.597	0.000	16.200
1.00	MN+2		1.00	PO4-3		1.00	H+			
MNNH3+2		2.0	-1.00	0.00	0.00	-258.755	-301.898	-144.704	0.000	0.700
1.00	MN+2		1.00	NH3						
MNNH32+2		2.0	-4.00	0.00	0.00	-288.267	-383.046	-317.889	0.000	1.200
1.00	MN+2		2.00	NH3						
MNNTA-		-1.0	2.00	0.00	0.00	-280.613	-220.750	200.781	0.000	9.200
1.00	MN+2		1.00	NTA-3						
MNOH+		1.0	2.00	0.00	0.00	-404.793	-446.330	-139.316	60.250	-10.590
1.00	MN+2		-1.00	H+		1.00	H2O			
MNOH3-		-1.0	2.00	0.00	0.00	-744.310	-1078.240	-1120.008	0.000	-34.200
1.00	MN+2		-3.00	H+		3.00	H2O			
MNOX		0.0	2.00	0.00	0.00	-246.365	-220.750	85.914	0.000	3.200
1.00	MN+2		1.00	OX-2						
MNOX2-2		-2.0	2.00	0.00	0.00	-256.069	-220.750	118.460	0.000	4.900
1.00	MN+2		2.00	OX-2						
MNS2O3		0.0	2.00	0.00	0.00	-758.235	-869.250	-372.346	0.000	1.900
1.00	MN+2		1.00	S2O3-2						
MNSO4		0.0	8.00	0.00	0.00	-984.943	-1115.990	-439.534	14.100	2.250
1.00	MN+2		1.00	SO4-2						
NACIT-2		-2.0	0.00	0.00	0.00	-269.599	-240.340	98.134	0.000	1.340
1.00	NA+		1.00	CIT-3						
NACO3-		-1.0	4.00	0.00	0.00	-797.118	-878.375	-272.536	37.279	1.270
1.00	NA+		1.00	CO3-2						
NAEDTA-3		-3.0	0.00	0.00	0.00	-276.791	-240.340	122.256	0.000	2.600
1.00	NA+		1.00	EDTA-4						
NAF		0.0	0.00	0.00	0.00	-542.100	-575.690	-112.661	0.000	-0.240
1.00	NA+		1.00	F-						
NAH3SiO4		0.0	0.00	0.00	0.00	-1522.823	-1622.300	-333.647	0.000	14.930
1.00	H+		1.00	H2SiO4-2		1.00	NA+			
NAHCO3		0.0	4.00	0.00	0.00	-847.405	-930.549	-278.868	-14.895	10.080
1.00	NA+		1.00	CO3-2		1.00	H+			
NANTA-2		-2.0	0.00	0.00	0.00	-275.649	-240.340	118.427	0.000	2.400
1.00	NA+		1.00	NTA-3						

Table B.4: Selected aqueous species and minerals in 0391 MINEQL-PSI data base. Page 12 of 37

		Charge	OPV	DH a	DH b	$\Delta_f G^0$	$\Delta_f H^0$	$\Delta_f S^0$	$\Delta_r H^0$	logK(25)
NAOH		0.0	0.00	0.00	0.00	-418.152	-526.170	-362.295	0.000	-14.180
	1.00	Na+		-1.00	H+		1.00	H2O		
NAS2O3-		-1.0	0.00	0.00	0.00	-784.665	-888.840	-349.406	0.000	0.600
	1.00	Na+		1.00	S2O3-2					
NASO4-		-1.0	6.00	0.00	0.00	-1009.946	-1144.994	-452.955	4.686	0.700
	1.00	Na+		1.00	SO4-2					
NH4+		1.0	-3.00	0.00	0.00	-78.400	-133.281	-180.716	-52.133	9.240
	1.00	H+		1.00	NH3					
NI2OH+3		3.0	0.00	0.00	0.00	-267.265	-393.830	-424.500	0.000	-10.700
	2.00	NI+2		-1.00	H+		1.00	H2O		
NI4OH4+4		4.0	0.00	0.00	0.00	-972.623	-1359.320	-1296.989	0.000	-27.740
	4.00	NI+2		-4.00	H+		4.00	H2O		
NIBR+		1.0	-1.00	0.00	0.00	-152.875	-175.410	-75.584	0.000	0.600
	1.00	NI+2		1.00	BR-					
NICIT-		-1.0	0.00	0.00	0.00	-83.443	-54.000	98.754	0.000	6.630
	1.00	NI+2		1.00	CIT-3					
NICL+		1.0	-1.00	0.00	0.00	-179.103	-221.080	-140.791	0.000	0.400
	1.00	NI+2		1.00	CL-					
NICL2		0.0	-2.00	0.00	0.00	-313.634	-388.160	-249.962	0.000	0.980
	1.00	NI+2		2.00	CL-					
NICO3		0.0	4.00	0.00	0.00	-606.511	-729.314	-411.884	0.000	5.780
	1.00	NI+2		1.00	CO3-2					
NICO32-2		-2.0	8.00	0.00	0.00	-1159.145	-1404.628	-823.354	0.000	10.110
	1.00	NI+2		2.00	CO3-2					
NIEDTA-2		-2.0	0.00	0.00	0.00	-165.466	-54.000	373.859	0.000	21.000
	1.00	NI+2		1.00	EDTA-4					
NIF+		1.0	0.00	0.00	0.00	-334.540	-389.350	-183.833	0.000	1.300
	1.00	NI+2		1.00	F-					
NIH2CIT+		1.0	0.00	0.00	0.00	-121.743	-54.000	227.213	0.000	13.340
	1.00	NI+2		1.00	CIT-3		2.00	H+		
NIH2PO4+		1.0	0.00	0.00	0.00	-1191.527	-1338.400	-492.615	0.000	21.100
	1.00	NI+2		1.00	PO4-3		2.00	H+		
NIHCIT		0.0	0.00	0.00	0.00	-105.875	-54.000	173.991	0.000	10.560
	1.00	NI+2		1.00	CIT-3		1.00	H+		
NIHCO3+		1.0	4.00	0.00	0.00	-650.062	-729.314	-265.812	0.000	13.410
	1.00	NI+2		1.00	CO3-2		1.00	H+		
NIHEDTA-		-1.0	0.00	0.00	0.00	-187.156	-54.000	446.608	0.000	24.800
	1.00	NI+2		1.00	EDTA-4		1.00	H+		
NIHPO4		0.0	0.00	0.00	0.00	-1158.307	-1338.400	-604.036	0.000	15.280
	1.00	NI+2		1.00	PO4-3		1.00	H+		
NINH32+2		2.0	-6.00	0.00	0.00	-128.200	-248.136	-402.270	-31.840	5.130
	1.00	NI+2		2.00	NH3					
NINH36+2		2.0	-18.00	0.00	0.00	-256.640	-635.195	-1269.682	-94.307	8.950
	1.00	NI+2		6.00	NH3					
NINO3+		1.0	5.00	0.00	0.00	-158.673	-260.850	-342.703	0.000	0.400
	1.00	NI+2		1.00	NO3-					

Table B.4: Selected aqueous species and minerals in 0391 MINEQL-PSI data base. Page 13 of 37

		Charge	OPV	DH a	DH b	$\Delta_f G^0$	$\Delta_f H^0$	$\Delta_f S^0$	$\Delta_r H^0$	logK(25)
NINO32		0.0	10.00	0.00	0.00	-263.755	-467.700	-684.034	0.000	-0.600
1.00	NI+2		2.00	NO3-						
NINTA-		-1.0	0.00	0.00	0.00	-120.374	-54.000	222.618	0.000	13.100
1.00	NI+2		1.00	NTA-3						
NIOH+		1.0	0.00	0.00	0.00	-227.316	-287.907	-203.221	51.923	-9.710
1.00	NI+2		-1.00	H+		1.00	H2O			
NIOH2		0.0	0.00	0.00	0.00	-405.722	-625.660	-737.676	0.000	-20.000
1.00	NI+2		-2.00	H+		2.00	H2O			
NIOH3-		-1.0	0.00	0.00	0.00	-585.783	-911.490	-1092.427	0.000	-30.000
1.00	NI+2		-3.00	H+		3.00	H2O			
NIOH4-2		-2.0	0.00	0.00	0.00	-743.012	-1197.320	-1523.756	0.000	-44.000
1.00	NI+2		-4.00	H+		4.00	H2O			
NIOX		0.0	0.00	0.00	0.00	-71.856	-54.000	59.891	0.000	4.600
1.00	NI+2		1.00	OX-2						
NIOX2-2		-2.0	0.00	0.00	0.00	-91.263	-54.000	124.982	0.000	8.000
1.00	NI+2		2.00	OX-2						
NIOX3-4		-4.0	0.00	0.00	0.00	-99.254	-54.000	151.784	0.000	9.400
1.00	NI+2		3.00	OX-2						
NIPO4-		-1.0	0.00	0.00	0.00	-1118.865	-1338.400	-736.323	0.000	8.370
1.00	NI+2		1.00	PO4-3						
NIS2O3		0.0	0.00	0.00	0.00	-577.447	-702.500	-419.428	0.000	2.200
1.00	NI+2		1.00	S2O3-2						
NISO4		0.0	6.00	0.00	0.00	-802.785	-949.365	-491.632	13.975	2.310
1.00	NI+2		1.00	SO4-2						
NISO42-2		-2.0	12.00	0.00	0.00	-1551.865	-1872.680	-1076.018	0.000	3.200
1.00	NI+2		2.00	SO4-2						
NP2OH2+4		4.0	6.00	0.00	0.00	-1428.569	-1626.060	-662.387	0.000	-14.000
2.00	NP+3		-2.00	H+		2.00	H2O			
NP3OH5+4		4.0	9.00	0.00	0.00	-2554.347	-3010.750	-1530.783	0.000	-32.000
3.00	NP+3		-5.00	H+		5.00	H2O			
NPCL+3		3.0	3.00	0.00	0.00	-640.969	-723.180	-275.735	0.000	1.200
1.00	NP+4		1.00	CL-						
NPCL2+2		2.0	2.00	0.00	0.00	-776.185	-890.260	-382.609	0.000	1.900
1.00	NP+4		2.00	CL-						
NPCO3+		1.0	7.00	0.00	0.00	-1099.815	-1202.514	-344.454	0.000	9.600
1.00	NP+3		1.00	CO3-2						
NPCO32-		-1.0	11.00	0.00	0.00	-1646.570	-1877.828	-775.643	0.000	12.900
1.00	NP+3		2.00	CO3-2						
NPCO33-3		-3.0	15.00	0.00	0.00	-2193.325	-2553.142	-1206.832	0.000	16.200
1.00	NP+3		3.00	CO3-2						
NPEDTA		0.0	4.00	0.00	0.00	-670.142	-556.100	382.498	0.000	29.300
1.00	NP+4		1.00	EDTA-4						
NPF+3		3.0	4.00	0.00	0.00	-831.796	-891.450	-200.082	0.000	8.300
1.00	NP+4		1.00	F-						
NPF2+2		2.0	4.00	0.00	0.00	-1148.705	-1226.800	-261.933	0.000	14.500
1.00	NP+4		2.00	F-						

Table B.4: Selected aqueous species and minerals in 0391 MINEQL-PSI data base. Page 14 of 37

		Charge	OPV	DH a	DH b	$\Delta_f G^0$	$\Delta_f H^0$	$\Delta_f S^0$	$\Delta_f H^0$	logK(25)
NPF3+		1.0	4.00	0.00	0.00	-1463.330	-1562.150	-331.442	0.000	20.300
1.00	NP+4		3.00	F-						
NPF4		0.0	4.00	0.00	0.00	-1772.248	-1897.500	-420.096	0.000	25.100
1.00	NP+4		4.00	F-						
NPNO3+3		3.0	9.00	0.00	0.00	-622.823	-762.950	-469.989	0.000	1.600
1.00	NP+4		1.00	NO3-						
NPNO32+2		2.0	14.00	0.00	0.00	-737.037	-969.800	-780.690	0.000	2.200
1.00	NP+4		2.00	NO3-						
NPO22OH+		3.0	12.00	0.00	0.00	-1805.908	-2007.030	-674.565	0.000	-4.000
2.00	NPO2+2		-1.00	H+		1.00	H2O			
NPO22OH2		2.0	12.00	0.00	0.00	-2029.349	-2292.860	-883.819	0.000	-6.400
2.00	NPO2+2		-2.00	H+		2.00	H2O			
NPO23OH5		1.0	18.00	0.00	0.00	-3473.212	-4010.950	-1803.583	0.000	-17.500
3.00	NPO2+2		-5.00	H+		5.00	H2O			
NPO2CL		0.0	4.00	0.00	0.00	-1045.649	-1145.280	-334.163	0.000	-0.100
1.00	NPO2+		1.00	CL-						
NPO2CL+		1.0	5.00	0.00	0.00	-928.447	-1027.680	-332.829	0.000	0.250
1.00	NPO2+2		1.00	CL-						
NPO2CO3		0.0	10.00	0.00	0.00	-1380.798	-1535.914	-520.261	0.000	10.000
1.00	NPO2+2		1.00	CO3-2						
NPO2CO32		-2.0	14.00	0.00	0.00	-1948.672	-2211.228	-880.616	0.000	17.000
1.00	NPO2+2		2.00	CO3-2						
NPO2CO33		-4.0	18.00	0.00	0.00	-2499.423	-2886.542	-1298.403	0.000	21.000
1.00	NPO2+2		3.00	CO3-2						
NPO2F+		1.0	6.00	0.00	0.00	-1103.006	-1195.950	-311.737	0.000	4.500
1.00	NPO2+2		1.00	F-						
NPO2F2		0.0	6.00	0.00	0.00	-1403.362	-1531.300	-429.107	0.000	7.800
1.00	NPO2+2		2.00	F-						
NPO2H2CO		-1.0	13.00	0.00	0.00	-2111.252	-2328.828	-729.752	0.000	24.600
1.00	NPO2+		2.00	CO3-2		2.00	H+			
NPO2HCO3		0.0	9.00	0.00	0.00	-1514.839	-1653.514	-465.120	0.000	12.600
1.00	NPO2+		1.00	CO3-2		1.00	H+			
NPO2HPO4		-1.0	5.00	0.00	0.00	-2031.246	-2262.600	-775.966	0.000	15.900
1.00	NPO2+		1.00	PO4-3		1.00	H+			
NPO2NO3		0.0	10.00	0.00	0.00	-1025.505	-1185.050	-535.118	0.000	-0.050
1.00	NPO2+		1.00	NO3-						
NPO2NO3+		1.0	11.00	0.00	0.00	-905.163	-1067.450	-544.313	0.000	-0.250
1.00	NPO2+2		1.00	NO3-						
NPO2OH		0.0	5.00	0.00	0.00	-1100.769	-1264.030	-547.581	0.000	-9.000
1.00	NPO2+		-1.00	H+		1.00	H2O			
NPO2OH+		1.0	6.00	0.00	0.00	-1003.830	-1146.430	-478.284	0.000	-5.100
1.00	NPO2+2		-1.00	H+		1.00	H2O			
NPO2OH2		0.0	6.00	0.00	0.00	-1204.439	-1432.260	-764.115	0.000	-11.500
1.00	NPO2+2		-2.00	H+		2.00	H2O			
NPO2OH3-		-1.0	6.00	0.00	0.00	-1389.066	-1718.090	-1103.551	0.000	-20.700
1.00	NPO2+2		-3.00	H+		3.00	H2O			

Table B.4: Selected aqueous species and minerals in 0391 MINEQL-PSI data base. Page 15 of 37

		Charge	OPV	DH a	DH b	$\Delta_f G^0$	$\Delta_f H^0$	$\Delta_f S^0$	$\Delta_r H^0$	logK(25)
NPO2SO4		0.0	12.00	0.00	0.00	-1558.636	-1769.940	-708.717	0.000	3.300
1.00	NPO2+2		1.00	SO4-2						
NPO2SO42		-2.0	18.00	0.00	0.00	-2310.627	-2679.280	-1236.468	0.000	4.700
1.00	NPO2+2		2.00	SO4-2						
NPOH+2		2.0	3.00	0.00	0.00	-714.285	-813.030	-331.194	0.000	-7.000
1.00	NP+3		-1.00	H+		1.00	H2O			
NPOH+3		3.0	4.00	0.00	0.00	-731.478	-841.930	-370.457	0.000	-1.500
1.00	NP+4		-1.00	H+		1.00	H2O			
NPOH2+		1.0	3.00	0.00	0.00	-905.761	-1098.860	-647.656	0.000	-15.000
1.00	NP+3		-2.00	H+		2.00	H2O			
NPOH2+2		2.0	4.00	0.00	0.00	-954.348	-1127.760	-581.625	0.000	-4.000
1.00	NP+4		-2.00	H+		2.00	H2O			
NPOH3		0.0	3.00	0.00	0.00	-1085.822	-1384.690	-1002.407	0.000	-25.000
1.00	NP+3		-3.00	H+		3.00	H2O			
NPOH3+		1.0	4.00	0.00	0.00	-1168.657	-1413.590	-821.510	0.000	-8.000
1.00	NP+4		-3.00	H+		3.00	H2O			
NPOH3CO3		-1.0	8.00	0.00	0.00	-1736.531	-2088.904	-1181.865	0.000	-1.000
1.00	NP+4		1.00	CO3-2		-3.00	H+	3.00	H2O	
NPOH4-		-1.0	3.00	0.00	0.00	-1265.883	-1670.520	-1357.158	0.000	-35.000
1.00	NP+3		-4.00	H+		4.00	H2O			
NPOH4		0.0	4.00	0.00	0.00	-1377.257	-1699.420	-1080.539	0.000	-13.000
1.00	NP+4		-4.00	H+		4.00	H2O			
NPOH5-		-1.0	4.00	0.00	0.00	-1574.442	-1985.250	-1377.857	0.000	-20.000
1.00	NP+4		-5.00	H+		5.00	H2O			
NPSO4+2		2.0	10.00	0.00	0.00	-1269.161	-1465.440	-658.324	0.000	3.900
1.00	NP+4		1.00	SO4-2						
NPSO42		0.0	16.00	0.00	0.00	-2023.435	-2374.780	-1178.417	0.000	5.700
1.00	NP+4		2.00	SO4-2						
OH-		-1.0	0.00	0.00	0.00	-157.229	-229.932	-243.845	55.898	-14.000
-1.00	H+		1.00	H2O						
PDBR+		1.0	1.00	0.00	0.00	31.325	27.590	-12.526	0.000	7.240
1.00	PD+2		1.00	BR-						
PDBR3-		-1.0	-1.00	0.00	0.00	-203.887	-215.230	-38.043	0.000	12.060
1.00	PD+2		3.00	BR-						
PDBR4-2		-2.0	-2.00	0.00	0.00	-317.555	-384.338	-223.990	-47.698	13.780
1.00	PD+2		4.00	BR-						
PDCL+		1.0	1.00	0.00	0.00	22.620	-37.912	-203.025	-19.832	3.970
1.00	PD+2		1.00	CL-						
PDCL2		0.0	0.00	0.00	0.00	-128.806	-185.160	-189.011	0.000	7.510
1.00	PD+2		2.00	CL-						
PDCL3-		-1.0	-1.00	0.00	0.00	-276.066	-352.240	-255.490	0.000	10.320
1.00	PD+2		3.00	CL-						
PDCL4-2		-2.0	-2.00	0.00	0.00	-417.103	-549.863	-445.279	-30.543	12.040
1.00	PD+2		4.00	CL-						
PDI+		1.0	1.00	0.00	0.00	65.189	92.220	90.661	0.000	10.440
1.00	PD+2		1.00	I-						

