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JNC Thermodynamic Database for Performance Assessment of High-level Radioactive Waste Disposal System

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Abstract

This report is a summary of status, frozen datasets, and future tasks of the JNC thermodynamic database (JNC-TDB) for assessing performance of high-level radioactive waste in geological environments. The JNC-TDB development was carried out after the first progress report on geological disposal research in Japan (H3). In the development, thermodynamic data (equilibrium constants at 25 °C, I=0) for important radioactive elements were selected/determined based on original experimental data using different models (e.g., SIT, Pitzer). As a result, the reliability and traceability of the data for most of the important elements were improved over those of the PNC-TDB used in H-3 report.
For detailed information of data analysis and selections for each element, see the JNC technical reports listed in this document.

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高レベル放射性廃棄物の地層処分システムの性能評価のための放射性元素の熱力学データベース（JNC-TDB）開発（研究報告）

油井 三和*，東 侍郎*，柴田 雅博*

要旨

本報告書は，高レベル放射性廃棄物の地層処分の性能評価を行うために開発された放射性元素の熱力学データベース（JNC-TDB）について記述する。「地層処分研究開発第２次とりまとめ」に向けて行われた熱力学データベース開発の現状，第２次とりまとめにおいて用いられたデータセット，および今後の課題を示した。

本熱力学データベース（JNC-TDB）の開発は，第一次とりまとめ（H３報告書）での課題をもとに進められた。熱力学データは，原則として，実験データにまでさかのぼり，その評価を行って選定された。データは，標準状態（25℃，I＝0）での平衡定数として整理された。結果として，第一次とりまとめで用いられた熱力学データベースと比較し，データの追跡性が確保されるとともに，その信頼性が向上された。

各元素のデータの検討や選定に関しての詳細は，本報告書中で引用している個別の技術資料を参照されたい。

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CONTENTS

1. INTRODUCTION

Many radionuclides, especially actinides, have very long half-lives and are present in high-level radioactive wastes (HLW) in significant quantities, and therefore are expected to be present in repositories for very long periods. Developing capabilities to predict radionuclide behavior in specific geological environments is a problem, because: 1) In most cases the repositories have not yet been chosen, and 2) A considerable amount of inherent heterogeneity will exist within any chosen repository. It would be prohibitively expensive, as well as impossible based on empirical approaches, to gather sufficient and reliable data for performance assessment calculation. Therefore, it becomes necessary to gather generic information on the actinides and other important elements before their behavior can be predicted in any environment.

Recognizing these needs, repository programs in many countries are using thermodynamic data to predict radionuclide behavior in different environments. Thermodynamic data can provide information on types of aqueous species, as well as potential solubility-limiting solids under different selected geological environments. These data are necessary for 1) setting upper limits on concentrations of those elements that readily form sparingly soluble solids under expected repository condition, 2) determining the fundamental reactions for adsorptive characteristics of different geological materials, and 3) providing long-term predictions of expected concentrations of elements under any given conditions which are otherwise impossible to make.

In the first progress report (called "H-3 report") on geological disposal of high-level radioactive wastes in Japan (PNC, 1992), a thermodynamic database on radioactive elements (PNC-TDB_H-3, Yui et al., 1992) was used to estimate the solubility in the engineered barrier systems in the report. The thermodynamic database referred mainly to the Harwell R12324 (Cross et al., 1987), and was discussed element by element. For some elements, the other databases, such as OECD/NEA (Grenthe et al.,1992) were adopted. However, most of the data used in the PNC-TDB_H-3 were not based on critical review of the available literature, and the sources of the data were not sufficiently documented. Therefore, it was

necessary to establish a more traceable and scientifically reliable thermodynamic database based on the critical review of original literatures.

Unfortunately, critically reviewed databases with a traceable data selection are rare, and ongoing projects are slow in progress. International efforts have been undertaken, e.g., by the International Atomic Energy Agency (IAEA) and the Nuclear Energy Agency (NEA). The IAEA project "The Chemical Thermodynamics of Actinide Elements and Compounds" (e.g., Fuger et al. 1992), in which 10 volumes (out of 14 volumes planned) have been published between 1976 and 1992, has been closed after the last publication had appeared in 1992. The OECD/NEA-TDB project has a high quality review standard and includes international reviewers, but its progress is slow. The first database was published in 1992 on uranium (Grenthe et al. 1992), the second one in 1995 on americium (Silva et al. 1995). Databases on technetium, neptunium and plutonium are close to completion, and critical reviews on nickel, selenium and zirconium have been started recently. This pace does not meet the needs of JNC to prepare the second progress report for geological disposal of HLW, which will be submitted in 1999. Therefore, JNC decided to start its own project in which it would develop a thermodynamic database of radioactive elements for performance analysis of geological disposal systems of HLW (JNC-TDB). International specialists have assisted JNC with the aim of developing critically reviewed datasets for a large number of elements: Ac, Am, Cm, Np, Pu, Sm, Th, U, Bi, Nb, Pb, Pd, Sb, Sn, Cs, Ni, Pa, Po, Ra, Se, Tc, and Zr. These elements were selected on the basis of their potential hazard index reported in PNC(1991). The potential hazard index for each nuclide was determined based on the maximum permissible concentration of the radionuclide in water. This index was calculated by estimating a very conservative scenario. The nuclides that exceeded 1 μSv/y in the scenario were selected as the important nuclides. Ni was added as a hazardous corrosion product (PNC, 1991). Key reactions in the solubility estimation for the performance analysis of the geological disposal system are oxidation/reduction, hydrolysis and complex formation with carbonate, sulfate, phosphate, nitrate, fluoride and chloride. These have been mainly discussed in the JNC-TDB development.

In the JNC-TDB development project, the responsibilities of different specialists are depicted in Figure 1-1. At the initial stage of JNC-TDB development, the general review guideline was agreed to (see Appendix-1). However, as might be expected of such a large technical undertaking, and because of funding and time limitations and the quality and extent of available data, it was not possible to critically evaluate and use the same evaluation criteria as shown in Appendix-1 for each element. The general procedure for data collection and the review process for different elements are shown in Figure 1-2. In all cases, an effort was made to tabulate all of the available data. In the case of trivalent (Ac(III), Am(III), Cm(III), Np(III), Pu(III), and Sm(III)) and tetravalent (Th(IV), U(IV), Np(IV), and Pu(IV)) actinides and rare earths, decisions were made primarily based on recent experimental data obtained in simple systems and validated in mixed and complex systems where the Pitzer model (Pitzer, 1973; Pitzer and Mayorga, 1973) was used. In the case of Bi, Nb, Pb, Pd, Sb, and Sn, all available experimental data were evaluated, and selected experimental data were extrapolated to zero ionic strength using the Specific Ion Interaction theory (SIT) model, which was described in the literature (e. g., Grenthe et al., 1992; Silver et al., 1995). In the case of pentavalent actinides (Np(V) and Pu(V)), recently obtained data for Np(V) (Neck et al. 1995, Runde et al. 1996) using the Pitzer model approach for many of the ligands, were used as the basis for both Np(V) and Pu(V). In the case of hexavalent actinides (U(VI), Np(VI), Pu(VI)), recently available U(VI) data (Grenthe et al. 1992) were the primary reference source. Data for the remaining elements were tabulated by JNC staff using primarily the existing compilations. For Ra and Po, the thermodynamic datasets are the same as the PNC-TDB_H-3, because no new thermodynamic data have been reported since 1992. For Tc, the OECD/NEA database (as a draft version) will be published in a few months. In the near future, it will be necessary to discuss the Tc data to be adopted in the JNC-TDB. For Ni, Zr and Se, the thermodynamic data reported by Cross et al. (1987) were the primary reference data in the PNC-TDB_H-3. For Ni, Zr and Se, the reliability and traceability of data in the literature are not discussed in enough detail in the JNC-TDB development.

These collective efforts have resulted in this report and several JNC reports, which are referred to in the following sections. Based on these reports and on the recommendations of the scientific advisory

committee, selected thermodynamic data for various elements for use in JNC's program are summarized in this report. The recommendations of the scientific advisory committee were determined based on the following three criteria: i) the reliability and traceability of thermodynamic data could be confirmed, ii) data selections were carried out by using a suitable method for activity correction based on some experiments which were adequate to obtain thermodynamic data, and iii) in the case of data selection from other thermodynamic databases, the data were reviewed by experts.

Furthermore, because of 1) analogous behavior exhibited by trivalent actinides and rare earths, 2) the unavailability of comprehensive data for several important trivalent rare earths and actinides (e.g., Ac(III), Pu(III), Cm(III), Sm(III)), and 3) the recommendation of the scientific advisory committee, it was decided that the comprehensive data provided in this report for Am(III) could be used for the other trivalent rare earths and actinides. Similarly, because of the scarcity of thermodynamic data for Pu(V) and the difficulties of experimentally determining such data for Pu(V), the scientific advisory committee recommended that data for Np(V) was an excellent analog for Pu(V).