Table B.4: Selected aqueous species and minerals in 0391 MINEQL-PSI data base. Page 16 of 37

		Charge	OPV	DH a	DH b	$\Delta_f G^0$	$\Delta_f H^0$	$\Delta_f S^0$	$\Delta_f H^0$	logK(25)
PDI4-2 1.00	PD+2	-2.0 4.00	-2.00 I-	0.00	0.00	-159.607	-78.120	273.309	0.000	22.640
PDNH3+2 1.00	PD+2	2.0 1.00	-1.00 NH3	0.00	0.00	95.045	67.852	-91.206	0.000	9.600
PDNH32+2 1.00	PD+2	2.0 2.00	-4.00 NH3	0.00	0.00	17.586	-13.296	-103.578	0.000	18.500
PDNH33+2 1.00	PD+2	2.0 3.00	-7.00 NH3	0.00	0.00	-51.883	-94.444	-142.752	0.000	26.000
PDNH34+2 1.00	PD+2	2.0 4.00	-10.00 NH3	0.00	0.00	-117.355	-175.582	-195.327	0.000	32.800
PDNO34-2 1.00	PD+2	2.0 4.00	2.00 NO3-	0.00	0.00	-385.955	-678.400	-980.865	0.000	20.900
PDOH+ 1.00	PD+2	1.0 -1.00	2.00 H+	0.00	0.00	-50.023	-136.830	-291.151	0.000	-1.860
PDOH2 1.00	PD+2	0.0 -2.00	2.00 H+	0.00	0.00	-276.147	-422.660	-491.407	0.000	-3.790
PDOH3- 1.00	PD+2	-1.0 -3.00	2.00 H+	0.00	0.00	-443.936	-708.490	-887.319	0.000	-15.940
PDOH4-2 1.00	PD+2	-2.0 -4.00	2.00 H+	0.00	0.00	-604.362	-994.320	-1307.926	0.000	-29.380
PDSO42-2 1.00	PD+2	-2.0 2.00	14.00 SO4-2	0.00	0.00	-1335.702	-1669.680	-1120.169	0.000	4.240
PUCL+2 1.00	PU+3	2.0 1.00	2.00 CL-	0.00	0.00	-714.386	-759.080	-149.903	0.000	0.800
PUCL+3 1.00	PU+4	3.0 1.00	3.00 CL-	0.00	0.00	-617.957	-686.075	-228.467	17.405	0.900
PUCL2+2 1.00	PU+4	2.0 2.00	2.00 CL-	0.00	0.00	-754.885	-870.560	-387.976	0.000	1.900
PUCO3+ 1.00	PU+3	1.0 1.00	7.00 CO3-2	0.00	0.00	-1161.315	-1267.314	-355.523	0.000	9.600
PUCO3+2 1.00	PU+4	2.0 1.00	8.00 CO3-2	0.00	0.00	-1243.543	-1398.404	-519.406	-186.690	41.000
PUCO32- 1.00	PU+3	-1.0 2.00	11.00 CO3-2	0.00	0.00	-1708.070	-1942.628	-786.711	0.000	12.900
PUCO33-3 1.00	PU+3	-3.0 3.00	15.00 CO3-2	0.00	0.00	-2254.825	-2617.942	-1217.900	0.000	16.200
PUEDTA- 1.00	PU+3	-1.0 1.00	3.00 EDTA-4	0.00	0.00	-696.754	-592.000	351.345	0.000	20.700
PUF+3 1.00	PU+4	3.0 1.00	4.00 F-	0.00	0.00	-808.212	-847.064	-130.310	24.686	7.900
PUH2PO4+ 1.00	PU+3	2.0 1.00	3.00 PO4-3	0.00	0.00	-1729.721	-1861.840	-443.128	14.560	22.010
PUH2PO42 1.00	PU+4	0.0 2.00	4.00 PO4-3	0.00	0.00	-2812.267	-3107.752	-991.061	-2.552	49.000
PUH2SO42 1.00	PU+3	1.0 2.00	15.00 SO4-2	0.00	0.00	-2105.985	-2410.680	-1021.954	0.000	6.900

Table B.4: Selected aqueous species and minerals in 0391 MINEQL-PSI data base. Page 17 of 37

		Charge	OPV	DH a	DH b	$\Delta_f G^0$	$\Delta_f H^0$	$\Delta_f S^0$	$\Delta_r H^0$	logK(25)
PUH3PO43		-2.0	4.00	0.00	0.00	-3957.623	-4438.511	-1612.905	-48.911	70.000
1.00	PU+4		3.00	PO4-3		3.00	H+			
PUH4PO44		-4.0	4.00	0.00	0.00	-5110.971	-5806.549	-2332.982	-132.549	92.400
1.00	PU+4		4.00	PO4-3		4.00	H+			
PUHPO4+2		2.0	4.00	0.00	0.00	-1654.925	-1794.776	-469.062	26.024	25.900
1.00	PU+4		1.00	PO4-3		1.00	H+			
PUNO3+3		3.0	9.00	0.00	0.00	-602.664	-743.250	-471.527	0.000	1.800
1.00	PU+4		1.00	NO3-						
PUO22OH+		3.0	12.00	0.00	0.00	-1726.396	-1930.230	-683.663	0.000	-4.300
2.00	PUO2+2		-1.00	H+		1.00	H2O			
PUO22OH2		2.0	12.00	0.00	0.00	-1940.704	-2158.195	-729.468	57.865	-8.300
2.00	PUO2+2		-2.00	H+		2.00	H2O			
PUO23OH5		1.0	18.00	0.00	0.00	-3332.538	-3756.004	-1420.312	139.746	-21.700
3.00	PUO2+2		-5.00	H+		5.00	H2O			
PUO2CL		0.0	4.00	0.00	0.00	-981.990	-1081.680	-334.361	0.000	0.170
1.00	PUO2+		1.00	CL-						
PUO2CL+		1.0	5.00	0.00	0.00	-889.262	-977.690	-296.591	11.590	0.200
1.00	PUO2+2		1.00	CL-						
PUO2CL2		0.0	4.00	0.00	0.00	-1017.913	-1156.360	-464.353	0.000	-0.250
1.00	PUO2+2		2.00	CL-						
PUO2CO3		0.0	10.00	0.00	0.00	-1360.163	-1497.514	-460.676	0.000	13.200
1.00	PUO2+2		1.00	CO3-2						
PUO2CO32		-2.0	14.00	0.00	0.00	-1897.786	-2145.758	-831.701	27.070	14.900
1.00	PUO2+2		2.00	CO3-2						
PUO2CO33		-4.0	18.00	0.00	0.00	-2459.952	-2848.142	-1301.995	0.000	20.900
1.00	PUO2+2		3.00	CO3-2						
PUO2EDTA		-2.0	6.00	0.00	0.00	-860.213	-822.200	127.497	0.000	18.100
1.00	PUO2+2		1.00	EDTA-4						
PUO2F+		1.0	6.00	0.00	0.00	-1070.955	-1162.947	-308.544	-5.397	5.700
1.00	PUO2+2		1.00	F-						
PUO2F2		0.0	6.00	0.00	0.00	-1382.727	-1508.255	-421.024	-15.355	11.000
1.00	PUO2+2		2.00	F-						
PUO2F3-		-1.0	6.00	0.00	0.00	-1691.645	-1857.412	-555.987	-29.162	15.800
1.00	PUO2+2		3.00	F-						
PUO2F4-2		-2.0	6.00	0.00	0.00	-1989.718	-2203.808	-718.063	-40.208	18.700
1.00	PUO2+2		4.00	F-						
PUO2H2PO		1.0	6.00	0.00	0.00	-1916.583	-2127.394	-707.066	-20.794	23.510
1.00	PUO2+2		1.00	PO4-3		2.00	H+			
PUO2OH		0.0	5.00	0.00	0.00	-1031.573	-1131.101	-333.818	69.329	-9.700
1.00	PUO2+		-1.00	H+		1.00	H2O			
PUO2OH+		1.0	6.00	0.00	0.00	-962.076	-1062.801	-337.834	45.229	-5.600
1.00	PUO2+2		-1.00	H+		1.00	H2O			
PUO2OH2		0.0	6.00	0.00	0.00	-1168.393	-1393.860	-756.220	0.000	-11.000
1.00	PUO2+2		-2.00	H+		2.00	H2O			
PUO2OH2C		-2.0	10.00	0.00	0.00	-1730.559	-2069.174	-1135.719	0.000	-5.000
1.00	PUO2+2		1.00	CO3-2		-2.00	H+	2.00	H2O	

Table B.4: Selected aqueous species and minerals in 0391 MINEQL-PSI data base. Page 18 of 37

		Charge	OPV	DH a	DH b	$\Delta_f G^0$	$\Delta_f H^0$	$\Delta_f S^0$	$\Delta_f H^0$	logK(25)
PUO2OH3-	1.00	-1.0	6.00	0.00	0.00	-1350.166	-1679.690	-1105.228	0.000	-20.700
					3.00	H2O				
PUO2OHCO	1.00	-1.0	10.00	0.00	0.00	-1578.182	-1783.344	-688.117	0.000	9.850
					1.00	CO3-2	-1.00	H+	1.00	H2O
PUO2SO4	1.00	0.0	12.00	0.00	0.00	-1518.024	-1711.457	-648.778	20.083	3.000
					1.00	SO4-2				
PUOH+2	1.00	2.0	3.00	0.00	0.00	-775.785	-824.191	-162.356	53.639	-7.000
					-1.00	H+	1.00	H2O		
PUOH+3	1.00	3.0	4.00	0.00	0.00	-714.744	-773.947	-198.565	48.283	-0.700
					-1.00	H+	1.00	H2O		
PUOH2+	1.00	1.0	3.00	0.00	0.00	-967.261	-1163.660	-658.724	0.000	-15.000
					-2.00	H+	2.00	H2O		
PUOH2+2	1.00	2.0	4.00	0.00	0.00	-942.752	-1033.543	-304.515	74.517	-2.300
					-2.00	H+	2.00	H2O		
PUOH3	1.00	0.0	3.00	0.00	0.00	-1141.614	-1449.490	-1032.620	0.000	-26.000
					-3.00	H+	3.00	H2O		
PUOH3+	1.00	1.0	4.00	0.00	0.00	-1162.768	-1297.365	-451.441	96.525	-5.300
					-3.00	H+	3.00	H2O		
PUOH3CO3	1.00	-1.0	8.00	0.00	0.00	-1715.231	-2069.204	-1187.231	0.000	-1.000
					1.00	CO3-2	-3.00	H+	3.00	H2O
PUOH4-	1.00	-1.0	3.00	0.00	0.00	-1338.799	-1735.320	-1329.938	0.000	-33.000
					-4.00	H+	4.00	H2O		
PUOH4	1.00	0.0	4.00	0.00	0.00	-1375.935	-1570.476	-652.493	109.244	-9.500
					-4.00	H+	4.00	H2O		
PUOH5-	1.00	-1.0	4.00	0.00	0.00	-1581.681	-1839.695	-865.383	125.855	-15.000
					-5.00	H+	5.00	H2O		
PUSO4+	1.00	1.0	9.00	0.00	0.00	-1340.295	-1486.738	-491.173	14.602	3.100
					1.00	SO4-2				
PUSO4+2	1.00	2.0	10.00	0.00	0.00	-1258.706	-1433.272	-585.497	12.468	5.800
					1.00	SO4-2				
PUSO42	1.00	0.0	16.00	0.00	0.00	-2027.821	-2313.742	-958.985	41.338	10.200
					2.00	SO4-2				
PUSO43-2	1.00	-2.0	22.00	0.00	0.00	-2779.241	-3264.420	-1627.299	0.000	11.500
					3.00	SO4-2				
S-2	-1.00	-2.0	-2.00	0.00	0.00	120.690	-16.300	-459.467	0.000	-19.000
					1.00	HS-				
SE-2	1.00	-2.0	-2.00	0.00	0.00	129.447	15.900	-380.840	0.000	-14.970
					-1.00	H+				
SIF6-2	6.00	-2.0	0.00	0.00	0.00	-2220.560	-2393.791	-581.021	-143.051	53.320
					1.00	H2SiO4-2	6.00	F-	-4.00	H2O
SNBR+	1.00	1.0	1.00	0.00	0.00	-137.729	-130.310	24.882	0.000	1.100
					1.00	BR-				
SNBR2	1.00	0.0	0.00	0.00	0.00	-245.003	-251.720	-22.527	0.000	1.700
					2.00	BR-				
SNBR3-	1.00	-1.0	-1.00	0.00	0.00	-347.141	-373.130	-87.167	0.000	1.400
					3.00	BR-				

Table B.4: Selected aqueous species and minerals in 0391 MINEQL-PSI data base. Page 19 of 37

		Charge	OPV	DH a	DH b	$\Delta_f G^0$	$\Delta_f H^0$	$\Delta_f S^0$	$\Delta_r H^0$	logK(25)
SNEDTA-2 1.00	SN+2	-2.0	2.00	0.00	0.00	-168.014	-8.900	533.673	0.000	24.600
				1.00	EDTA-4					
SNF+ 1.00	SN+2	1.0	2.00	0.00	0.00	-348.505	-344.250	14.270	0.000	6.900
				1.00	F-					
SNF2 1.00	SN+2	0.0	2.00	0.00	0.00	-646.007	-679.600	-112.673	0.000	9.700
				2.00	F-					
SNF3- 1.00	SN+2	-1.0	2.00	0.00	0.00	-930.381	-1014.950	-283.647	0.000	10.200
				3.00	F-					
SNOH+ 1.00	SN+2	1.0	2.00	0.00	0.00	-246.475	-294.730	-161.849	0.000	-3.200
				-1.00	H+	1.00	H2O			
SRCIT- 1.00	SR+2	-1.0	0.00	0.00	0.00	-587.289	-550.900	122.051	0.000	4.110
				1.00	CIT-3					
SRCL2 1.00	SR+2	0.0	-2.00	0.00	0.00	-826.270	-885.060	-197.183	0.000	0.000
				2.00	CL-					
SRCO3 1.00	SR+2	0.0	4.00	0.00	0.00	-1107.788	-1204.374	-323.949	21.840	2.810
				1.00	CO3-2					
SREDITA-2 1.00	SR+2	-2.0	0.00	0.00	0.00	-623.192	-550.900	242.469	0.000	10.400
				1.00	EDTA-4					
SRHCO3+ 1.00	SR+2	1.0	4.00	0.00	0.00	-1157.447	-1215.796	-195.703	10.418	11.510
				1.00	CO3-2	1.00	H+			
SRHEDTA- 1.00	SR+2	-1.0	0.00	0.00	0.00	-647.736	-550.900	324.790	0.000	14.700
				1.00	EDTA-4	1.00	H+			
SRHPO4 1.00	SR+2	0.0	0.00	0.00	0.00	-1669.801	-1835.300	-555.085	0.000	14.100
				1.00	PO4-3	1.00	H+			
SRNO3+ 1.00	SR+2	1.0	5.00	0.00	0.00	-679.186	-757.750	-263.504	0.000	0.800
				1.00	NO3-					
SRNO32 1.00	SR+2	0.0	10.00	0.00	0.00	-789.976	-964.600	-585.691	0.000	0.800
				2.00	NO3-					
SRNTA- 1.00	SR+2	-1.0	0.00	0.00	0.00	-603.215	-550.900	175.464	0.000	6.900
				1.00	NTA-3					
SROH+ 1.00	SR+2	1.0	0.00	0.00	0.00	-725.112	-776.062	-170.887	60.668	-13.290
				-1.00	H+	1.00	H2O			
SROX 1.00	SR+2	0.0	0.00	0.00	0.00	-574.675	-550.900	79.742	0.000	1.900
				1.00	OX-2					
SRPO4- 1.00	SR+2	-1.0	0.00	0.00	0.00	-1623.567	-1835.300	-710.154	0.000	6.000
				1.00	PO4-3					
SRS2O3 1.00	SR+2	0.0	0.00	0.00	0.00	-1094.536	-1199.400	-351.716	0.000	2.000
				1.00	S2O3-2					
SRSO4 1.00	SR+2	0.0	6.00	0.00	0.00	-1320.901	-1451.537	-438.156	8.703	2.290
				1.00	SO4-2					
TCOOH+ 1.00	TCO+2	1.0	4.00	0.00	0.00	-329.749	-285.830	147.305	0.000	-1.400
				-1.00	H+	1.00	H2O			
TCOOH2 1.00	TCO+2	0.0	4.00	0.00	0.00	-555.473	-571.660	-54.291	0.000	-3.400
				-2.00	H+	2.00	H2O			
TH2OH2+6 2.00	TH+4	6.0	0.00	0.00	0.00	-1849.462	-2047.737	-665.018	61.923	-6.100
				-2.00	H+	2.00	H2O			

Table B.4: Selected aqueous species and minerals in 0391 MINEQL-PSI data base. Page 20 of 37