At present, most thermodynamic data for elements have been obtained at standard state (25 °C and 0.1 MPa), and are given by equilibrium constants or molar Gibbs free energy. Unfortunately, reliable thermodynamic data at temperatures higher than ambient are not available. Hence, the JNC-TDB includes equilibrium constants only for zero ionic strength and 25 °C. The selected thermodynamic data at 25 °C, for use in JNC's calculations are listed in the following sections. For details of the available data, selection criteria, and the specific reasons for choosing the data reported in this compilation, the reader is directed to detailed JNC technical reports referred to in the following sections. This compilation contains referenceable and internally consistent data for most of the important elements. Those data are expected to serve JNC's interim needs and to form the basis for future improvements in thermodynamic data at 25 °C and at elevated temperatures.

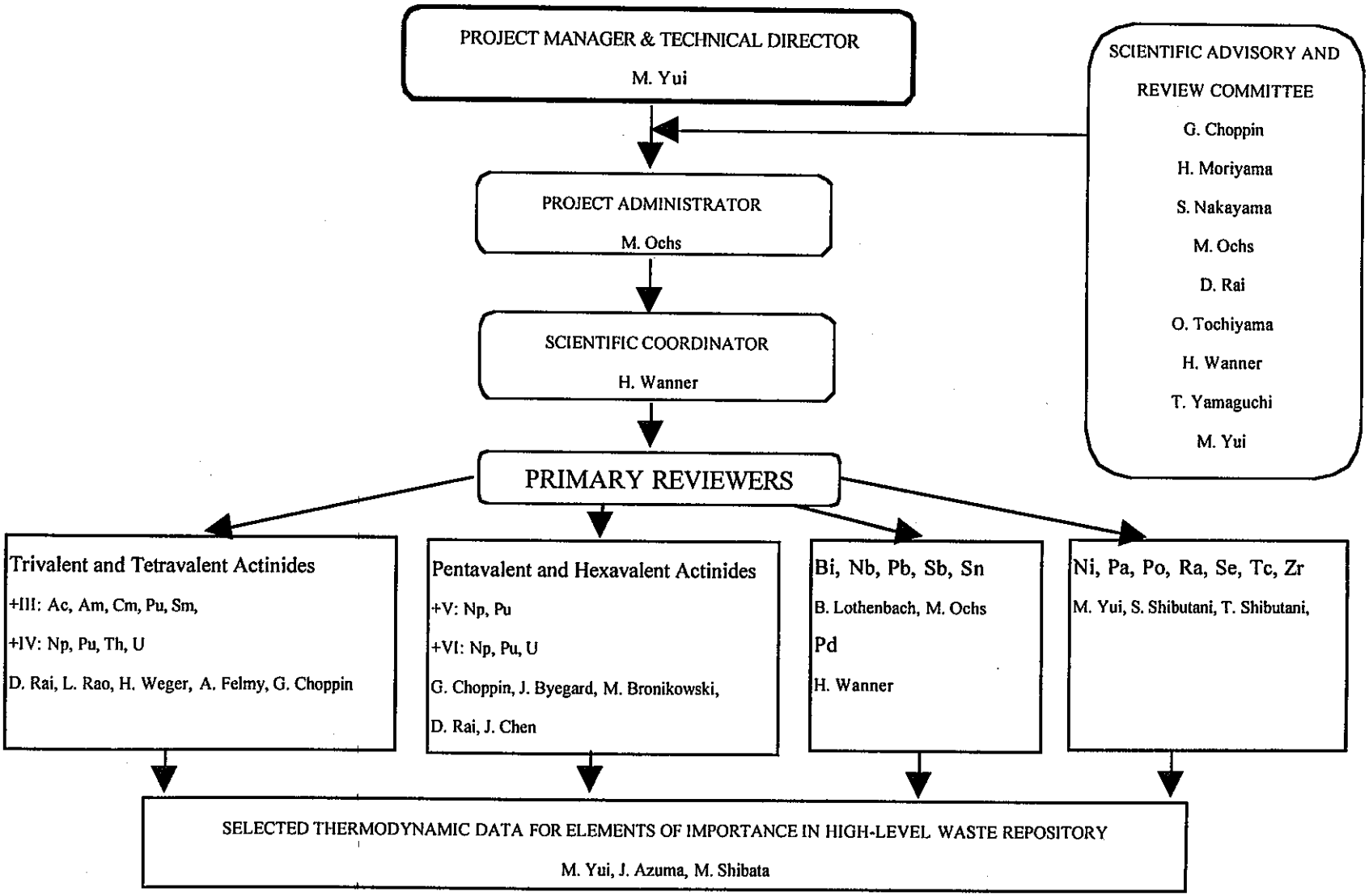

Figure 1-1 Programmatic and technical responsibilities for developing thermodynamic data for use in performance assessment