		Charge	OPV	DH a	DH b	$\Delta_f G^0$	$\Delta_f H^0$	$\Delta_f S^0$	$\Delta_r H^0$	logK(25)
TH4OH8+8	4.00	TH+4	8.0 -8.00	0.00 H+	0.00 8.00	-4596.683 H2O	-5120.805 15.00	-1757.913	241.835	-21.100
TH6OH15+	6.00	TH+4	9.0 -15.00	0.00 H+	0.00 15.00	-7577.620 H2O	-8447.904 34.220	-2918.949	453.546	-36.700
THCIT+	1.00	TH+4	1.0 1.00	0.00 CIT-3	0.00 2.00	-779.203 CIT-3	-769.000 187.376	34.220 0.000	0.000	13.000
THCIT2-2	1.00	TH+4	-2.0 2.00	0.00 CIT-3	0.00 2.00	-824.866 CIT-3	-769.000 187.376	187.376 0.000	0.000	21.000
THCL+3	1.00	TH+4	3.0 1.00	-1.00 CL-	0.00 1.00	-842.499 CL-	-936.917 -316.680	-316.680 -0.837	-0.837	1.100
THCL2+2	1.00	TH+4	2.0 2.00	-2.00 CL-	0.00 2.00	-972.006 CL-	-1015.714 -146.598	-146.598 87.446	87.446	0.800
THCL3+	1.00	TH+4	1.0 3.00	-3.00 CL-	0.00 3.00	-1108.078 CL-	-1204.342 -322.871	-322.871 65.898	65.898	1.650
THCL4	1.00	TH+4	0.0 4.00	-4.00 CL-	0.00 4.00	-1237.072 CL-	-1385.857 -499.027	-499.027 51.463	51.463	1.260
THCO3+2	1.00	TH+4	2.0 1.00	4.00 CO3-2	0.00 1.00	-1295.706 CO3-2	-1444.314 -498.434	-498.434 0.000	0.000	11.000
THEDETA	1.00	TH+4	0.0 1.00	0.00 EDTA-4	0.00 1.00	-857.401 EDTA-4	-769.000 296.499	296.499 0.000	0.000	26.700
THF+3	1.00	TH+4	3.0 1.00	0.00 F-	0.00 1.00	-1032.183 F-	-1110.208 -261.695	-261.695 -5.858	-5.858	8.000
THF2+2	1.00	TH+4	2.0 2.00	0.00 F-	0.00 2.00	-1349.092 F-	-1448.486 -333.370	-333.370 -8.786	-8.786	14.200
THF3+	1.00	TH+4	1.0 3.00	0.00 F-	0.00 3.00	-1657.439 F-	-1787.602 -436.567	-436.567 -12.552	-12.552	18.900
THF4	1.00	TH+4	0.0 4.00	0.00 F-	0.00 4.00	-1958.366 F-	-2126.299 -563.250	-563.250 -15.899	-15.899	22.300
THH2PO4+	1.00	TH+4	3.0 1.00	0.00 PO4-3	0.00 2.00	-1868.051 PO4-3	-1999.426 H+	-440.637 53.974	53.974	24.100
THH2PO42	1.00	TH+4	0.0 2.00	0.00 PO4-3	0.00 2.00	-3047.654 PO4-3	-3380.686 H+	-1116.995 -42.886	-42.886	51.100
THH3PO4+	1.00	TH+4	4.0 1.00	0.00 PO4-3	0.00 3.00	-1865.197 PO4-3	-1996.079 H+	-438.982 57.321	57.321	23.600
THH3PO43	1.00	TH+4	-2.0 3.00	0.00 PO4-3	0.00 3.00	-4192.439 PO4-3	-4687.889 H+	-1661.746 -65.689	-65.689	72.000
THH4PO42	1.00	TH+4	2.0 2.00	0.00 PO4-3	0.00 4.00	-3030.074 PO4-3	-3353.699 H+	-1085.445 -15.899	-15.899	48.020
THHEDTA+	1.00	TH+4	1.0 1.00	0.00 EDTA-4	0.00 1.00	-868.817 EDTA-4	-769.000 H+	334.788 0.000	0.000	28.700
THHPO4+2	1.00	TH+4	2.0 1.00	0.00 PO4-3	0.00 1.00	-1876.327 PO4-3	-2068.462 H+	-644.425 -15.062	-644.425 -15.062	25.550
THNO3+3	1.00	TH+4	3.0 1.00	5.00 NO3-	0.00 1.00	-821.155 NO3-	-975.850 -518.848	-518.848 0.000	0.000	0.940
THNO32+2	1.00	TH+4	2.0 2.00	10.00 NO3-	0.00 2.00	-937.825 NO3-	-1182.700 -821.316	-821.316 0.000	0.000	1.970

Table B.4: Selected aqueous species and minerals in 0391 MINEQL-PSI data base. Page 21 of 37

		Charge	OPV	DH a	DH b	$\Delta_f G^0$	$\Delta_f H^0$	$\Delta_f S^0$	$\Delta_f H^0$	logK(25)
THNTA+		1.0	0.00	0.00	0.00	-802.605	-769.000	112.712	0.000	17.100
	1.00	TH+4		1.00	NTA-3					
THOH+3		3.0	0.00	0.00	0.00	-923.875	-1029.935	-355.729	24.895	-3.200
	1.00	TH+4		-1.00	H+		1.00	H2O		
THOH2+2		2.0	0.00	0.00	0.00	-1139.610	-1282.921	-480.667	57.739	-6.950
	1.00	TH+4		-2.00	H+		2.00	H2O		
THOH2EDT		-2.0	0.00	0.00	0.00	-2129.720	-2109.660	67.281	0.000	43.000
	2.00	TH+4		2.00	EDTA-4		-2.00	H+	2.00	H2O
THOH3+		1.0	0.00	0.00	0.00	-1349.637	-1541.136	-642.290	85.354	-11.700
	1.00	TH+4		-3.00	H+		3.00	H2O		
THOH4		0.0	0.00	0.00	0.00	-1562.804	-1808.975	-825.661	103.345	-15.900
	1.00	TH+4		-4.00	H+		4.00	H2O		
THOHEDTA		-1.0	0.00	0.00	0.00	-1053.444	-1054.830	-4.648	0.000	19.500
	1.00	TH+4		1.00	EDTA-4		-1.00	H+	1.00	H2O
THOX+2		2.0	0.00	0.00	0.00	-758.084	-769.000	-36.614	0.000	9.300
	1.00	TH+4		1.00	OX-2					
THOX2		0.0	0.00	0.00	0.00	-810.596	-769.000	139.515	0.000	18.500
	1.00	TH+4		2.00	OX-2					
THOX3-2		-2.0	0.00	0.00	0.00	-851.693	-769.000	277.354	0.000	25.700
	1.00	TH+4		3.00	OX-2					
THSO4+2		2.0	6.00	0.00	0.00	-1480.108	-1662.859	-612.950	15.481	5.450
	1.00	TH+4		1.00	SO4-2					
THSO42		0.0	12.00	0.00	0.00	-2248.652	-2556.300	-1031.856	31.380	9.750
	1.00	TH+4		2.00	SO4-2					
THSO43-2		-2.0	18.00	0.00	0.00	-2996.933	-3448.067	-1513.111	48.953	10.500
	1.00	TH+4		3.00	SO4-2					
THSO44-4		-4.0	24.00	0.00	0.00	-3729.517	-4351.550	-2086.307	54.810	8.500
	1.00	TH+4		4.00	SO4-2					
UBR+3		3.0	3.00	0.00	0.00	-641.986	-712.610	-236.873	0.000	1.450
	1.00	U+4		1.00	BR-					
UCL+3		3.0	3.00	0.00	0.00	-670.898	-777.275	-356.793	-18.995	1.720
	1.00	U+4		1.00	CL-					
UCO34-4		-4.0	20.00	0.00	0.00	-2841.998	-3292.456	-1510.845	0.000	35.120
	1.00	U+4		4.00	CO3-2					
UCO35-6		-6.0	24.00	0.00	0.00	-3363.524	-3987.770	-2093.730	-20.000	34.000
	1.00	U+4		5.00	CO3-2					
UEDTA		0.0	4.00	0.00	0.00	-696.531	-591.200	353.281	0.000	29.200
	1.00	U+4		1.00	EDTA-4					
UF+3		3.0	4.00	0.00	0.00	-864.406	-932.198	-227.375	-5.648	9.290
	1.00	U+4		1.00	F-					
UF2+2		2.0	4.00	0.00	0.00	-1185.539	-1265.415	-267.903	-3.515	16.230
	1.00	U+4		2.00	F-					
UF3+		1.0	4.00	0.00	0.00	-1497.597	-1596.748	-332.555	0.502	21.580
	1.00	U+4		3.00	F-					
UF4		0.0	4.00	0.00	0.00	-1801.606	-1936.240	-451.566	-3.640	25.520
	1.00	U+4		4.00	F-					

Table B.4: Selected aqueous species and minerals in 0391 MINEQL-PSI data base. Page 22 of 37

		Charge	OPV	DH a	DH b	$\Delta_f G^0$	$\Delta_f H^0$	$\Delta_f S^0$	$\Delta_r H^0$	logK(25)
UF5-	1.00	U+4	-1.0 5.00	4.00 F-	0.00	0.00 -2091.745	-2267.950	-590.995	0.000	27.030
UF6-2	1.00	U+4	-2.0 6.00	4.00 F-	0.00	0.00 -2385.137	-2603.300	-731.722	0.000	29.110
UI+3	1.00	U+4	3.0 1.00	3.00 I-	0.00	0.00 -588.715	-647.980	-198.776	0.000	1.250
UL2EDTA	2.00	UO2+2	0.0 1.00	12.00 EDTA-4	0.00	0.00 -2022.114	-2038.000	-53.282	0.000	20.500
UL2EDTA2	2.00	UO2+2	-4.0 2.00	12.00 EDTA-4	0.00	0.00 -2053.508	-2038.000	52.013	0.000	26.000
ULCO33-4	1.00	UO2+2	-4.0 3.00	18.00 CO3-2	0.00	0.00 -2659.713	-3083.226	-1420.468	-38.284	21.620
UNO3+3	1.00	U+4	3.0 1.00	9.00 NO3-	0.00	0.00 -649.041	-798.050	-499.780	0.000	1.470
UNO32+2	1.00	U+4	2.0 2.00	14.00 NO3-	0.00	0.00 -764.568	-1004.900	-806.077	0.000	2.300
UO21609	11.00	UO2+2	-2.0 6.00	90.00 CO3-2	0.00 -16698.566	-18690.844	-6682.133	0.000	36.320	
UO22CO3O	2.00	UO2+2	-1.0 1.00	16.00 CO3-2	0.00 -3139.418	-3570.804	-1446.876	0.000	-0.880	
UO22OH+3	2.00	UO2+2	3.0 -1.00	12.00 H+	0.00 -2126.716	-2323.830	-661.122	0.000	-2.720	
UO22OH2+	2.00	UO2+2	2.0 -2.00	12.00 H+	0.00 -2347.189	-2572.004	-754.032	37.656	-5.640	
UO23CO36	3.00	UO2+2	-6.0 6.00	42.00 CO3-2	0.00 -6333.280	-7177.585	-2831.815	-68.701	53.980	
UO23OH4+	3.00	UO2+2	2.0 -4.00	18.00 H+	0.00 -3738.118	-4200.320	-1550.234	0.000	-11.930	
UO23OH5+	3.00	UO2+2	1.0 -5.00	18.00 H+	0.00 -3954.424	-4389.081	-1457.848	97.069	-15.580	
UO23OH5C	3.00	UO2+2	1.0 1.00	22.00 CO3-2	0.00 -4338.470	-4875.634	-1801.657	0.000	0.760	
UO23OH7-	3.00	UO2+2	-1.0 -7.00	18.00 H+	0.00 -4340.517	-5057.810	-2405.814	0.000	-31.030	
UO24OH7+	4.00	UO2+2	1.0 -7.00	24.00 H+	0.00 -5345.181	-6076.810	-2453.896	0.000	-21.900	
UO2BR+	1.00	UO2+2	1.0 1.00	5.00 BR-	0.00 -1057.543	-1140.410	-277.939	0.000	0.200	
UO2CL+	1.00	UO2+2	1.0 1.00	5.00 CL-	0.00 -1084.171	-1178.089	-315.003	7.991	0.070	
UO2CL2	1.00	UO2+2	0.0 2.00	4.00 CL-	0.00 -1208.712	-1338.139	-434.101	15.021	-1.100	
UO2CO3	1.00	UO2+2	0.0 1.00	10.00 CO3-2	0.00 -1535.380	-1689.293	-516.227	5.021	9.620	
UO2CO32-	1.00	UO2+2	-2.0 2.00	14.00 CO3-2	0.00 -2105.366	-2351.177	-824.452	18.451	16.990	

Table B.4: Selected aqueous species and minerals in 0391 MINEQL-PSI data base. Page 23 of 37

		Charge	OPV	DH a	DH b	$\Delta_f G^0$	$\Delta_f H^0$	$\Delta_f S^0$	$\Delta_r H^0$	logK(25)
UO2CO33-		-5.0	17.00	0.00	0.00	-2587.188	-3051.069	-1555.865	0.000	7.430
1.00	UO2+		3.00	CO3-2						
UO2EDTA-		-2.0	6.00	0.00	0.00	-1021.046	-1019.000	6.862	0.000	12.000
1.00	UO2+2		1.00	EDTA-4						
UO2F+		1.0	6.00	0.00	0.00	-1263.124	-1352.635	-300.219	1.715	5.080
1.00	UO2+2		1.00	F-						
UO2F2		0.0	6.00	0.00	0.00	-1564.793	-1687.608	-411.923	2.092	8.620
1.00	UO2+2		2.00	F-						
UO2F3-		-1.0	6.00	0.00	0.00	-1859.327	-2022.707	-547.978	2.343	10.900
1.00	UO2+2		3.00	F-						
UO2F4-2		-2.0	6.00	0.00	0.00	-2145.471	-2360.107	-719.894	0.293	11.710
1.00	UO2+2		4.00	F-						
UO2H2PO4		1.0	6.00	0.00	0.00	-2108.352	-2303.400	-654.193	0.000	22.830
1.00	UO2+2		1.00	PO4-3		2.00	H+			
UO2H3PO4		2.0	6.00	0.00	0.00	-2106.355	-2303.400	-660.893	0.000	22.480
1.00	UO2+2		1.00	PO4-3		3.00	H+			
UO2H4PO4		0.0	6.00	0.00	0.00	-3256.391	-3587.800	-1111.550	0.000	44.300
1.00	UO2+2		2.00	PO4-3		4.00	H+			
UO2H5PO4		1.0	6.00	0.00	0.00	-3261.072	-3587.800	-1095.852	0.000	45.120
1.00	UO2+2		2.00	PO4-3		5.00	H+			
UO2HEDTA		-1.0	6.00	0.00	0.00	-1064.997	-1019.000	154.274	0.000	19.700
1.00	UO2+2		1.00	EDTA-4		1.00	H+			
UO2HPO4		0.0	6.00	0.00	0.00	-2092.599	-2303.400	-707.031	0.000	20.070
1.00	UO2+2		1.00	PO4-3		1.00	H+			
UO2NO3+		1.0	11.00	0.00	0.00	-1064.996	-1225.850	-539.506	0.000	0.290
1.00	UO2+2		1.00	NO3-						
UO2OH+		1.0	6.00	0.00	0.00	-1159.953	-1261.693	-341.238	43.137	-5.210
1.00	UO2+2		-1.00	H+		1.00	H2O			
UO2OH2		0.0	6.00	0.00	0.00	-1367.925	-1590.660	-747.055	0.000	-10.320
1.00	UO2+2		-2.00	H+		2.00	H2O			
UO2OH3-		-1.0	6.00	0.00	0.00	-1554.322	-1876.490	-1080.556	0.000	-19.210
1.00	UO2+2		-3.00	H+		3.00	H2O			
UO2OH4-2		-2.0	6.00	0.00	0.00	-1712.693	-2162.320	-1508.056	0.000	-33.010
1.00	UO2+2		-4.00	H+		4.00	H2O			
UO2OHEDT		-3.0	6.00	0.00	0.00	-1221.084	-1304.830	-280.884	0.000	5.500
1.00	UO2+2		1.00	EDTA-4		-1.00	H+	1.00	H2O	
UO2PO4-		-1.0	6.00	0.00	0.00	-2056.182	-2303.400	-829.172	0.000	13.690
1.00	UO2+2		1.00	PO4-3						
UO2S2O3		0.0	6.00	0.00	0.00	-1487.823	-1667.500	-602.639	0.000	2.800
1.00	UO2+2		1.00	S2O3-2						
UO2SO3		0.0	10.00	0.00	0.00	-1477.636	-1654.500	-593.204	0.000	6.590
1.00	UO2+2		1.00	SO3-2						
UO2SO4		0.0	12.00	0.00	0.00	-1714.474	-1908.884	-652.056	19.456	3.140
1.00	UO2+2		1.00	SO4-2						
UO2SO42-		-2.0	18.00	0.00	0.00	-2464.182	-2802.660	-1135.261	35.020	4.140
1.00	UO2+2		2.00	SO4-2						

Table B.4: Selected aqueous species and minerals in 0391 MINEQL-PSI data base. Page 24 of 37

	Charge	OPV	DH a	DH b	$\Delta_f G^0$	$\Delta_f H^0$	$\Delta_f S^0$	$\Delta_f H^0$	logK(25)
UOH+	1.00 U+4	3.0 -1.00	4.00 H+	0.00 1.00	0.00 -763.975	-830.127	-221.877	46.903	-0.530
UOH2EDTA	2.00 U+4	-2.0 2.00	8.00 EDTA-4	0.00 -2.00	-1830.240 H+	-1754.060 2.00	255.510 H2O	0.000	51.900
UOH4	1.00 U+4	0.0 -4.00	4.00 H+	0.00 4.00	-1452.563 H2O	-1734.520	-945.688	0.000	-4.530
UOH5-	1.00 U+4	-1.0 -5.00	4.00 H+	0.00 5.00	-1621.151 H2O	-2020.350	-1338.919	0.000	-16.540
UOHEDTA-	1.00 U+4	-1.0 1.00	4.00 EDTA-4	0.00 -1.00	-905.702 H+	-877.030 1.00	96.167 H2O	0.000	24.300
USO4+2	1.00 U+4	2.0 1.00	10.00 SO4-2	0.00 1.00	0.00 -1311.418	-1492.590	-607.655	7.950	6.580
USO42	1.00 U+4	0.0 2.00	16.00 SO4-2	0.00 1.00	0.00 -2077.850	-2377.287	-1004.315	32.593	10.510

Table B.4: Selected aqueous species and minerals in 0391 MINEQL-PSI data base. Page 25 of 37