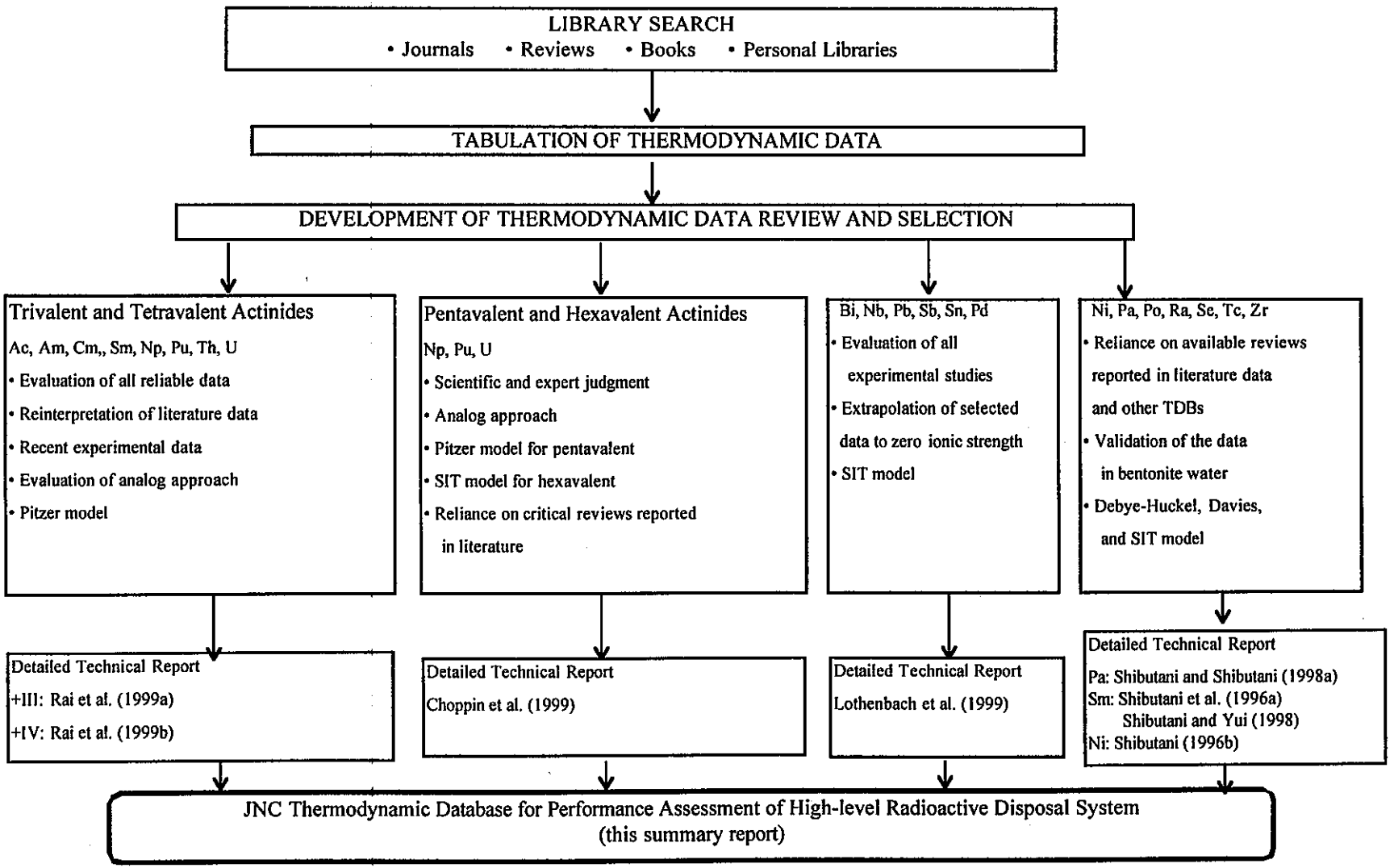

Figure 1-2 General technical approach, review, process, and technical output for developing of thermodynamic data for performance assessment calculations

2. SELECTED AND FROZEN DATASETS IN JNC-TDB

Status of selected and frozen thermodynamic datasets for each radioactive element in the JNC-TDB is briefly mentioned in the following subsections, which show equilibrium constants of reactions including solids and aqueous species for each radioactive element at 25 °C, zero ionic strength.

Abbreviations for different types of solids and aqueous species used in this report are listed in Table 2-1. In the reactions involving solids, designator "(cr)" means the solid is in crystalline phase, designator "(am)" means the solid is in amorphous phase, and designator "(s)" means solid phase, which was not identified as crystalline or amorphous. For minerals, designators are given by the name of minerals. For aqueous species with neutral charge, designator "(aq)" is used. An equilibrium constant is represented by K, and K_{sp} is used for solubility product.

The JNC-TDB is used in solubility estimation for the performance analysis of the geological disposal system. The JNC-TDB development and the solubility estimation for the second progress report (H12) have been carried out in parallel. Some parts of the selected and frozen datasets were consequently not used in the solubility estimation for the second progress report. In such cases, datasets used in the solubility estimation are given in Appendix-2.

Table 2-1 Abbreviations for Differential Types of Solid, Aqueous Species and Constants in JNC-TDB

Abbreviation	Meaning
(cr)	crystalline phase
(am)	amorphous phase
(s)	undecided solid phase
(minerals name)	minerals
(aq)	aqueous species with neutral charge
K	equilibrium constant
K_{sp}	solubility product constant

2.1 Lanthanide and Actinide Elements

This section shows the status and frozen thermodynamic data of the JNC-TDB development for lanthanides and actinides of the radioactive elements as mentioned in the introduction.

2.1.1 Actinium (Ac), Americium (Am), Curium (Cm), and Samarium (Sm)

Sm, Ac, Am and Cm of lanthanide and actinide elements have chemically analogous properties in aquatic chemistry, because these elements tend to form trivalent species and solids in aquatic system, and have similar ionic radii. Pu(III) mentioned in subsection 2.1.6 is also analogous to these elements. Of these elements, thermodynamic data for Am have been reviewed in detail by experts.

For Am, the PNC-TDB_H-3 included thermodynamic data given by Rai et al. (1983) and Felmy et al. (1990). In 1995, OECD/NEA published carefully reviewed thermodynamic data for Am (Silva et al., 1995), where the activity corrections were carried out with the use of specific ion interaction theory (SIT). These data were discussed comparing with PNC-TDB_H-3 and some related experimental data by Shibutani (1997a). Rai et al. (1999a) compiled thermodynamic data (equilibrium constants and Pitzer parameters) for actinide (III) in detail based on the Pitzer model for activity corrections. Choppin et al. (1999) compiled thermodynamic data of redox reactions for Am. Based on these four reports and the discussion in the scientific advisory and review committee in the JNC-TDB development, thermodynamic data for Am adopted in the JNC-TDB were determined. Thermodynamic dataset for Am selected by Rai et al. (1999a) was recommended by the scientific advisory and review committee. The thermodynamic dataset for Am(III) adopted in the JNC-TDB is shown in Tables 2.1.1-1 and 2.1.1-2. As only trivalent is relevant redox state to expected repository conditions and ambient conditions, thermodynamic data only for Am(III) are adopted in the JNC-TDB. Data for chloride and nitrate complexes were not included because complexation with Cl^- and NO_3^- are very weak. Ion-interaction parameters for Pitzer model were only determined. Detailed information on the data selection is described in Rai et al. (1999a).

The JNC-TDB development and the solubility estimation had been carried out in parallel for the last phase for the second progress report on the geological disposal research. For the solubility estimation, the

dataset is shown in Appendix-2.

For the other trivalent actinides and rare earths, the compilations were carried out in the JNC-TDB development.

For Sm, the PNC-TDB_H-3 did not include the thermodynamic data. In the JNC-TDB development, equilibrium constants of Sm(III)-OH and Sm(III)-CO_3 systems were obtained from the solubility measurements of $Sm(OH)_3$(cr) and $SmOHCO_3$(cr) by Shibutani (1996a), and a datum on $Sm(OH)_2^+$ was revised by Shibutani and Yui (1998).

For Ac, thermodynamic data for Am, which is chemically analogous to Ac, were used in the PNC-TDB_H-3. In the JNC-TDB development, thermodynamic data for Ac were not discussed. Rai et al. (1999a) discussed the data for actinides (III), but could not select the data for Ac because of the lack of reliable experimental measurements.

The PNC-TDB_H-3 did not include the thermodynamic data for Cm. In the JNC-TDB development, Ashida and Shibutani (1995) selected thermodynamic data for Cm-OH and Cm-CO_3 systems comparing with experimental results of Cm-doped glass leaching (Ashida and Shibutani, 1995) and of solubility in bentonite porewater (Shibutani, 1997b).