	Charge	OPV	DH a	DH b	$\Delta_f G^0$	$\Delta_f H^0$	$\Delta_f S^0$	$\Delta_r H^0$	logK(25)
MINERALS									
A_NA2UO4		6.00			-1679.149	-1899.001	-737.388	172.339	-47.580
1.00 UO2+2		2.00	NA+		-4.00 H+	2.00	H2O		
A_U3O8		16.00			-3369.421	-3574.849	-689.006	66.065	3.600
1.00 UO2+2		2.00	UO2+		-4.00 H+	2.00	H2O		
A_UF5		5.00			-1968.772	-2075.323	-357.373	54.894	13.040
1.00 UO2+		5.00	F-		4.00 H+	-2.00	H2O		
AL(OH)3CR		0.00			-1141.275	-1285.014	-482.104	110.876	-10.800
1.00 AL+3		-3.00	H+		3.00 H2O				
ALASO4		5.00			-1234.661	-1426.540	-643.565	-0.000	16.600
1.00 AL+3		1.00	ASO4-3						
ALPO4CR		0.00			-1645.418	-1822.800	-594.943	-0.000	22.500
1.00 AL+3		1.00	PO4-3						
AM(OH)3CR		3.00			-1203.782	-1474.190	-906.952	-0.000	-18.700
1.00 AM+3		-3.00	H+		3.00 H2O				
ANHYDRIT		6.00			-1321.693	-1445.185	-414.194	7.155	4.360
1.00 CA+2		1.00	SO4-2						
ARAGONIT		4.00			-1128.330	-1207.477	-265.462	10.837	8.340
1.00 CA+2		1.00	CO3-2						
AS_ELEM		0.00			0.028	-0.002	-0.102	-255.182	52.580
1.00 ASO4-3		8.00	H+		5.00 E-	-4.00	H2O		
B_SRUO4		6.00			-1881.298	-1989.597	-363.239	151.963	-19.160
1.00 UO2+2		1.00	SR+2		-4.00 H+	2.00	H2O		
B_U3O7		14.00			-3241.749	-3426.059	-618.179	72.885	13.740
2.00 UO2+		1.00	U+4		-6.00 H+	3.00	H2O		
B_U4O9		18.00			-4277.910	-4513.272	-789.408	148.532	19.350
2.00 UO2+		2.00	U+4		-10.00 H+	5.00	H2O		
B_UF5		5.00			-1970.713	-2083.231	-377.387	46.986	13.380
1.00 UO2+		5.00	F-		4.00 H+	-2.00	H2O		
B_UO2OH2		6.00			-1398.634	-1533.799	-453.347	56.861	-4.940
1.00 UO2+2		-2.00	H+		2.00 H2O				
BA(OH)2CR		0.00			-2787.487	-3390.800	-2023.521	-0.000	-24.400
1.00 BA+2		-2.00	H+		10.00 H2O				
BA3ASO42		10.00			-3275.693	-3373.780	-328.985	-0.000	54.800
3.00 BA+2		2.00	ASO4-3						
BAF2CR		0.00			-1153.218	-1203.200	-167.640	-0.000	6.100
1.00 BA+2		2.00	F-						
BAOXAL		0.00			-590.749	-532.500	195.368	-0.000	6.200
1.00 BA+2		1.00	OX-2						
BARITE		6.00			-1356.268	-1468.408	-376.121	-26.568	9.970
1.00 BA+2		1.00	SO4-2						
BASE		-2.00			-383.674	-387.733	-13.613	128.867	-22.370
1.00 BA+2		1.00	HSE-		-1.00 H+				
BASEO3		4.00			-962.718	-1035.424	-243.857	6.276	6.580
1.00 BA+2		1.00	SEO3-2						

Table B.4: Selected aqueous species and minerals in 0391 MINEQL-PSI data base. Page 26 of 37

		Charge	OPV	DH a	DH b	$\Delta_f G^0$	$\Delta_f H^0$	$\Delta_f S^0$	$\Delta_f H^0$	logK(25)
BASEO3CR			4.00			-962.832	-1041.700	-264.524	-0.000	6.600
1.00	BA+2		1.00	SEO3-2						
BASEO4CR			6.00			-1039.298	-1141.223	-341.859	-9.623	7.470
1.00	BA+2		1.00	SEO4-2						
BAUO4			6.00			-1886.983	-1997.096	-369.321	126.064	-16.680
1.00	UO2+2		1.00	BA+2		-4.00	H+	2.00	H2O	
BRUCITE			0.00			-833.559	-925.274	-307.613	113.386	-16.840
1.00	MG+2		-2.00	H+		2.00	H2O			
CA3ASO42			10.00			-3085.952	-3405.280	-1071.031	-0.000	22.900
3.00	CA+2		2.00	ASO4-3						
CA4HPO43			0.00			-5555.399	-6025.200	-1575.721	-0.000	46.900
4.00	CA+2		3.00	PO4-3		1.00	H+			
CAHPO4			0.00			-2160.628	-2417.888	-862.855	-18.828	18.930
1.00	CA+2		1.00	PO4-3		1.00	H+	2.00	H2O	
CALCIT			4.00			-1129.129	-1208.691	-266.851	9.623	8.480
1.00	CA+2		1.00	CO3-2						
CAMOO4			0.00			-1431.346	-1540.900	-367.448	-0.000	7.400
1.00	CA+2		1.00	MOO4-2						
CAOXAL			0.00			-598.470	-543.000	186.048	-0.000	8.000
1.00	CA+2		1.00	OX-2						
CASECR			-2.00			-363.427	-368.108	-15.701	158.992	-25.470
1.00	CA+2		1.00	HSE-		-1.00	H+			
CASEO3			4.00			-954.000	-1052.200	-329.363	-0.000	5.500
1.00	CA+2		1.00	SEO3-2						
CASEO3_2			4.00			-1427.938	-1623.860	-657.126	-0.000	5.440
1.00	CA+2		1.00	SEO3-2		2.00	H2O			
CASEO4_2			6.00			-1486.024	-1706.856	-740.674	6.904	3.090
1.00	CA+2		1.00	SEO4-2		2.00	H2O			
CASO3			4.00			-1077.378	-1178.500	-339.164	-0.000	6.500
1.00	CA+2		1.00	SO3-2						
CAUO4			6.00			-1888.083	-2001.697	-381.061	131.963	-16.040
1.00	UO2+2		1.00	CA+2		-4.00	H+	2.00	H2O	
CELESTIT			6.00			-1345.673	-1455.889	-369.664	4.351	6.630
1.00	SR+2		1.00	SO4-2						
CH4_GAS			-4.00			-50.741	-74.800	-80.695	13.807	2.860
1.00	CH4(AQ)									
CHALCEDO			0.00			-853.718	-905.068	-172.227	-94.768	26.690
2.00	H+		1.00	H2SiO4-2		-2.00	H2O			
CO2_GAS			4.00			-394.377	-393.501	2.941	-4.017	18.150
2.00	H+		1.00	CO3-2		-1.00	H2O			
CO3_CH4			0.00			-0.011	-0.005	0.018	-270.788	38.180
-1.00	CH4(AQ)		1.00	CO3-2		10.00	H+	8.00	E-	
CRYOLITE			0.00			-3159.626	-3309.553	-502.858	-38.033	33.840
1.00	AL+3		3.00	NA+		6.00	F-			
DOLO_DIS			8.00			-2158.454	-2314.227	-522.467	46.401	16.540
1.00	CA+2		1.00	MG+2		2.00	CO3-2			

Table B.4: Selected aqueous species and minerals in 0391 MINEQL-PSI data base. Page 27 of 37

	Charge	OPV	DH a	DH b	$\Delta_f G^0$	$\Delta_f H^0$	$\Delta_f S^0$	$\Delta_r H^0$	logK(25)
DOLOMITE		8.00			-2161.593	-2321.131	-535.093	39.497	17.090
	1.00 CA+2	1.00 MG+2		2.00 CO3-2					
FAYALITE		4.00			-1366.217	-1469.367	-345.966	90.793	5.740
	2.00 FE+2	1.00 H2SIO4-2		-2.00 H+					
FE(OH)2CR		2.00			-479.548	-569.549	-301.864	91.211	-12.900
	1.00 FE+2	-2.00 H+		2.00 H2O					
FE2SEO32		18.00			-1298.936	-1624.800	-1092.954	-0.000	31.600
	2.00 FE+3	3.00 SEO3-2							
FEASO4CR		8.00			-772.859	-936.740	-549.659	-0.000	21.000
	1.00 FE+3	1.00 ASO4-3							
FEOH3_AG		3.00			-711.437	-824.502	-379.223	81.588	-0.800
	1.00 FE+3	-3.00 H+		3.00 H2O					
FEOH3CR		3.00			-698.879	-824.502	-421.341	81.588	-3.000
	1.00 FE+3	-3.00 H+		3.00 H2O					
FEPO4CR		3.00			-1177.337	-1333.000	-522.096	-0.000	25.800
	1.00 FE+3	1.00 PO4-3							
FESCR		0.00			-90.633	-105.400	-49.528	-0.000	4.200
	1.00 FE+2	1.00 HS-		-1.00 H+					
FESEZ		0.00			-97.410	-102.906	-18.434	-45.606	18.660
	1.00 FE+2	2.00 HSE-		-2.00 H+	-2.00 E-				
FLUORAP		0.00			-6458.791	-6911.500	-1518.391	-7.950	59.000
	5.00 CA+2	3.00 PO4-3		1.00 F-					
FLUORITE		0.00			-1176.351	-1233.365	-191.226	-19.665	10.600
	1.00 CA+2	2.00 F-							
GIBBS_MC		0.00			-1149.551	-1293.382	-482.411	102.508	-9.350
	1.00 AL+3	-3.00 H+		3.00 H2O					
GIBBSI_C		0.00			-1156.629	-1300.495	-482.529	95.395	-8.110
	1.00 AL+3	-3.00 H+		3.00 H2O					
GOETHHITE		3.00			-476.009	-560.429	-283.145	59.831	-0.500
	1.00 FE+3	-3.00 H+		2.00 H2O					
GYPSUM		6.00			-1797.229	-2023.540	-759.049	0.460	4.580
	1.00 CA+2	1.00 SO4-2		2.00 H2O					
H2_GAS		-2.00			-0.026	-0.022	0.011	4.017	3.110
	1.00 H2(AQ)								
H2S_GAS		-2.00			-33.423	-16.300	57.432	-0.000	8.000
	1.00 H+	1.00 HS-							
H2TCO42		6.00			-576.367	-572.230	13.877	-0.000	19.900
	2.00 ASO2-	2.00 H+		-1.00 H2O					
HAUSMANN		8.00			-1284.506	-1384.492	-335.354	421.078	-61.030
	3.00 MN+2	-8.00 H+		-2.00 E-	4.00 H2O				
HEMATITE		6.00			-742.276	-826.660	-283.024	128.030	3.800
	2.00 FE+3	-6.00 H+		3.00 H2O					
HYDROXAP		0.00			-6323.085	-6746.920	-1421.548	107.110	43.000
	5.00 CA+2	3.00 PO4-3		-1.00 H+	1.00 H2O				
K2SE		-2.00			-369.932	-383.780	-46.447	104.600	-26.470
	2.00 K+	1.00 HSE-		-1.00 H+					

Table B.4: Selected aqueous species and minerals in 0391 MINEQL-PSI data base. Page 28 of 37

	Charge	OPV	DH a	DH b	$\Delta_f G^0$	$\Delta_f H^0$	$\Delta_f S^0$	$\Delta_f H^0$	logK(25)
K2SEO3		4.00			-877.969	-966.619	-297.333	46.861	-9.960
2.00 K+		1.00	SEO3-2						
K2SEO4CR		6.00			-1009.973	-1128.066	-396.084	-24.686	0.640
2.00 K+		1.00	SEO4-2						
K4PUSO44		28.00			-4690.382	-5182.320	-1649.967	-0.000	18.000
1.00 PU+4		4.00	K+		4.00	SO4-2			
KAOLINIT		0.00			-3793.200	-4128.893	-1125.919	-2.343	38.850
2.00 AL+3		2.00	H2SiO4-2		-2.00 H+	1.00 H2O			
LARNITE		0.00			-2191.083	-2295.579	-350.482	172.381	-15.800
2.00 CA+2		1.00	H2SiO4-2		-2.00 H+				
LI2SE		-2.00			-392.464	-400.876	-28.214	140.164	-26.170
2.00 Li+		1.00	HSE-		-1.00 H+				
LI2SEO3		4.00			-969.396	-1057.772	-296.414	8.368	2.410
2.00 Li+		1.00	SEO3-2						
LI2SEO4		6.00			-1020.005	-1138.049	-395.920	17.991	-1.250
2.00 Li+		1.00	SEO4-2						
LI2UO4		6.00			-1846.457	-1961.496	-385.842	186.104	-29.120
1.00 UO2+2		2.00	Li+		-4.00 H+	2.00 H2O			
MAGNETIT		8.00			-1013.224	-1120.420	-359.539	209.200	-4.100
2.00 FE+3		1.00	FE+2		-8.00 H+	4.00 H2O			
MANGANIT		3.00			-557.742	-792.410	-787.081	-0.000	-25.340
1.00 MN+2		-3.00	H+		-1.00 E-	2.00 H2O			
MELANTER		8.00			-2495.494	-3019.793	-1758.507	-20.543	2.210
1.00 FE+2		1.00	SO4-2		7.00 H2O				
MG3ASO42		10.00			-2802.293	-3177.280	-1257.713	-0.000	24.400
3.00 MG+2		2.00	ASO4-3						
MG3PO42C		0.00			-3579.285	-3969.800	-1309.795	-0.000	28.400
3.00 MG+2		2.00	PO4-3						
MGCO3CR		4.00			-1029.211	-1116.373	-292.345	25.941	8.040
1.00 MG+2		1.00	CO3-2						
MGF2CR		0.00			-1065.131	-1129.332	-215.332	8.368	8.180
1.00 MG+2		2.00	F-						
MGOXAL		0.00			-476.519	-467.000	31.928	-0.000	3.700
1.00 MG+2		1.00	OX-2						
MGSE		-2.00			-288.280	-333.948	-153.170	117.152	-21.570
1.00 MG+2		1.00	HSE-		-1.00 H+				
MGSEO3CR		4.00			-853.169	-976.200	-412.649	-0.000	4.900
1.00 MG+2		1.00	SEO3-2						
MGUO4		6.00			-1749.237	-1856.995	-361.424	200.665	-23.300
1.00 UO2+2		1.00	MG+2		-4.00 H+	2.00 H2O			
MILLERIT		-2.00			-86.044	-83.521	8.461	-13.221	9.230
1.00 NI+2		1.00	HS-		-1.00 H+				
MIN32521		16.00			-3369.366	-3574.784	-688.975	197.736	-2.480
2.00 UO2+2		1.00	U+4		-8.00 H+	4.00 H2O			
MIN41506		14.00			-3241.979	-3426.998	-620.558	203.552	7.710
1.00 UO2+2		2.00	U+4		-10.00 H+	5.00 H2O			

Table B.4: Selected aqueous species and minerals in 0391 MINEQL-PSI data base. Page 29 of 37

	Charge	OPV	DH a	DH b	$\Delta_f G^0$	$\Delta_f H^0$	$\Delta_f S^0$	$\Delta_f H^0$	logK(25)
MIN41511		18.00			-4277.855	-4513.208	-789.377	280.202	13.270
1.00 UO2+2		3.00	U+4	-14.00	H+	7.00	H2O		
MN3ASO42		16.00			-2150.074	-2438.530	-967.486	-0.000	29.600
3.00 MN+2		2.00	ASO4-3						
MNH2SIO4		2.00			-1464.829	-1602.710	-462.456	-0.000	10.700
1.00 MN+2		1.00	H2SIO4-2						
MNO2		4.00			-462.648	-792.410	-1106.027	-0.000	-42.000
1.00 MN+2		-4.00	H+	-2.00	E-	2.00	H2O		
MNSCR		0.00			-213.577	-237.050	-78.729	-0.000	-0.400
1.00 MN+2		1.00	HS-	-1.00	H+				
MNSEO3CR		6.00			-639.568	-729.950	-303.144	-0.000	7.300
1.00 MN+2		1.00	SEO3-2						
N2_GAS		0.00			-0.020	-0.019	0.005	10.418	3.190
1.00 N2(AQ)									
N2AQ_NH3		0.00			0.043	-0.020	-0.212	-151.879	12.520
-2.00 NH3		1.00	N2(AQ)	6.00	H+	6.00	E-		
NA2SE		-2.00			-327.099	-343.026	-53.417	121.754	-26.770
2.00 NA+		1.00	HSE-	-1.00	H+				
NA2SE2		-2.00			-370.031	-388.212	-60.980	60.668	-11.540
2.00 NA+		2.00	HSE-	-2.00	H+	-2.00	E-		
NA2SEO3		4.00			-871.268	-959.755	-296.788	30.125	-3.930
2.00 NA+		1.00	SEO3-2						
NA2SEO4		6.00			-962.289	-1079.989	-394.769	-0.209	-0.510
2.00 NA+		1.00	SEO4-2						
NA2U207		12.00			-3011.309	-3203.789	-645.581	172.381	-22.620
2.00 UO2+2		2.00	NA+	-6.00	H+	3.00	H2O		
NA3UO4		5.00			-1899.739	-2024.007	-416.796	293.800	-56.310
1.00 UO2+		3.00	NA+	-4.00	H+	2.00	H2O		
NA4UO2CO		18.00			-3737.822	-4006.302	-900.487	-0.000	26.930
1.00 UO2+2		4.00	NA+	3.00	CO3-2				
NH42PUO2		8.00			-1988.205	-2335.124	-1163.571	-0.000	21.400
1.00 PUO2+2		2.00	CO3-2	2.00	NH3	2.00	H+		
NI-SPINE		0.00			-1280.724	-1386.615	-355.160	103.345	2.430
2.00 NI+2		1.00	H2SIO4-2	-2.00	H+				
NI-OLIVI		0.00			-1288.715	-1393.310	-350.811	96.650	3.830
2.00 NI+2		1.00	H2SIO4-2	-2.00	H+				
NI(OH)2CR		0.00			-447.218	-529.721	-276.715	95.939	-12.730
1.00 NI+2		-2.00	H+	2.00	H2O				
NI_ELEM		-2.00			-1.192	-1.909	-2.404	52.091	-7.780
1.00 NI+2		2.00	E-						
NI2OH3CL		-1.00			-824.248	-1132.570	-1034.116	-0.000	-19.200
2.00 NI+2		1.00	CL-	-3.00	H+	3.00	H2O		
NI3ASO42		10.00			-1605.999	-1938.280	-1114.477	-0.000	30.200
3.00 NI+2		2.00	ASO4-3						
NI3PO42CR		0.00			-2356.734	-2578.502	-743.815	152.298	29.600
3.00 NI+2		2.00	PO4-3						