Because of the paucity of available thermodynamic data for these elements (Sm, Ac, Cm, and Pu(III)), it was not possible to develop comprehensive datasets as was developed for Am. It is considered that the thermodynamic data for these elements are analogous to those for Am. Therefore, the scientific advisory and review committee recommended that the dataset for Am shown in Tables 2.1.1-1 and 2.1.1-2 should be applied to those for Sm(III), Ac(III), Cm(III) and Pu(III). In freezing, the datasets for Sm(III), Ac(III), Cm(III) and Pu(III) were adopted in the JNC-TDB as being chemically analogous to Am(III). For Sm, Ac, and Cm, only trivalent solid and aqueous species are adopted in JNC-TDB, as same as Am, considering their stable redox state.

Table 2.1.1-1 log Ksp values of Reactions Involving Solid Compounds of Americium(III)

Reaction	log Ksp	Reference
$Am(OH)_3(am) <=> Am^{3+} +3OH^-$	-25.0	Silva et al. (1995)
$Am(OH)_3(cr) <=> Am^{3+} +3OH^-$	-26.8	Silva et al. (1995)
$Am_2(CO_3)_3(cr) <=> 2Am^{3+} +3CO_3^{2-}$	-33.4	Silva et al. (1995)
$AmOHCO_3(cr) <=> Am^{3+} +OH^- +CO_3^{2-}$	-22.5	Felmy et al. (1990)
$NaAm(CO_3)_2 \cdot 6H_2O (cr) <=> Na^+ +Am^{3+} +2CO_3^{2-} +6H_2O$	-21.40	Rai et al. (1999a)
$AmPO_4 \cdot xH_2O (am) <=> Am^{3+} +PO_4^{3-} +xH_2O$	-24.79	Rai et al. (1992)
$AmF_3(cr) <=> Am^{3+} +3F^-$	-19.5	Rai et al. (1999a)

Table 2.1.1-2 log K values of Reactions Involving Solution Species of Americium (III)

Reaction	log K	Reference
$Am^{3+} +H_2O <=> AmOH^{2+} +H^+$	-6.4	Silva et al. (1995)
$Am^{3+} +2\ H_2O <=> Am(OH)_2^+ +2H^+$	-14.1	Silva et al. (1995)
$Am^{3+} +3\ H_2O <=> Am(OH)_3(aq) +3H^+$	$< -28.6^{*1}$	Felmy et al. (1990)
$Am^{3+} +F^- <=> AmF^{2+}$	3.4	Silva et al. (1995)
$Am^{3+} +2F^- <=> AmF_2^+$	5.8	Silva et al. (1995)
$Am^{3+} +3F^- <=> AmF_3(aq)$	$< 11.2^{*1}$	Rai et al. (1999a)
$Am^{3+} + CO_3^{2-} <=> AmCO_3^+$	7.6	Felmy et al. (1990)
$Am^{3+} + 2CO_3^{2-} <=> Am(CO_3)_2^-$	12.3	Felmy et al. (1990)
$Am^{3+} + 3CO_3^{2-} <=> Am(CO_3)_3^{3-}$	15.2	Felmy et al. (1990)
$Am^{3+} + H_2PO_4^- <=> AmH_2PO_4^{2+}$	2.74	Rai et al. (1999a)

*1 This value is the detection limit in literature.

2.1.2 Thorium (Th)

The PNC-TDB_H-3 included thermodynamic data for Th given by Harwell R12324 (Cross et al., 1987). Solids and aqueous species of Th(IV) are considered to be dominant in geological disposal system. In the JNC-TDB development, Rai et al. (1999b) selected thermodynamic data (equilibrium constants and Pitzer parameters) for Th(IV) based on the Pitzer model for activity corrections. As a result, the data for OH^-, CO_3^{2-}, SO_4^{2-}, F^-, and NO_3^- complexes were more developed than those of the PNC-TDB_H-3, that were recommended by the scientific advisory and review committee. In freezing, the thermodynamic dataset for Th(IV) were adopted in the JNC-TDB as shown in Tables 2.1.2-1 and 2.1.2-2.

Table 2.1.2-1 log Ksp Values of Reactions Involving Solid Compounds of Thorium (IV)

Reaction	log Ksp	Reference
$ThO_2(am) + 2H_2O <=> Th^{4+} + 4OH^-$	-45.5	Felmy et al. (1991)
$ThO_2(cr) + 2H_2O <=> Th^{4+} + 4OH^-$	-54.2	Rai et al. (1987)
$ThO_2(am) + H^+ + H_2O + CO_3^{2-} <=> Th(OH)_3CO_3^-$	6.78	Östhols et al. (1994)
$ThO_2(am) + 4H^+ + 5CO_3^{2-} <=> Th(CO_3)_5^{6-} + 2H_2O$	37.6	Felmy et al. (1997)
$ThF_4 \cdot nH_2O(s) + 4H^+ <=> Th^{4+} + 4HF + nH_2O$	-16.29	Felmy et al. (1993)
$ThF_4 \cdot NaF \cdot H_2O(cr) + 5H^+ <=> Th^{4+} + Na^+ + 5HF + H_2O$	-18.23	Felmy et al. (1993)
$ThF_4 \cdot NH_4F(s) + 5H^+ <=> Th^{4+} + NH_4^+ + 5HF$	-18.09	Felmy et al. (1993)

Table 2.1.2-2 log K Values of Reactions Involving Solution Species of Thorium (IV) *1

Reaction	log K	Reference
$Th^{4+} + 4H_2O <=> Th(OH)_4(aq) + 4H^+$	≤ -19.7	Ryan and Rai (1987)
$Th^{4+} + 3SO_4^{2-} <=> Th(SO_4)_3^{2-}$	12.42	Felmy and Rai (1992)
$Th^{4+} + 3F^- <=> ThF_3^+$	18.89	Felmy et al. (1993)
$Th^{4+} + 4F^- <=> ThF_4(aq)$	22.33	Felmy et al. (1993)
$Th^{4+} + 5F^- <=> ThF_5^-$	24.76	Felmy et al. (1993)
$Th^{4+} + 6F^- <=> ThF_6^{2-}$	25.56	Felmy et al. (1993)
$Th^{4+} + NO_3^- <=> ThNO_3^{3+}$	2.5 *2	Rai et al. (1999b)

*1 For accurate thermodynamic model, associated ion-interaction parameters for these species and for chloride are required and reported in Rai et al. (1999b).

*2 estimated value.

2.1.3 Protactinium (Pa)

The PNC-TDB_H-3 included thermodynamic data for Pa in the Harwell R12324 (Cross et al., 1987). In the JNC-TDB development, Shibutani and Shibutani (1998a) selected thermodynamic data for Pa for the redox and hydrolysis reactions as shown in Tables 2.1.3-1 and 2.1.3-2. At present, there is no thermodynamic data for Pa-CO_3 system. In case of no data for an object element, chemical analogy is generally adopted. However, the chemical properties of Pa are very different from those of other actinides, because the pentavalent state is ordinarily stable in aquatic system of Pa. Hence the scientific advisory and review committee recommended that chemical analogy with other actinides is inadequate for Pa.

In freezing, the dataset by Shibutani and Shibutani (1998a) was adopted in the JNC-TDB. In future, it will be necessary to carry out solubility measurement for Pa in high carbonate-concentrated water system for the thermodynamic data development.

Table 2.1.3-1 log K Values of Reactions Involving Solid Compounds of Protactinium

Reaction	log K	Reference
$PaO_2(cr) + 4H^+ <=> Pa^{4+} + 2H_2O$	0.6	Baes and Mesmer (1976)
$Pa_2O_5(s) + 10H^+ + 2e^- <=> 2Pa^{4+} + 5H_2O$	-8.72	Shibutani and Shibutani (1998a)
$PaCl_4(cr) <=> Pa^{4+} + 4Cl^-$	24.01	Shibutani and Shibutani (1998a)
$PaCl_5(cr) <=> Pa^{4+} + 5Cl^- - e^-$	32.85	Shibutani and Shibutani (1998a)

Table 2.1.3-2 log K Values of Reactions Involving Solution Species of Protactinium

Reaction	log K	Reference
$Pa^{4+} + H_2O <=> PaOH^{3+} + H^+$	0.84	Baes and Mesmer (1976)
$Pa^{4+} + 2H_2O <=> Pa(OH)_2^{2+} + 2H^+$	-0.02	Baes and Mesmer (1976)
$Pa^{4+} + 3H_2O <=> Pa(OH)_3^{+} + 3H^+$	-1.5	Baes and Mesmer (1976)
$Pa^{4+} + 2H_2O <=> PaOOH^{2+} + 3H^+ + e^-$	1.86	Fuger and Oetting (1976)
$Pa^{4+} + 3H_2O <=> PaO(OH)_2^{+} + 4H^+ + e^-$	0.85	Shibutani and Shibutani (1998a)
$Pa^{4+} + 4H_2O <=> PaO(OH)_3(aq) + 5H^+ + e^-$	-3.6	Shibutani and Shibutani (1998a)