Table B.4: Selected aqueous species and minerals in 0391 MINEQL-PSI data base. Page 30 of 37

	Charge	OPV	DH a	DH b	$\Delta_f G^0$	$\Delta_f H^0$	$\Delta_f S^0$	$\Delta_r H^0$	logK(25)
NI3S2		-6.00			-196.626	-181.630	50.297	12.970	14.770
3.00	NI+2	2.00	HS-		-2.00 H+	2.00	E-		
NI3S4		-6.00			-331.168	-217.995	379.584	9.205	42.630
3.00	NI+2	4.00	HS-		-4.00 H+	-2.00	E-		
NI4OH7CL		-1.00			-1722.452	-2383.890	-2218.473	-0.000	-44.000
4.00	NI+2	1.00	CL-		-7.00 H+	7.00	H2O		
NIBO22		0.00			-1454.153	-1599.834	-488.617	-0.000	8.700
1.00	NI+2	2.00	B(OH)4-		-4.00 H2O				
NIBR2		-2.00			-199.532	-213.977	-48.450	82.843	-9.420
1.00	NI+2	2.00	BR-						
NICL2_2H		-2.00			-760.116	-922.164	-543.511	37.656	-3.890
1.00	NI+2	2.00	CL-		2.00 H2O				
NICL2_4H		-2.00			-1234.910	-1516.418	-944.181	15.062	-3.800
1.00	NI+2	2.00	CL-		4.00 H2O				
NICL2_6H		-2.00			-1713.243	-2103.140	-1307.722	-0.000	-3.090
1.00	NI+2	2.00	CL-		6.00 H2O				
NICL2CR		-2.00			-260.322	-307.409	-157.930	80.751	-8.360
1.00	NI+2	2.00	CL-						
NICO3CR		4.00			-613.303	-691.240	-261.400	38.074	6.970
1.00	NI+2	1.00	CO3-2						
NIF2_4H2		0.00			-1586.482	-1868.020	-944.285	-0.000	5.130
1.00	NI+2	2.00	F-		4.00 H2O				
NIF2CR		0.00			-610.638	-659.011	-162.245	65.689	0.350
1.00	NI+2	2.00	F-						
NIFE2O4		6.00			-973.074	-1083.646	-370.861	210.874	-5.300
1.00	NI+2	2.00	FE+3		-8.00 H+	4.00	H2O		
NII2		-2.00			-81.744	-80.114	5.465	87.446	-11.790
1.00	NI+2	2.00	I-						
NIO		0.00			-211.677	-239.707	-94.014	100.123	-12.450
1.00	NI+2	-2.00	H+		1.00 H2O				
NIOH2BOH		0.00			-2526.803	-2743.154	-725.646	-0.000	30.440
1.00	NI+2	2.00	B(OH)4-						
NIS_ALPH		-2.00			-64.753	-70.300	-18.603	-0.000	5.500
1.00	NI+2	1.00	HS-		-1.00 H+				
NIS_BETA		-2.00			-96.147	-70.300	86.691	-0.000	11.000
1.00	NI+2	1.00	HS-		-1.00 H+				
NIS_GAMM		-2.00			-105.850	-70.300	119.237	-0.000	12.700
1.00	NI+2	1.00	HS-		-1.00 H+				
NIS2		-2.00			-135.107	-140.574	-18.335	-53.974	19.970
1.00	NI+2	2.00	HS-		-2.00 H+	-2.00	E-		
NISEO3CR		4.00			-445.652	-563.200	-394.258	-0.000	5.300
1.00	NI+2	1.00	SEO3-2						
NISIO3		0.00			-1127.953	-1150.130	-74.381	-0.000	25.200
1.00	NI+2	1.00	H2SiO4-2		-1.00 H2O				
NISO4_6H		6.00			-2223.913	-2682.922	-1539.525	-4.602	2.010
1.00	NI+2	1.00	SO4-2		6.00 H2O				

Table B.4: Selected aqueous species and minerals in 0391 MINEQL-PSI data base. Page 31 of 37

	Charge	OPV	DH a	DH b	$\Delta_f G^0$	$\Delta_f H^0$	$\Delta_f S^0$	$\Delta_f H^0$	logK(25)
NISO4_7H 1.00 NI+2		6.00 1.00 SO4-2		-2461.110 7.00 H2O	-2976.284	-1727.901	-12.134	2.020	
NISO4CR 1.00 NI+2		6.00 1.00 SO4-2		-759.177	-872.966	-381.649	90.374	-5.330	
NO3_NH3 -1.00 NH3		0.00 1.00 NO3-		-0.010 9.00 H+	0.006 8.00 E-	0.055 -3.00 H2O	-731.782 109.900		
NP(OH)3CR 1.00 NP+3		3.00 -3.00 H+		-1102.946 3.00 H2O	-1384.690	-944.974	-0.000	-22.000	
NP(OH)4CR 1.00 NP+4		4.00 -4.00 H+		-1446.894 4.00 H2O	-1699.420	-846.977	-0.000	-0.800	
NPO2 1.00 NP+4		4.00 -4.00 H+		-992.591 2.00 H2O	-1127.760	-453.358	-0.000	2.700	
NPO2OH2C 1.00 NPO2+2		6.00 -2.00 H+		-1239.828 2.00 H2O	-1432.260	-645.420	-0.000	-5.300	
NPO2OHCR 1.00 NPO2+		5.00 -1.00 H+		-1124.171 1.00 H2O	-1264.030	-469.089	-0.000	-4.900	
O2_GAS 1.00 O2(AQ)		4.00		0.025	-0.009	-0.115	12.050	2.890	
PD_ELEM 1.00 PD+2		0.00 2.00 E-		-0.046	0.050	0.319	-148.950	30.930	
PDBR2CR 1.00 PD+2		0.00 2.00 BR-		-107.172	-105.117	6.894	-11.297	13.310	
PDCL2CR 1.00 PD+2		0.00 2.00 CL-		-126.409	-173.026	-156.355	12.134	7.090	
PDI2CR 1.00 PD+2		0.00 2.00 I-		-62.617	-63.721	-3.702	-99.161	23.770	
PDO 1.00 PD+2		2.00 -2.00 H+		-85.755 1.00 H2O	-85.367	1.301	51.463	4.400	
PDOH2CR 1.00 PD+2		2.00 -2.00 H+		-306.970 2.00 H2O	-395.046	-295.408	27.614	1.610	
PDS 1.00 PD+2		0.00 1.00 HS-		-69.828 -1.00 H+	-73.153	-11.151	-205.853	45.300	
PDS2 1.00 PD+2		0.00 2.00 HS-		-80.991 -2.00 H+	-82.758 -2.00 E-	-5.929 -199.158	-199.158	49.400	
PLCO3CR 1.00 PUO2+2		10.00 1.00 CO3-2		-1364.730	-1497.514	-445.361	-0.000	14.000	
PLHPO4CR 1.00 PUO2+2		6.00 1.00 PO4-3		-1927.371 1.00 H+	-2110.617	-614.610	-4.017	25.400	
PORLAND 1.00 CA+2		0.00 -2.00 H+		-896.890 2.00 H2O	-984.956	-295.376	129.704	-22.810	
PU(OH)3CR 1.00 PU+3		3.00 -3.00 H+		-1162.734 3.00 H2O	-1301.167	-464.308	148.323	-22.300	
PU(OH)4CR 1.00 PU+4		4.00 -4.00 H+		-1424.452 4.00 H2O	-1610.810	-625.046	68.910	-1.000	
PU2O3 2.00 PU+3		6.00 -6.00 H+		-1594.070 3.00 H2O	-1681.164	-292.115	360.326	-48.100	

Table B.4: Selected aqueous species and minerals in 0391 MINEQL-PSI data base. Page 32 of 37

		Charge	OPV	DH a	DH b	$\Delta_f G^0$	$\Delta_f H^0$	$\Delta_f S^0$	$\Delta_r H^0$	logK(25)
PUCL3CR			0.00			-1037.330	-1093.240	-187.523	-0.000	11.400
1.00	PU+3		3.00	CL-						
PUF3CR			3.00			-1480.239	-1551.733	-239.792	46.317	10.000
1.00	PU+3		3.00	F-						
PUF4CR			4.00			-1681.883	-1777.802	-321.716	99.998	13.000
1.00	PU+4		4.00	F-						
PUH2P42C			4.00			-2833.387	-3099.928	-893.985	5.272	52.700
1.00	PU+4		2.00	PO4-3		2.00	H+			
PUO2			4.00			-995.835	-1055.969	-201.690	52.091	7.000
1.00	PU+4		-4.00	H+		2.00	H2O			
PUO2OHCR			5.00			-1055.547	-1157.753	-342.803	42.677	-5.500
1.00	PUO2+		-1.00	H+		1.00	H2O			
PUO3			6.00			-1211.202	-1357.961	-492.232	35.899	-3.500
1.00	PUO2+2		-2.00	H+		2.00	H2O			
PYRITE			0.00			-154.308	-121.700	109.369	-0.000	17.500
1.00	FE+2		2.00	HS-		-2.00	E-	-2.00	H+	
PYROCHRO			2.00			-615.620	-792.410	-592.957	-0.000	-15.200
1.00	MN+2		-2.00	H+		2.00	H2O			
PYROLUSI			4.00			-466.187	-519.990	-180.456	272.420	-41.380
1.00	MN+2		-4.00	H+		-2.00	E-	2.00	H2O	
QUARTZ			0.00			-856.172	-910.381	-181.817	-100.081	27.120
2.00	H+		1.00	H2SiO4-2		-2.00	H2O			
RHODO_SY			6.00			-815.324	-896.064	-270.803	-0.000	10.390
1.00	MN+2		1.00	CO3-2						
RHODOCHR			6.00			-819.548	-890.081	-236.568	5.983	11.130
1.00	MN+2		1.00	CO3-2						
S_ELEM_R			0.00			0.025	-0.024	-0.165	16.276	2.140
1.00	HS-		-1.00	H+		-2.00	E-			
SE_ELEM			0.00			-0.122	-0.125	-0.009	-16.025	7.730
1.00	HSE-		-1.00	H+		-2.00	E-			
SE205			2.00			229.745	275.488	153.424	-72.802	19.600
1.00	SEO3-2		6.00	H+		2.00	E-	-3.00	H2O	
SECL4CR			0.00			-100.952	-188.652	-294.149	131.378	-14.420
1.00	SEO3-2		6.00	H+		4.00	CL-	-3.00	H2O	
SEO2			4.00			-171.360	-225.044	-180.057	-1.674	6.780
1.00	SEO3-2		2.00	H+		-1.00	H2O			
SEO3CR			6.00			-94.568	-170.177	-253.594	143.093	-19.200
1.00	SEO4-2		2.00	H+		-1.00	H2O			
SIDER_PR			6.00			-666.467	-764.414	-328.517	-0.000	10.450
1.00	FE+2		1.00	CO3-2						
SIDERITE			6.00			-668.978	-754.038	-285.291	10.376	10.890
1.00	FE+2		1.00	CO3-2						
SIO2_AM			0.00			-848.923	-899.336	-169.083	-89.036	25.850
2.00	H+		1.00	H2SiO4-2		-2.00	H2O			
SISE2			-2.00			-185.948	-150.357	119.373	72.383	0.500
1.00	H2SiO4-2		1.00	HSE-		4.00	H+	-4.00	H2O	

Table B.4: Selected aqueous species and minerals in 0391 MINEQL-PSI data base. Page 33 of 37

		Charge	OPV	DH a	DH b	$\Delta_f G^0$	$\Delta_f H^0$	$\Delta_f S^0$	$\Delta_r H^0$	logK(25)
SN(OH)2CR		2.00				-254.694	-294.730	-134.281	-0.000	-1.760
1.00 SN+2		-2.00	H+		1.00 H2O					
SN(OH)4CR		4.00				-500.453	-571.160	-237.154	-0.000	5.000
1.00 SN+4		-4.00	H+		2.00 H2O					
SNS		0.00				-83.855	-25.200	196.729	-0.000	12.000
1.00 SN+2		1.00	HS-		-1.00 H+					
SO2_GAS		4.00				-301.701	-349.670	-160.888	-0.000	9.000
2.00 H+		1.00	SO3-2		-1.00 H2O					
SR3ASO42		10.00				-3118.450	-3428.980	-1041.522	-0.000	22.800
3.00 SR+2		2.00	ASO4-3							
SRF2CR		0.00				-1175.616	-1225.784	-168.266	-4.184	8.540
1.00 SR+2		2.00	F-							
SRH2SIO4		0.00				-1753.183	-1932.860	-602.640	-0.000	2.400
1.00 SR+2		1.00	H2SIO4-2							
SROXAL		0.00				-602.073	-550.900	171.635	-0.000	6.700
1.00 SR+2		1.00	OX-2							
SRSE		-2.00				-392.144	-396.928	-16.045	138.072	-22.370
1.00 SR+2		1.00	HSE-		-1.00 H+					
SRSEO3CR		4.00				-968.448	-1060.100	-307.402	-0.000	6.100
1.00 SR+2		1.00	SEO3-2							
STRONTIT		4.00				-1144.661	-1224.540	-267.916	1.674	9.270
1.00 SR+2		1.00	CO3-2							
TC_ELEM		0.00				0.029	0.000	-0.098	-0.000	13.520
1.00 TC+2		2.00	E-							
TCO2		4.00				-342.877	-285.830	191.337	-0.000	0.900
1.00 TCO+2		-2.00	H+		1.00 H2O					
TH(OH)4CR		0.00				-1574.791	-1880.940	-1026.829	31.380	-13.800
1.00 TH+4		-4.00	H+		4.00 H2O					
THF4_AQ		0.00				-2612.862	-2854.891	-811.769	-29.916	33.100
1.00 TH+4		4.00	F-		2.50 H2O					
THF4CR		0.00				-2002.888	-2098.685	-321.304	11.715	30.100
1.00 TH+4		4.00	F-							
THH2P42C		0.00				-3998.497	-4489.488	-1646.791	-8.368	51.500
1.00 TH+4		2.00	PO4-3		2.00 H+	4.00	H2O			
THO2		0.00				-1143.320	-1226.855	-280.178	113.805	-6.300
1.00 TH+4		-4.00	H+		2.00 H2O					
THSO32		8.00				-1796.952	-2040.000	-815.187	-0.000	20.500
1.00 TH+4		2.00	SO3-2							
U2O3F6		12.00				-3373.920	-3580.383	-692.480	183.887	2.950
2.00 UO2+2		6.00	F-		2.00 H+	-1.00	H2O			
U3O5F8		18.00				-4889.511	-5199.457	-1039.564	254.513	2.950
3.00 UO2+2		8.00	F-		2.00 H+	-1.00	H2O			
U5O12CL		24.00				-5517.971	-5854.417	-1128.447	9.958	18.810
5.00 UO2+		1.00	CL-		-4.00 H+	2.00	H2O			
UBR2CL		0.00				-715.676	-750.594	-117.114	148.406	-17.470
1.00 U+3		1.00	CL-		2.00 BR-					

Table B.4: Selected aqueous species and minerals in 0391 MINEQL-PSI data base. Page 34 of 37

		Charge	OPV	DH a	DH b	$\Delta_f G^0$	$\Delta_f H^0$	$\Delta_f S^0$	$\Delta_r H^0$	logK(25)
UBR3CR				0.00		-674.322	-698.689	-81.730	154.641	-19.920
1.00	U+3			3.00	BR-					
UBR4CR				0.00		-767.287	-802.119	-116.824	274.721	-31.180
1.00	U+4			4.00	BR-					
UBR5				0.00		-769.056	-810.439	-138.801	250.078	-41.510
1.00	UO2+			5.00	BR-	4.00	H+	-2.00	H2O	
UBRCL2				0.00		-761.654	-812.079	-169.128	132.591	-14.210
1.00	U+3			2.00	CL-	1.00	BR-			
UCL2BR2				0.00		-850.795	-907.852	-191.367	260.328	-26.140
1.00	U+4			2.00	CL-	2.00	BR-			
UCL2F2				2.00		-1376.060	-1465.979	-301.592	130.081	3.630
1.00	U+4			2.00	CL-	2.00	F-			
UCL2I2				0.00		-723.418	-768.006	-149.548	270.914	-30.190
1.00	U+4			2.00	CL-	2.00	I-			
UCL3BR				0.00		-893.463	-963.061	-233.435	250.789	-23.460
1.00	U+4			3.00	CL-	1.00	BR-			
UCL3CR				0.00		-800.268	-866.033	-220.577	124.307	-12.240
1.00	U+3			3.00	CL-					
UCL3F				1.00		-1146.648	-1242.941	-322.967	184.849	-10.230
1.00	U+4			3.00	CL-	1.00	F-			
UCL3I				0.00		-829.974	-898.222	-228.905	250.998	-25.450
1.00	U+4			3.00	CL-	1.00	I-			
UCL4CR				0.00		-929.623	-1018.731	-298.870	240.789	-21.920
1.00	U+4			4.00	CL-					
UCL5CR				0.00		-949.800	-1058.538	-364.710	230.329	-33.820
1.00	UO2+			5.00	CL-	4.00	H+	-2.00	H2O	
UCL6				0.00		-951.371	-1091.879	-471.266	357.941	-55.050
1.00	UO2+2			6.00	CL-	4.00	H+	-2.00	H2O	
UCLBR3				0.00		-806.987	-852.265	-151.866	270.245	-29.020
1.00	U+4			1.00	CL-	3.00	BR-			
UCLF3				3.00		-1606.442	-1689.980	-280.190	74.350	17.660
1.00	U+4			1.00	CL-	3.00	F-			
UCLI3				0.00		-672.914	-643.773	97.740	284.847	-25.110
1.00	U+4			1.00	CL-	3.00	I-			
UF3CR				3.00		-1434.620	-1502.095	-226.313	-6.945	19.900
1.00	U+3			3.00	F-					
UF4_2.5A				4.00		-2440.347	-2671.484	-775.236	-24.309	33.560
1.00	U+4			4.00	F-	2.50	H2O			
UF4CR				4.00		-1823.581	-1914.190	-303.905	18.410	29.370
1.00	U+4			4.00	F-					
UF6_CRYs				6.00		-2068.587	-2197.020	-430.764	262.420	-17.310
1.00	UO2+2			6.00	F-	4.00	H+	-2.00	H2O	
UH2P424H				4.00		-3844.648	-4337.880	-1654.309	-34.560	55.230
1.00	U+4			2.00	PO4-3	2.00	H+	4.00	H2O	
UI3CR				0.00		-468.044	-467.394	2.180	192.046	-28.660
1.00	U+3			3.00	I-					

Table B.4: Selected aqueous species and minerals in 0391 MINEQL-PSI data base. Page 35 of 37

	Charge	OPV	DH a	DH b	$\Delta_f G^0$	$\Delta_f H^0$	$\Delta_f S^0$	$\Delta_f H^0$	logK(25)
UI4		0.00			-513.218	-518.787	-18.679	299.533	-39.160
	1.00 U+4	4.00 I-							
UL3P424H		18.00			-6138.992	-6742.091	-2022.804	27.029	49.370
3.00 UO2+2		2.00 PO4-3		4.00 H2O					
UL3P426H		18.00			-6618.067	-7340.780	-2423.991	-0.000	50.210
3.00 UO2+2		2.00 PO4-3		6.00 H2O					
UL3P42CR		18.00			-5116.058	-5494.297	-1268.618	131.503	36.340
3.00 UO2+2		2.00 PO4-3							
ULNO32_H		16.00			-1362.925	-1663.887	-1009.431	54.643	-8.470
1.00 UO2+2		2.00 NO3-		1.00 H2O					
ULNO322H		16.00			-1620.442	-1978.587	-1201.222	25.773	-4.900
1.00 UO2+2		2.00 NO3-		2.00 H2O					
ULNO323H		16.00			-1864.603	-2280.316	-1394.307	9.874	-3.670
1.00 UO2+2		2.00 NO3-		3.00 H2O					
ULNO326H		16.00			-2584.128	-3167.387	-1956.258	-19.707	-2.250
1.00 UO2+2		2.00 NO3-		6.00 H2O					
ULNO32CR		16.00			-1106.036	-1350.903	-821.288	81.797	-11.930
1.00 UO2+2		2.00 NO3-							
ULSO3CR		10.00			-1530.377	-1654.500	-416.310	-0.000	15.830
1.00 UO2+2		1.00 SO3-2							
ULSO4_3		12.00			-2416.533	-2755.329	-1136.327	30.501	1.500
1.00 UO2+2		1.00 SO4-2		3.00 H2O					
ULSO4_35		12.00			-2535.559	-2901.633	-1227.815	27.112	1.580
1.00 UO2+2		1.00 SO4-2		3.50 H2O					
UO2_AMOR		4.00			-1003.569	-1162.860	-534.264	-0.000	-0.100
1.00 U+4		-4.00 H+		2.00 H2O					
UO2_CRYs		4.00			-1032.337	-1084.996	-176.618	77.864	4.940
1.00 U+4		-4.00 H+		2.00 H2O					
UO2BR2		4.00			-1066.242	-1137.388	-238.625	124.432	-16.470
1.00 UO2+2		2.00 BR-							
UO2BR2_1		4.00			-1328.439	-1455.895	-427.487	91.755	-12.080
1.00 UO2+2		2.00 BR-		1.00 H2O					
UO2BR2_3		4.00			-1818.359	-2058.014	-803.808	61.296	-9.340
1.00 UO2+2		2.00 BR-		3.00 H2O					
UO2BROH		5.00			-1744.076	-1957.985	-717.453	39.915	-4.160
1.00 UO2+2		1.00 BR-		-1.00 H+ 3.00 H2O					
UO2CL2_1		4.00			-1404.984	-1559.745	-519.072	79.245	-8.260
1.00 UO2+2		2.00 CL-		1.00 H2O					
UO2CL2_3		4.00			-1894.618	-2163.957	-903.366	46.693	-5.570
1.00 UO2+2		2.00 CL-		3.00 H2O					
UO2CL2CR		4.00			-1145.811	-1243.539	-327.781	109.621	-12.120
1.00 UO2+2		2.00 CL-							
UO2CLCR		4.00			-1095.323	-1169.990	-250.433	22.217	0.540
1.00 UO2+		1.00 CL-							
UO2CLOH		5.00			-1782.177	-2010.391	-765.433	33.179	-2.280
1.00 UO2+2		1.00 CL-		-1.00 H+ 3.00 H2O					

Table B.4: Selected aqueous species and minerals in 0391 MINEQL-PSI data base. Page 36 of 37

		Charge	OPV	DH a	DH b	$\Delta_f G^0$	$\Delta_f H^0$	$\Delta_f S^0$	$\Delta_f H^0$	logK(25)
UO2CO3CR			10.00			-1562.892	-1689.628	-425.074	4.686	14.440
1.00	UO2+2		1.00	CO3-2						
UO2F2_3A			6.00			-2269.706	-2534.387	-887.744	12.803	7.480
1.00	UO2+2		2.00	F-		3.00	H2O			
UO2F2CR			6.00			-1557.316	-1653.508	-322.632	36.192	7.310
1.00	UO2+2		2.00	F-						
UO2FOH_1			6.00			-1721.650	-1894.504	-579.755	31.506	2.330
1.00	UO2+2		1.00	F-		-1.00	H+	2.00	H2O	
UO2FOH_2			6.00			-1960.959	-2190.292	-769.187	21.548	2.710
1.00	UO2+2		1.00	F-		-1.00	H+	3.00	H2O	
UO2HPO4_-			6.00			-3064.789	-3471.489	-1364.078	-24.769	24.210
1.00	UO2+2		1.00	PO4-3		1.00	H+	4.00	H2O	
UO2SO4_2			12.00			-2298.477	-2607.560	-1036.672	35.355	1.590
1.00	UO2+2		1.00	SO4-2		2.50	H2O			
UO2SO4CR			12.00			-1685.763	-1845.162	-534.627	83.178	-1.890
1.00	UO2+2		1.00	SO4-2						
UO2UO2CL			8.00			-2234.799	-2404.450	-569.013	140.917	-12.690
1.00	UO2+2		3.00	CL-		1.00	UO2+			
UO3_2H2O			6.00			-1636.459	-1826.115	-636.108	50.375	-4.820
1.00	UO2+2		-2.00	H+		3.00	H2O			
UO3_ALF			6.00			-1140.375	-1217.510	-258.713	87.320	-8.640
1.00	UO2+2		-2.00	H+		1.00	H2O			
UO3_ALF_-			6.00			-1374.577	-1506.304	-441.814	55.773	-5.000
1.00	UO2+2		-2.00	H+		1.90	H2O			
UO3_BETA			6.00			-1142.258	-1220.313	-261.797	84.517	-8.310
1.00	UO2+2		-2.00	H+		1.00	H2O			
UO3_GAMM			6.00			-1145.626	-1223.786	-262.150	81.044	-7.720
1.00	UO2+2		-2.00	H+		1.00	H2O			
UOBR2			2.00			-929.493	-973.619	-147.999	146.231	-7.920
1.00	U+4		2.00	BR-		-2.00	H+	1.00	H2O	
UOBR3			2.00			-901.352	-954.033	-176.691	149.494	-23.490
1.00	UO2+		3.00	BR-		2.00	H+	-1.00	H2O	
UOCL2CR			2.00			-996.106	-1066.842	-237.250	144.348	-5.840
1.00	U+4		2.00	CL-		-2.00	H+	1.00	H2O	
UOCL3			2.00			-1068.853	-1162.966	-315.657	77.571	-8.530
1.00	UO2+		3.00	CL-		2.00	H+	-1.00	H2O	
UOCLCR			2.00			-787.126	-832.891	-153.497	109.119	-10.110
1.00	U+3		1.00	CL-		-2.00	H+	1.00	H2O	
UOF2_1AQ			4.00			-1674.489	-1802.013	-427.718	31.547	18.800
1.00	U+4		2.00	F-		-2.00	H+	2.00	H2O	
UOF2CR			4.00			-1434.095	-1504.593	-236.451	43.137	18.230
1.00	U+4		2.00	F-		-2.00	H+	1.00	H2O	
UOF4			6.00			-1816.319	-1924.615	-363.228	149.955	-4.410
1.00	UO2+2		4.00	F-		2.00	H+	-1.00	H2O	
UOFOH			4.00			-1342.625	-1426.705	-282.008	71.505	9.980
1.00	U+4		1.00	F-		-3.00	H+	2.00	H2O	

Table B.4: Selected aqueous species and minerals in 0391 MINEQL-PSI data base. Page 37 of 37

	Charge	OPV	DH a	DH b	$\Delta_f G^0$	$\Delta_f H^0$	$\Delta_f S^0$	$\Delta_r H^0$	logK(25)
UOFOH_0.		4.00			-1458.113	-1576.106	-395.750	65.019	9.440
1.00 U+4		1.00 F-		-3.00 H+	2.50	H2O			
UOH2SO4		10.00			-1766.234	-2072.200	-1026.215	-0.000	3.170
1.00 U+4		1.00 SO4-2		-2.00 H+	2.00	H2O			
USIO4		4.00			-1882.288	-1973.160	-304.787	-0.000	30.970
1.00 U+4		1.00 H2SIO4-2		-2.00 H+					
USO32		12.00			-1712.796	-1862.200	-501.103	-0.000	36.440
1.00 U+4		2.00 SO3-2							
USO42_4A		16.00			-3033.260	-3483.285	-1509.394	69.915	11.710
1.00 U+4		2.00 SO4-2		4.00 H2O					
USO42_8A		16.00			-3987.870	-4662.671	-2263.295	33.849	12.770
1.00 U+4		2.00 SO4-2		8.00 H2O					
USO42CR		16.00			-2084.471	-2309.673	-755.331	100.207	11.670
1.00 U+4		2.00 SO4-2							
UU3F17		17.00			-7464.231	-7849.734	-1292.985	78.283	105.480
1.00 UO2+		17.00 F-		3.00 U+4	4.00 H+		-2.00 H2O		
UUF9		9.00			-3812.160	-4015.914	-683.396	46.903	45.880
1.00 UO2+		9.00 F-		1.00 U+4	4.00 H+		-2.00 H2O		
UUO2CL5		4.00			-2037.332	-2197.340	-536.668	254.387	-19.210
1.00 UO2+		1.00 U+4		5.00 CL-					
VIVIANIT		6.00			-2493.165	-2836.100	-1150.211	-0.000	36.000
3.00 FE+2		2.00 PO4-3							
WITHERIT		4.00			-1132.139	-1210.743	-263.640	-2.929	8.560
1.00 BA+2		1.00 CO3-2							

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Table B.5: Selected aqueous species and minerals in 0491 PHREEQE-PSI data base. Page 1 of 12

Charge	OPV	DH a	DH b	$\Delta_f G^0$	$\Delta_f H^0$	$\Delta_f S^0$	$\Delta_f I^0$	logK(25)
MASTER SPECIES								
AL+3	3.0	0.00	6.65	0.19	-491.500	-538.400	-157.303	
AM+3	3.0	0.00	9.00	0.00	-598.100	-616.700	-59.031	
ASO4-3	-3.0	5.00	4.00	0.00	-648.410	-888.140	-804.058	
BA+2	2.0	0.00	4.55	0.09	-555.360	-532.500	76.673	
BR-	-1.0	0.00	3.00	0.00	-103.850	-121.410	-58.897	
CA+2	2.0	0.00	4.86	0.15	-552.807	-543.000	32.893	
CH4(AQ)	0.0	-4.00	0.00	0.00	-34.416	-88.607	-181.758	
CIT-3	-3.0	0.00	0.00	0.00	0.000	0.000	0.000	
CL-	-1.0	0.00	3.71	0.01	-131.220	-167.080	-120.275	
CO3-2	-2.0	4.00	5.40	0.00	-527.919	-675.314	-494.365	
E-	-1.0	-1.00	0.00	0.00	0.000	0.000	0.000	
EDTA-4	-4.0	0.00	0.00	0.00	0.000	0.000	0.000	
F-	-1.0	0.00	3.46	0.08	-281.520	-335.350	-180.547	
FE+2	2.0	2.00	5.08	0.16	-78.900	-89.100	-34.211	
H+	1.0	0.00	9.00	0.00	0.000	0.000	0.000	
H2(AQ)	0.0	2.00	0.00	0.00	17.726	-4.039	-73.000	
H2O	0.0	0.00	0.00	0.00	-237.140	-285.830	-163.307	
H2S(AQ)	-2.0	-2.00	0.00	0.00	-27.600	-38.600	-36.894	
H3ASO3	0.0	3.00	0.00	0.00	-639.800	-742.200	-343.451	
H3BO3	0.0	0.00	0.00	0.00	-969.300	-1072.800	-347.141	
H4SiO4	0.0	0.00	0.00	0.00	-1307.735	-1456.960	-500.503	
I-	-1.0	0.00	3.00	0.00	-51.720	-56.780	-16.971	
K+	1.0	0.00	3.71	0.01	-282.510	-252.140	101.861	
Li+	1.0	0.00	4.76	0.20	-292.920	-278.470	48.466	
Mg+2	2.0	0.00	5.46	0.22	-455.400	-467.000	-38.907	
Mn+2	2.0	2.00	7.04	0.22	-228.100	-220.750	24.652	
MOO4-2	-2.0	0.00	5.00	0.00	-836.300	-997.900	-542.009	
N2(AQ)	0.0	0.00	0.00	0.00	18.188	-10.437	-96.009	
NA+	1.0	0.00	4.32	0.06	-261.950	-240.340	72.480	
NH4+	1.0	-3.00	2.50	0.00	-79.400	-133.260	-180.647	
NI2+	2.0	0.00	5.51	0.22	-45.600	-54.000	-28.174	
NO3-	-1.0	5.00	3.00	0.00	-110.790	-206.850	-322.187	
NP+4	4.0	4.00	11.00	0.00	-502.900	-556.100	-178.434	
NTA-3	-3.0	0.00	0.00	0.00	0.000	0.000	0.000	
O2(AQ)	0.0	4.00	0.00	0.00	16.521	-12.059	-95.858	
OX-2	-2.0	0.00	0.00	0.00	0.000	0.000	0.000	
PD2+	2.0	0.00	5.50	0.00	176.500	149.000	-92.235	
PO4-3	-3.0	0.00	4.00	0.00	-1025.497	-1284.400	-868.365	
PU+4	4.0	4.00	11.00	0.00	-481.600	-536.400	-183.800	
SEO4-2	-2.0	6.00	4.50	0.00	-441.300	-599.100	-529.264	
SN+2	2.0	2.00	6.00	0.00	-27.600	-8.900	62.720	
SO4-2	-2.0	6.00	5.31	-0.07	-744.000	-909.340	-554.553	
SR+2	2.0	0.00	5.48	0.11	-563.830	-550.900	43.367	
TCO+2	2.0	2.00	5.00	0.00	-100.600	0.000	337.414	
TH+4	4.0	0.00	11.00	0.00	-705.000	-769.000	-214.657	
U4+	4.0	4.00	11.00	0.00	-529.860	-591.200	-205.735	
ZR+4	4.0	0.00	11.00	0.00	-524.500	0.000	1759.182	

Table B.5: Selected aqueous species and minerals in 0491 PHREEQE-PSI data base. Page 2 of 12

	Charge	OPV	DH a	DH b	$\Delta_f G^0$	$\Delta_f H^0$	$\Delta_f S^0$	$\Delta_r H^0$	logK(25)
PRODUCT SPECIES									
AL(OH)+2 1.00	2.0 AL+3	0.00 1.00	5.00 H2O	0.00 -1.00	-700.100 H+	-774.231	-248.636	49.999	-5.000
AL(OH)2+ 1.00	1.0 AL+3	0.00 2.00	4.00 H2O	0.00 -2.00	-907.559 H+	-1020.058	-377.322	90.002	-10.200
AL(OH)4- 1.00	-1.0 AL+3	0.00 4.00	4.00 H2O	0.00 -4.00	-1313.344 H+	-1510.302	-660.597	171.418	-22.200
ALF+2 1.00	2.0 AL+3	0.00 1.00	5.00 F-	0.00	-813.032	-873.750	-203.648	0.000	7.010
ALF2+ 1.00	1.0 AL+3	0.00 2.00	4.00 F-	0.00	-1127.316	-1125.399	6.429	83.701	12.750
ALF3 1.00	0.0 AL+3	0.00 3.00	0.00 F-	0.00	-1433.209	-1533.990	-338.023	10.460	17.020
ALF4- 1.00	-1.0 AL+3	0.00 4.00	4.00 F-	0.00	-1730.140	-1879.800	-501.962	0.000	19.720
BACO3 1.00	0.0 BA+2	4.00 1.00	0.00 CO3-2	0.00	-1098.765	-1192.973	-315.978	14.841	2.713
BAHCO3+ 1.00	1.0 BA+2	4.00 1.00	5.40 CO3-2	0.00 1.00	-1147.841 H+	-1199.454	-173.112	8.360	11.311
BAOH+ 1.00	1.0 BA+2	0.00 1.00	4.00 H2O	0.00 -1.00	-715.615 H+	-755.168	-132.664	63.162	-13.470
BASO4 1.00	0.0 BA+2	6.00 1.00	0.00 SO4-2	0.00	-1312.374	-1435.690	-413.602	6.150	2.280
CACO3 1.00	0.0 CA+2	4.00 1.00	0.00 CO3-2	0.00	-1099.128	-1203.482	-350.003	14.832	3.224
CAF+ 1.00	1.0 CA+2	0.00 1.00	4.00 F-	0.00	-839.692	-862.459	-76.360	15.891	0.940
CAHCO3+ 1.00	1.0 CA+2	4.00 1.00	5.40 CO3-2	0.00 1.00	-1145.990 H+	-1221.950	-254.770	-3.636	11.434
CAOH+ 1.00	1.0 CA+2	0.00 1.00	4.00 H2O	0.00 -1.00	-716.600 H+	-768.020	-172.461	60.810	-12.850
CASO4 1.00	0.0 CA+2	6.00 1.00	0.00 SO4-2	0.00	-1309.987	-1446.190	-456.827	6.150	2.309
FE(OH)2+ 1.00	1.0 FE+2	3.00 2.00	4.00 H2O	0.00 -1.00	-446.442 E-	-618.920 -2.00	-578.494 H+	41.840	-18.700
FE(OH)20 1.00	0.0 FE+2	2.00 2.00	0.00 H2O	0.00 -2.00	-435.597 H+	-541.261	-354.398	119.499	-20.600
FE(OH)3- 1.00	-1.0 FE+2	2.00 3.00	4.00 H2O	0.00 -3.00	-613.375 H+	-819.790	-692.319	126.800	-31.000
FE(OH)30 1.00	0.0 FE+2	3.00 3.00	0.00 H2O	0.00 -1.00	-638.261 E-	-904.750 -3.00	-893.807 H+	41.840	-26.640
FE(OH)4- 1.00	-1.0 FE+2	3.00 4.00	4.00 H2O	0.00 -1.00	-829.795 E-	-1190.580 -4.00	-1210.078 H+	41.840	-34.630
FE(SO4)2 1.00	-1.0 FE+2	15.00 2.00	4.00 SO4-2	0.00 -1.00	-1523.463 E-	-1846.689	-1084.107	61.091	-7.610

Table B.5: Selected aqueous species and minerals in 0491 PHREEQE-PSI data base. Page 3 of 12

		Charge	OPV	DH a	DH b	$\Delta_f G^0$	$\Delta_f H^0$	$\Delta_f S^0$	$\Delta_r H^0$	logK(25)
FE+3		3.0	3.00	9.00	0.00	-4.526	-47.260	-143.331	41.840	-13.030
1.00	FE+2		-1.00	E-						
FECL+2		2.0	3.00	4.00	0.00	-144.194	-181.240	-124.255	74.940	-11.550
1.00	FE+2		1.00	CL-		-1.00	E-			
FECL2+		1.0	3.00	4.00	0.00	-279.124	-348.069	-231.244	75.191	-10.900
1.00	FE+2		2.00	CL-		-1.00	E-			
FECL30		0.0	3.00	0.00	0.00	-404.636	-505.451	-338.135	84.889	-11.900
1.00	FE+2		3.00	CL-		-1.00	E-			
FECL4-		-1.0	3.00	4.00	0.00	-524.954	-657.590	-444.863	99.830	-13.810
1.00	FE+2		4.00	CL-		-1.00	E-			
FEOH+		1.0	2.00	4.00	0.00	-261.815	-319.710	-194.180	55.220	-9.500
1.00	FE+2		1.00	H2O		-1.00	H+			
FEOH+2		2.0	3.00	4.00	0.00	-229.166	-289.589	-202.661	85.341	-15.220
1.00	FE+2		1.00	H2O		-1.00	E-			
FESO4+		1.0	9.00	4.00	0.00	-770.901	-940.241	-567.968	58.199	-9.110
1.00	FE+2		1.00	SO4-2		-1.00	E-			
FESO40		0.0	8.00	0.00	0.00	-835.743	-991.741	-523.222	6.699	2.250
1.00	FE+2		1.00	SO4-2						
H2ASO3-		-1.0	3.00	4.00	0.00	-587.127	-714.791	-428.184	27.409	-9.228
1.00	H3ASO3		-1.00	H+						
H2ASO4-		-1.0	5.00	4.50	0.00	-753.173	-909.562	-524.532	-21.422	18.354
1.00	ASO4-3		2.00	H+						
H2BO3-		-1.0	0.00	4.00	0.00	-916.559	-1059.311	-478.792	13.489	-9.240
1.00	H3BO3		-1.00	H+						
H2CO3		0.0	4.00	0.00	0.00	-623.133	-699.322	-255.540	-24.008	16.681
1.00	CO3-2		2.00	H+						
H2PO4-		-1.0	0.00	4.50	0.00	-1137.104	-1303.312	-557.464	-18.912	19.553
1.00	PO4-3		2.00	H+						
H2SE		0.0	-2.00	0.00	0.00	22.145	19.212	-9.839	-525.008	84.990
1.00	SEO4-2		10.00	H+		8.00	E-	-4.00	H2O	
H2SEO3		0.0	4.00	0.00	0.00	-433.732	-509.207	-253.144	-195.937	40.220
1.00	SEO4-2		4.00	H+		2.00	E-	-1.00	H2O	
H3SIO4-		-1.0	0.00	4.00	0.00	-1251.061	-1419.576	-565.201	37.384	-9.929
1.00	H4SIO4		-1.00	H+						
HASO4-2		-2.0	5.00	4.00	0.00	-714.599	-906.340	-643.104	-18.200	11.596
1.00	ASO4-3		1.00	H+						
HCO3-		-1.0	4.00	5.50	0.00	-586.876	-690.213	-346.595	-14.899	10.329
1.00	CO3-2		1.00	H+						
HF(AQ)		0.0	0.00	0.00	0.00	-299.608	-320.869	-71.309	14.481	3.169
1.00	H+		1.00	F-						
HPO4-2		-2.0	0.00	4.00	0.00	-1095.967	-1299.170	-681.545	-14.770	12.346
1.00	PO4-3		1.00	H+						
HS-		-1.0	-2.00	3.50	0.00	12.310	67.259	184.302	105.859	-6.992
1.00	H2S(AQ)		-1.00	H+						
HSE-		-1.0	-2.00	0.00	0.00	43.949	15.906	-94.056	-528.314	81.170
1.00	SEO4-2		9.00	H+		8.00	E-	-4.00	H2O	

Table B.5: Selected aqueous species and minerals in 0491 PHREEQE-PSI data base. Page 4 of 12

		Charge	OPV	DH a	DH b	$\Delta_f G^0$	$\Delta_f H^0$	$\Delta_f S^0$	$\Delta_f H^0$	logK(25)
HSEO3-		-1.0	4.00	0.00	0.00	-417.750	-504.186	-289.908	-190.916	37.420
1.00	SEO4-2		3.00	H+	2.00	E-	-1.00	H2O		
HSEO4-		-1.0	6.00	0.00	0.00	-451.574	-575.293	-414.955	23.807	1.800
1.00	SEO4-2		1.00	H+						
I2		0.0	2.00	0.00	0.00	16.141	-113.560	-435.018	0.000	-20.950
2.00	I-		-2.00	E-						
I3-		-1.0	2.00	0.00	0.00	-51.961	-170.340	-397.045	0.000	-18.080
3.00	I-		-2.00	E-						
KSO4-		-1.0	6.00	4.00	0.00	-1031.362	-1152.070	-404.858	9.410	0.850
1.00	K+		1.00	SO4-2						
MGCO3		0.0	4.00	0.00	0.00	-1000.329	-1130.963	-438.149	11.351	2.980
1.00	MG+2		1.00	CO3-2						
MGF+		1.0	0.00	4.00	0.00	-747.308	-782.794	-119.019	19.556	1.820
1.00	MG+2		1.00	F-						
MGHCO3+		1.0	4.00	5.40	0.00	-1048.361	-1152.887	-350.583	-10.573	11.395
1.00	MG+2		1.00	H+	1.00	CO3-2				
MGOH+		1.0	0.00	4.00	0.00	-627.242	-686.158	-197.607	66.672	-11.440
1.00	MG+2		1.00	H2O	-1.00	H+				
MGSO4		0.0	6.00	0.00	0.00	-1212.243	-1370.491	-530.766	5.849	2.250
1.00	MG+2		1.00	SO4-2						
MN(OH)3-		-1.0	2.00	4.00	0.00	-740.885	-1078.240	-1131.495	0.000	-34.800
1.00	MN+2		3.00	H2O	-3.00	H+				
MN2(OH)3		1.0	4.00	4.00	0.00	-1031.201	-1298.990	-898.169	0.000	-23.900
2.00	MN+2		3.00	H2O	-3.00	H+				
MNCL+		1.0	2.00	4.00	0.00	-362.785	-387.830	-84.002	0.000	0.607
1.00	MN+2		1.00	CL-						
MNCL20		0.0	2.00	0.00	0.00	-490.774	-554.910	-215.113	0.000	0.041
1.00	MN+2		2.00	CL-						
MNCL3-		-1.0	2.00	4.00	0.00	-620.019	-721.990	-342.012	0.000	-0.305
1.00	MN+2		3.00	CL-						
MNHCO3+		1.0	6.00	5.40	0.00	-822.231	-911.164	-298.284	-15.100	11.600
1.00	MN+2		1.00	CO3-2	1.00	H+				
MNOH+		1.0	2.00	4.00	0.00	-404.793	-446.330	-139.316	60.250	-10.590
1.00	MN+2		1.00	H2O	-1.00	H+				
MNSO40		0.0	8.00	0.00	0.00	-985.000	-1121.011	-456.183	9.079	2.260
1.00	MN+2		1.00	SO4-2						
NACO3-		-1.0	4.00	4.00	0.00	-797.107	-878.370	-272.560	37.284	1.268
1.00	NA+		1.00	CO3-2						
NAHCO3		0.0	4.00	0.00	0.00	-847.405	-930.733	-279.485	-15.079	10.080
1.00	NA+		1.00	H+	1.00	CO3-2				
NASO4-		-1.0	6.00	4.00	0.00	-1009.946	-1144.994	-452.955	4.686	0.700
1.00	NA+		1.00	SO4-2						
NH3		0.0	-3.00	0.00	0.00	-26.590	-81.065	-182.707	52.195	-9.252
1.00	NH4+		-1.00	H+						
NI(CO3)2		-2.0	8.00	0.00	0.00	-1159.145	-1404.628	-823.354	0.000	10.110

Table B.5: Selected aqueous species and minerals in 0491 PHREEQE-PSI data base. Page 5 of 12

	Charge	OPV	DH a	DH b	$\Delta_f G^0$	$\Delta_f H^0$	$\Delta_f S^0$	$\Delta_r H^0$	logK(25)
1.00	NI2+	2.00	CO3-2						
NI(NH3)2		2.0	-6.00	0.00	0.00	-128.085	-247.969	-402.093	72.551
1.00	NI2+	2.00	NH4+		-2.00	H+			
NI(NH3)6		2.0	-18.00	0.00	0.00	-256.240	-634.695	-1269.345	218.865
1.00	NI2+	6.00	NH4+		-6.00	H+			
NI(NO3)2		0.0	5.00	0.00	0.00	-263.755	-467.700	-684.034	0.000
1.00	NI2+	2.00	NO3-						
NI(OH)2		0.0	0.00	0.00	0.00	-405.722	-625.660	-737.676	0.000
1.00	NI2+	2.00	H2O		-2.00	H+			
NI(OH)3-		-1.0	0.00	0.00	0.00	-585.783	-911.490	-1092.427	0.000
1.00	NI2+	3.00	H2O		-3.00	H+			
NI(OH)4-		-2.0	0.00	0.00	0.00	-743.012	-1197.320	-1523.756	0.000
1.00	NI2+	4.00	H2O		-4.00	H+			
NI(SO4)2		-2.0	12.00	0.00	0.00	-1551.865	-1872.680	-1076.018	0.000
1.00	NI2+	2.00	SO4-2						
NI2OH3+		3.0	0.00	0.00	0.00	-267.265	-393.830	-424.500	0.000
2.00	NI2+	1.00	H2O		-1.00	H+			
NI4(OH)4		4.0	0.00	0.00	0.00	-972.623	-1359.320	-1296.989	0.000
4.00	NI2+	4.00	H2O		-4.00	H+			
NICl+		1.0	0.00	0.00	0.00	-179.103	-221.080	-140.791	0.000
1.00	NI2+	1.00	Cl-						
NICl2		0.0	0.00	0.00	0.00	-313.520	-388.160	-250.345	0.000
1.00	NI2+	2.00	Cl-						
NICO3		0.0	4.00	0.00	0.00	-606.511	-729.314	-411.884	0.000
1.00	NI2+	1.00	CO3-2						
NIF+		1.0	0.00	0.00	0.00	-334.540	-389.350	-183.833	0.000
1.00	NI2+	1.00	F-						
NIH2PO4+		1.0	0.00	0.00	0.00	-1191.534	-1338.400	-492.592	0.000
1.00	NI2+	1.00	PO4-3		2.00	H+			
NIHC03+		1.0	4.00	0.00	0.00	-650.062	-729.314	-265.812	0.000
1.00	NI2+	1.00	CO3-2		1.00	H+			
NIHP207-		-1.0	0.00	0.00	0.00	-2053.237	-2336.970	-951.644	0.000
1.00	NI2+	2.00	PO4-3		-1.00	H2O	3.00	H+	
NIHPO4		0.0	0.00	0.00	0.00	-1158.314	-1338.400	-604.012	0.000
1.00	NI2+	1.00	PO4-3		1.00	H+			
NINO3+		1.0	5.00	0.00	0.00	-158.673	-260.850	-342.703	0.000
1.00	NI2+	1.00	NO3-						
NIOH+		1.0	0.00	0.00	0.00	-227.316	-287.907	-203.221	51.923
1.00	NI2+	1.00	H2O		-1.00	H+			
NIP207-2		-2.0	0.00	0.00	0.00	-2018.020	-2356.593	-1135.581	-19.623
1.00	NI2+	2.00	PO4-3		-1.00	H2O	2.00	H+	
NIPO4-		-1.0	0.00	0.00	0.00	-1118.872	-1338.400	-736.300	0.000
1.00	NI2+	1.00	PO4-3						
NISO4		0.0	6.00	0.00	0.00	-802.785	-949.365	-491.632	13.975
1.00	NI2+	1.00	SO4-2						2.310

Table B.5: Selected aqueous species and minerals in 0491 PHREEQE-PSI data base. Page 6 of 12

		Charge	OPV	DH a	DH b	$\Delta_f G^0$	$\Delta_f H^0$	$\Delta_f S^0$	$\Delta_r H^0$	logK(25)
OH-		-1.0	0.00	3.50	0.00	-157.241	-229.995	-244.017	55.835	-13.998
	1.00 H2O		-1.00 H+							
PD(NH3)1		2.0	-3.00	0.00	0.00	95.114	15.740	-266.221	0.000	0.348
	1.00 PD2+		1.00 NH4+		-1.00 H+					
PD(NH3)2		2.0	-6.00	0.00	0.00	17.723	-117.520	-453.607	0.000	-0.004
	1.00 PD2+		2.00 NH4+		-2.00 H+					
PD(NH3)3		2.0	-9.00	0.00	0.00	-51.677	-250.780	-667.795	0.000	-1.756
	1.00 PD2+		3.00 NH4+		-3.00 H+					
PD(NH3)4		2.0	-12.00	0.00	0.00	-117.081	-384.040	-895.384	0.000	-4.208
	1.00 PD2+		4.00 NH4+		-4.00 H+					
PD(NO2)4		-2.0	6.00	0.00	0.00	-89.466	464.920	1859.421	0.000	135.140
	1.00 PD2+		4.00 NO3-		8.00 H+		8.00 E-		-4.00 H2O	
PD(OH)2		0.0	0.00	0.00	0.00	-276.090	-422.660	-491.598	0.000	-3.800
	1.00 PD2+		-2.00 H+		2.00 H2O					
PD(OH)3-		-1.0	0.00	0.00	0.00	-443.936	-708.490	-887.319	0.000	-15.940
	1.00 PD2+		-3.00 H+		3.00 H2O					
PD(OH)4-		-2.0	0.00	0.00	0.00	-604.476	-994.320	-1307.544	0.000	-29.360
	1.00 PD2+		-4.00 H+		4.00 H2O					
PD(SO4)2		-2.0	0.00	0.00	0.00	-1335.245	-1669.680	-1121.701	0.000	4.160
	1.00 PD2+		2.00 SO4-2							
PDBR+		1.0	0.00	0.00	0.00	31.439	27.590	-12.909	0.000	7.220
	1.00 PD2+		1.00 BR-							
PDBR3-		-1.0	0.00	0.00	0.00	-203.887	-215.230	-38.043	0.000	12.060
	1.00 PD2+		3.00 BR-							
PDBR4-2		-2.0	0.00	0.00	0.00	-317.555	-384.338	-223.990	-47.698	13.780
	1.00 PD2+		4.00 BR-							
PDCL+		1.0	0.00	0.00	0.00	22.620	-37.912	-203.025	-19.832	3.970
	1.00 PD2+		1.00 CL-							
PDCL2		0.0	0.00	0.00	0.00	-128.806	-185.160	-189.011	0.000	7.510
	1.00 PD2+		2.00 CL-							
PDCL3-		-1.0	0.00	0.00	0.00	-276.066	-352.240	-255.490	0.000	10.320
	1.00 PD2+		3.00 CL-							
PDCL4-2		-2.0	0.00	0.00	0.00	-417.103	-549.863	-445.279	-30.543	12.040
	1.00 PD2+		4.00 CL-							
PDI+		1.0	0.00	0.00	0.00	65.304	92.220	90.278	0.000	10.420
	1.00 PD2+		1.00 I-							
PDI4-2		-2.0	0.00	0.00	0.00	-159.607	-78.120	273.309	0.000	22.640
	1.00 PD2+		4.00 I-							
PDOH+		1.0	0.00	0.00	0.00	-49.966	-136.830	-291.343	0.000	-1.870
	1.00 PD2+		-1.00 H+		1.00 H2O					
S-2		-2.0	-2.00	5.00	0.00	86.039	117.882	106.802	156.482	-19.909
	1.00 H2S(AQ)		-2.00 H+							
SE-2		-2.0	-2.00	0.00	0.00	129.282	544.220	1391.707	0.000	66.220
	1.00 SEO4-2		8.00 H+		8.00 E-		-4.00 H2O			
SEO3-2		-2.0	4.00	0.00	0.00	-369.803	-509.207	-467.561	-195.937	29.020
	1.00 SEO4-2		2.00 H+		2.00 E-		-1.00 H2O			

Table B.5: Selected aqueous species and minerals in 0491 PHREEQE-PSI data base. Page 7 of 12

		Charge	OPV	DH a	DH b	$\Delta_f G^0$	$\Delta_f H^0$	$\Delta_f S^0$	$\Delta_r H^0$	$\log K(25)$
SRCO3		0.0	4.00	0.00	0.00	-1107.760	-1204.386	-324.087	21.828	2.805
1.00	SR+2		1.00	CO3-2						
SRHC03+		1.0	4.00	5.40	0.00	-1157.470	-1215.813	-195.683	10.401	11.514
1.00	SR+2		1.00	CO3-2		1.00	H+			
SROH+		1.0	0.00	4.00	0.00	-725.112	-776.079	-170.944	60.651	-13.290
1.00	SR+2		1.00	H2O		-1.00	H+			
SRSO4		0.0	6.00	0.00	0.00	-1320.901	-1468.939	-496.520	-8.699	2.290
1.00	SR+2		1.00	SO4-2						
U(OH)4		0.0	4.00	0.00	0.00	-1429.903	-1630.761	-673.682	103.759	-8.500
1.00	U4+		4.00	H2O		-4.00	H+			
U(OH)5-		-1.0	4.00	4.00	0.00	-1640.501	-1904.872	-886.703	115.478	-13.150
1.00	U4+		5.00	H2O		-5.00	H+			
UL(OH)2		0.0	6.00	0.00	0.00	-1357.412	-1517.370	-536.502	217.150	-21.200
1.00	U4+		4.00	H2O		-6.00	H+	-2.00	E-	
UL=UO2+2		2.0	6.00	5.00	0.00	-951.627	-1018.512	-224.333	144.348	-9.200
1.00	U4+		2.00	H2O		-4.00	H+	-2.00	E-	
ULCO3		0.0	10.00	0.00	0.00	-1536.911	-1705.545	-565.603	132.629	0.850
1.00	U4+		2.00	H2O		1.00	CO3-2	-4.00	H+	-2.00 E-
ULCO32-2		-2.0	14.00	4.00	0.00	-2104.500	-2354.078	-837.088	159.410	7.800
1.00	U4+		2.00	H2O		2.00	CO3-2	-4.00	H+	-2.00 E-
ULCO33-4		-4.0	18.00	6.00	0.00	-2657.533	-3085.043	-1433.874	103.759	12.200
1.00	U4+		2.00	H2O		3.00	CO3-2	-4.00	H+	-2.00 E-
ULOH+		1.0	6.00	4.50	0.00	-1155.661	-1258.318	-344.312	190.372	-15.000
1.00	U4+		3.00	H2O		-5.00	H+	-2.00	E-	
UO2+		1.0	5.00	4.00	0.00	-967.427	-1032.612	-218.633	130.248	-6.432
1.00	U4+		2.00	H2O		-4.00	H+	-1.00	E-	

Table B.5: Selected aqueous species and minerals in 0491 PHREEQE-PSI data base. Page 8 of 12

	Charge	OPV	DH a	DH b	$\Delta_f G^0$	$\Delta_f H^0$	$\Delta_f S^0$	$\Delta_r H^0$	logK(25)
MINERALS									
ANHYDRIT		6.00			-1321.009	-1432.382	-373.550	19.958	4.240
1.00	CA+2		1.00	SO4-2					
BARITE		6.00			-1356.268	-1468.408	-376.121	-26.568	9.970
1.00	BA+2		1.00	SO4-2					
BASE		-2.00			-383.725	-387.852	-13.842	-399.572	58.800
1.00	SEO4-2		1.00	BA+2	8.00	H+	-4.00	H2O	8.00 E-
BASEO3S		4.00			-962.721	-1035.473	-244.008	-189.703	35.600
1.00	BA+2		1.00	SEO4-2	2.00	H+	2.00	E-	-1.00 H2O
BASEO4S		6.00			-1039.298	-1141.265	-341.999	-9.665	7.470
1.00	BA+2		1.00	SEO4-2					
CALCITE		4.00			-1129.129	-1208.691	-266.851	9.623	8.480
1.00	CO3-2		1.00	CA+2					
CASE		-2.00			-363.477	-368.227	-15.931	-369.447	55.700
1.00	SEO4-2		1.00	CA+2	8.00	H+	-4.00	H2O	8.00 E-
CASEO3AQ		4.00			-1427.941	-1623.867	-657.137	-195.937	34.460
1.00	CA+2		1.00	SEO4-2	2.00	H+	2.00	E-	1.00 H2O
CASEO4AQ		6.00			-1486.024	-1706.856	-740.674	6.904	3.090
1.00	CA+2		1.00	SEO4-2	2.00	H2O			
CELESTIT		6.00			-1345.673	-1462.750	-392.678	-2.510	6.630
1.00	SR+2		1.00	SO4-2					
CHALCEDO		0.00			-1090.858	-1190.878	-335.470	-19.748	3.550
1.00	H4SiO4		-1.00	H2O					
DOLOMITE		8.00			-2161.079	-2325.943	-552.954	34.685	17.000
1.00	CA+2		1.00	Mg+2	2.00	CO3-2			
FE(OH)3(3.00			-701.676	-823.162	-407.465	123.428	-15.530
1.00	FE+2		-1.00	E-	3.00	H2O	-3.00	H+	
FE3SE4		0.00			-221.409	-209.616	39.555	-2119.196	352.800
4.00	SEO4-2		3.00	FE+2	-16.00	H2O	32.00	H+	30.00 E-
FESE2		0.00			-97.511	-102.726	-17.490	-1102.066	181.000
1.00	FE+2		2.00	SEO4-2	16.00	H+	-8.00	H2O	14.00 E-
FLUORITE		0.00			-1175.266	-1229.599	-182.233	-15.899	10.410
1.00	CA+2		2.00	F-					
GOETHITE		3.00			-475.952	-558.336	-276.316	102.424	-13.530
1.00	FE+2		-1.00	E-	2.00	H2O	-3.00	H+	
GYPSUM		6.00			-1797.229	-2023.540	-759.049	0.460	4.580
1.00	CA+2		1.00	SO4-2	2.00	H2O			
HEMATITE		6.00			-816.879	-864.020	-158.115	171.670	-9.170
2.00	FE+2		-2.00	E-	3.00	H2O	-6.00	H+	
K2SE		-2.00			-369.982	-383.899	-46.677	-423.839	54.700
1.00	SEO4-2		2.00	K+	8.00	H+	-4.00	H2O	8.00 E-
K2SE04		6.00			-1009.973	-1127.982	-395.804	-24.602	0.640
2.00	K+		1.00	SEO4-2					
K2SEO3		4.00			-877.973	-966.500	-296.923	-148.950	19.060
2.00	K+		1.00	SEO4-2	2.00	H+	2.00	E-	-1.00 H2O

Table B.5: Selected aqueous species and minerals in 0491 PHREEQE-PSI data base. Page 9 of 12

	Charge	OPV	DH a	DH b	$\Delta_f G^0$	$\Delta_f H^0$	$\Delta_f S^0$	$\Delta_f H^0$	logK(25)
LI2SE		-2.00			-392.515	-400.995	-28.443	-388.275	55.000
2.00 LI+		1.00	SEO4-2	8.00 H+		-4.00	H2O	8.00 E-	
LI2SEO3		4.00			-969.399	-1057.988	-297.127	-187.778	31.430
2.00 LI+		1.00	SEO4-2	2.00 H+		2.00 E-		-1.00 H2O	
LI2SEO4		6.00			-1020.005	-1138.007	-395.780	18.033	-1.250
2.00 LI+		1.00	SEO4-2						
MAGNETIT		8.00			-1161.116	-1195.688	-115.956	214.932	-4.230
3.00 FE+2		-2.00	E-		4.00 H2O		-8.00 H+		
MANGANIT		3.00			-558.141	-792.410	-785.741	0.000	-25.270
1.00 MN+2		2.00	H2O		-1.00 E-		-3.00 H+		
MGSE		-2.00			-288.331	-292.227	-13.067	-369.447	59.600
1.00 MG+2		1.00	SEO4-2		8.00 H+		-4.00 H2O	8.00 E-	
NA2SE		-2.00			-327.150	-343.145	-53.647	-406.685	54.400
2.00 NA+		1.00	SEO4-2		8.00 H+		-4.00 H2O	8.00 E-	
NA2SE2		-2.00			-370.132	-388.032	-60.036	-995.792	150.800
2.00 NA+		2.00	SEO4-2		16.00 H+		-8.00 H2O	14.00 E-	
NA2SEO3		4.00			-871.271	-959.804	-296.939	-165.854	25.090
2.00 NA+		1.00	SEO4-2		2.00 H+		2.00 E-	-1.00 H2O	
NA2SEO4		6.00			-962.289	-1079.989	-394.769	-0.209	-0.510
2.00 NA+		1.00	SEO4-2						
NI.METAL		-2.00			-1.192	-1.909	-2.404	52.091	-7.780
1.00 NI2+		2.00	E-						
NI(BO2)2		0.00			-1454.097	-1627.940	-583.073	0.000	-9.780
1.00 NI2+		2.00	H3BO3		-2.00 H2O		-2.00 H+		
NI(OH)2B		0.00			-2526.747	-2771.260	-820.102	0.000	11.960
1.00 NI2+		2.00	H2O		-2.00 H+		2.00 H3BO3		
NI(OH)2S		0.00			-447.218	-529.721	-276.715	95.939	-12.730
1.00 NI2+		2.00	H2O		-2.00 H+				
NI2P2O7S		0.00			-2096.725	-2390.970	-986.901	0.000	33.580
2.00 NI2+		2.00	PO4-3		-1.00 H2O		2.00 H+		
NI2SiO4O		0.00			-1288.715	-1393.458	-351.308	171.502	-19.310
2.00 NI2+		1.00	H4SiO4		-4.00 H+				
NI2SiO4S		0.00			-1280.724	-1386.680	-355.376	178.280	-20.710
2.00 NI2+		1.00	H4SiO4		-4.00 H+				
NI3PO4.2		0.00			-2356.748	-2578.502	-743.768	152.298	29.600
3.00 NI2+		2.00	PO4-3						
NI3S2		-6.00			-310.102	-196.942	379.543	42.258	20.691
3.00 NI2+		2.00	H2S(AQ)		-4.00 H+		2.00 E-		
NI3S4		-6.00			-671.817	-353.219	1068.582	-36.819	74.391
3.00 NI2+		4.00	H2S(AQ)		-8.00 H+		-2.00 E-		
NIBR2S		0.00			-199.532	-213.977	-48.450	82.843	-9.420
1.00 NI2+		2.00	BR-						
NICL22AQ		0.00			-760.116	-922.038	-543.090	37.782	-3.890
1.00 NI2+		2.00	CL-		2.00 H2O				
NICL24AQ		0.00			-1234.910	-1516.543	-944.602	14.937	-3.800
1.00 NI2+		2.00	CL-		4.00 H2O				

Table B.5: Selected aqueous species and minerals in 0491 PHREEQE-PSI data base. Page 10 of 12

	Charge	OPV	DH a	DH b	$\Delta_f G^0$	$\Delta_f H^0$	$\Delta_f S^0$	$\Delta_r H^0$	logK(25)
NICL26AQ		0.00			-1713.243	-2103.056	-1307.442	0.084	-3.090
1.00 NI2+		2.00	CL-		6.00 H2O				
NICL2S		0.00			-260.322	-307.409	-157.930	80.751	-8.360
1.00 NI2+		2.00	CL-						
NICO3S		4.00			-613.303	-691.240	-261.400	38.074	6.970
1.00 NI2+		1.00	CO3-2						
NIF2.4AQ		0.00			-1586.482	-1868.020	-944.285	0.000	5.130
1.00 NI2+		2.00	F-		4.00 H2O				
NIF2S		0.00			-610.638	-659.011	-162.245	65.689	0.350
1.00 NI2+		2.00	F-						
NIFE2O4		6.00			-972.960	-1080.966	-362.255	294.554	-31.360
1.00 NI2+		2.00	FE+2		4.00 H2O	-8.00 H+	-2.00 E-		
NII2S		0.00			-81.744	-80.114	5.465	87.446	-11.790
1.00 NI2+		2.00	I-						
NIO		0.00			-211.677	-239.707	-94.014	100.123	-12.450
1.00 NI2+		1.00	H2O		-2.00 H+				
NIOHCL50		0.00			-452.091	-510.450	-195.736	55.835	-2.598
1.00 NI2+		1.50	H2O		-1.50 H+	0.50 CL-			
NIOHCL75		0.00			-490.557	-540.137	-166.291	55.835	-0.498
1.00 NI2+		1.75	H2O		-1.75 H+	0.25 CL-			
NIS		-2.00			-85.991	0.034	288.530	92.634	2.241
1.00 NI2+		1.00	H2S(AQ)		-2.00 H+				
NIS2		-2.00			-248.583	-129.945	397.916	1.255	25.891
1.00 NI2+		2.00	H2S(AQ)		-4.00 H+	-2.00 E-			
NISIO3		0.00			-1127.953	-1225.130	-325.932	0.000	2.060
1.00 NI2+		1.00	H4SiO4		-1.00 H2O	-2.00 H+			
NISO46AQ		6.00			-2223.913	-2682.881	-1539.385	-4.561	2.010
1.00 NI2+		1.00	SO4-2		6.00 H2O				
NISO47AQ		6.00			-2461.110	-2976.367	-1728.181	-12.217	2.020
1.00 NI2+		1.00	SO4-2		7.00 H2O				
NISO4S		6.00			-759.177	-872.966	-381.649	90.374	-5.330
1.00 NI2+		1.00	SO4-2						
P		4.00			-394.383	-393.492	2.988	-4.008	18.151
1.00 CO3-2		2.00	H+		-1.00 H2O				
PD.METAL		-2.00			-0.046	0.050	0.319	-148.950	30.930
1.00 PD2+		2.00	E-						
PD(OH)2S		0.00			-306.913	-395.046	-295.599	27.614	1.600
1.00 PD2+		-2.00	H+		2.00 H2O				
PD4S		-8.00			-72.138	12.225	282.955	-545.175	131.491
4.00 PD2+		1.00	H2S(AQ)		-2.00 H+	6.00 E-			
PDBR2S		0.00			-107.172	-105.284	6.333	-11.464	13.310
1.00 PD2+		2.00	BR-						
PDCL2S		0.00			-126.409	-173.194	-156.917	11.966	7.090
1.00 PD2+		2.00	CL-						
PDI2S		0.00			-62.617	-63.595	-3.281	-99.035	23.770

Table B.5: Selected aqueous species and minerals in 0491 PHREEQE-PSI data base. Page 11 of 12

	Charge	OPV	DH a	DH b	$\Delta_f G^0$	$\Delta_f H^0$	$\Delta_f S^0$	$\Delta_f H^0$	logK(25)
1.00	PD2+	2.00	I-						
PDO		0.00			-85.755	-85.367	1.301	51.463	4.400
1.00	PD2+	-2.00	H+	1.00	H2O				
PDS2		-2.00			-194.867	-72.130	411.662	-143.930	55.391
1.00	PD2+	2.00	H2S(AQ)	-4.00	H+	-2.00	E-		
PDSS		-2.00			-70.232	10.402	270.450	-99.998	38.391
1.00	PD2+	1.00	H2S(AQ)	-2.00	H+				
PORLAND		0.00			-897.746	-986.253	-296.855	128.407	-22.660
1.00	CA+2	2.00	H2O	-2.00	H+				
PYROLUSI		4.00			-465.217	-520.073	-183.991	272.337	-41.550
1.00	MN+2	2.00	H2O	-2.00	E-	-4.00	H+		
QUARTZ		0.00			-856.172	-910.362	-181.753	-25.062	3.980
1.00	H4SiO4	-2.00	H2O						
RHODOCHR		6.00			-816.180	-887.487	-239.163	8.577	10.540
1.00	MN+2	1.00	CO3-2						
SE		0.00			-0.173	-0.118	0.183	-544.338	88.900
1.00	SEO4-2	8.00	H+	-4.00	H2O	6.00	E-		
SE205		10.00			-283.055	-413.512	-437.554	-72.802	19.600
2.00	SEO4-2	6.00	H+	-3.00	H2O	2.00	E-		
SECL4S		4.00			-100.955	-188.534	-293.739	-64.434	14.600
1.00	SEO4-2	8.00	H+	4.00	CL-	-4.00	H2O	2.00	E-
SEO2		4.00			-171.363	-224.925	-179.647	-197.485	35.800
1.00	SEO4-2	4.00	H+	-2.00	H2O	2.00	E-		
SEO3		6.00			-94.568	-170.177	-253.594	143.093	-19.200
1.00	SEO4-2	2.00	H+	-1.00	H2O				
SIDERITE		6.00			-667.037	-742.113	-251.806	22.301	10.550
1.00	FE+2	1.00	CO3-2						
SISE2		-4.00			-142.049	-134.383	25.713	-909.183	139.700
1.00	H4SiO4	2.00	SEO4-2	20.00	H+	-12.00	H2O	16.00	E-
SRSE		-2.00			-392.195	-397.047	-16.275	-390.367	58.800
1.00	SR+2	1.00	SEO4-2	8.00	H+	-4.00	H2O	8.00	E-
STRONTIA		4.00			-1144.661	-1224.540	-267.916	1.674	9.270
1.00	SR+2	1.00	CO3-2						
URANINIT		4.00			-1030.396	-1084.619	-181.864	78.241	4.600
1.00	U4+	2.00	H2O	-4.00	H+				
WITHERIT		4.00			-1132.139	-1210.743	-263.640	-2.929	8.560
1.00	BA+2	1.00	CO3-2						
PE:AS(V)		1.00			-0.007	-0.011	-0.014	-69.956	20.020
0.50	ASO4-3	2.50	H+	-0.50	H3ASO3	-0.50	H2O		
PE:CO3-2		1.00			0.013	0.167	0.516	-33.681	4.770
0.13	CO3-2	1.25	H+	-0.13	CH4(AQ)	-0.38	H2O		
PE:H+/H2		1.00			-0.073	-0.073	0.001	-2.092	-1.540
1.00	H+	-0.50	H2(AQ)						
PE:N2(AQ)		1.00			0.196	-0.212	-1.367	-42.844	5.130
0.17	N2(AQ)	1.33	H+	-0.33	NH4+				

Table B.5: Selected aqueous species and minerals in 0491 PHREEQE-PSI data base. Page 12 of 12

	Charge	OPV	DH a	DH b	$\Delta_f G^0$	$\Delta_f H^0$	$\Delta_f S^0$	$\Delta_r H^0$	logK(25)
PE: NO ₃ - / 0.20	NO ₃ -	1.00 1.20	H+	-0.10	-0.531 N ₂ (AQ)	-0.122 -0.60	1.372 H ₂ O	-131.294	20.820
PE: O ₂ /H ₂ 0.25	O ₂ (AQ)	1.00 1.00	H+	-0.50	0.037 H ₂ O	-0.096	-0.449 -193.807	-139.997	21.490
PE: O ₂ (SA 0.25	O ₂ (AQ)	1.00 1.00	H+	-0.50	57.687 H ₂ O	-0.096	-139.997	11.390	
PE: SO ₄ -2 0.13	SO ₄ -2	1.00 1.25	H+	-0.13	0.024 H ₂ S(AQ)	-0.153 -0.50	-0.592 H ₂ O	-34.225	5.080