2.1.4 Uranium (U)

The PNC-TDB_H-3 used thermodynamic data for U as reported by Grenthe et al. (1992). Solids and aqueous species for U(IV) are considered to be very important under reducing conditions. In the JNC-TDB development, Yui and Makino (1996) discussed thermodynamic data for U(IV)O_2(am), U(IV)-OH^- and U(IV)-HPO_4^{2-} complexes focused on filtration technique, control of redox conditions in the experiments. The pore-size corresponding to the microstructure of highly compacted bentonite would be around 10 Å. Thermodynamic data for autunite minerals were also discussed by Yui and Makino (1996) based on natural analogue study. In the JNC-TDB development, Rai et al. (1999b) selected thermodynamic data (equilibrium constants and Pitzer parameters) for U(IV) based on chemical analogy with other tetravalent actinides, and recent experimental data that were interpreted using the Pitzer model for activity corrections. In this compilation, thermodynamic data for U(IV) hydroxide, sulfate, carbonate, hydroxo-carbonate complexes, and U(IV)O_2(am) were discussed in detail. Choppin et al. (1999) selected thermodynamic data for redox reactions for U and compiled data for reactions including solid and aqueous species of and U(VI).

Based on these reports in the JNC-TDB development, the scientific advisory and review committee reviewed the thermodynamic data. From views of experts, the committee consequently recommended:

1) thermodynamic data for redox reactions for U selected by Grenthe et al. (1992) and by Choppin et al. (1999) should be adopted in the JNC-TDB (see Table 2.1.4-1);

2) thermodynamic data for U(IV) recommended by Rai et al. (1999b) should be adopted in the JNC-TDB (see Tables 2.1.4-2 and 2.1.4-3);

3) the JNC-TDB should not include thermodynamic data for U(V) except for redox reaction of UO_2^{2+}/UO_2^+ because of the unavailability of reliable data for U(V) solids and complexes;

and

4) thermodynamic data for U(VI) from Grenthe et al. (1992) should be adopted in the JNC-TDB (see Tables 2.1.4-4 and 2.1.4-5).

In freezing, the dataset for U was adopted in the JNC-TDB as shown in Tables 2.1.4-1, 2.1.4-2, 2.1.4-3, 2.1.4-4 and 2.1.4-5. Table 2.1.4-4 shows a portion of U(VI) compounds selected by Grenthe et al. (1992).

Table 2.1.4-1 log K values of Redox Reactions of Uranium

Reaction	log K	Reference
$U^{4+} + e^- <=> U^{3+}$	-9.353	Grenthe et al. (1992)
$UO_2^{2+} + 2e^- + 4H^+ <=> U^{4+} + 2H_2O$	9.038	Grenthe et al. (1992)
$UO_2^{2+} + e^- <=> UO_2^+$	1.484	Grenthe et al. (1992)

Table 2.1.4-2 log Ksp values of Reactions Involving Solid Compounds of Uranium (IV)

Reaction	log Ksp	Reference
$UO_2(am) + 2H_2O <=> U^{4+} + 4OH^-$	-53.45	Rai et al. (1997)
$UO_2(am) + 2HCO_3^- <=> U(OH)_2(CO_3)_2^{2-}$	-4.8	Rai et al. (1998)
$UO_2(am) + 2H_2O <=> U(OH)_4(aq)$	< -8.7 *1	Yajima et al. (1995)
$UO_2(am) + 4H^+ + 5CO_3^{2-} <=> U(CO_3)_5^{6-} + 2H_2O$	33.8	Rai et al. (1998)

*1 This value is the detection limit in literature.

Table 2.1.4-3 log K values of Reactions Involving Solution Species of Uranium (IV) *1

Reaction	log K	Reference
$U^{4+} + H_2O <=> UOH^{3+} + H^+$	-0.50	Rai et al. (1990)
$U^{4+} + SO_4^{2-} <=> USO_4^{2+}$	9.0	Rai et al. (1999b)
$U^{4+} + 2SO_4^{2-} <=> U(SO_4)_2(aq)$	11.7	Rai et al. (1999b)
$U^{4+} + 5CO_3^{2-} <=> U(CO_3)_5^{6-}$	31.29	Rai et al. (1998)
$U^{4+} + 2CO_3^{2-} + 2OH^- <=> U(OH)_2(CO_3)_2^{2-}$	41.33	Rai et al. (1998)
$U^{4+} + NO_3^- <=> UNO_3^{3+}$	1.47	Grenthe et al. (1992)
$U^{4+} + 2NO_3^- <=> U(NO_3)_2^{2+}$	2.30	Grenthe et al. (1992)
$U^{4+} + F^- <=> UF^{3+}$	9.28	Grenthe et al. (1992)
$U^{4+} + 2F^- <=> UF_2^{2+}$	16.23	Grenthe et al. (1992)
$U^{4+} + 3F^- <=> UF_3^+$	21.60	Grenthe et al. (1992)
$U^{4+} + 4F^- <=> UF_4(aq)$	25.60	Grenthe et al. (1992)
$U^{4+} + 5F^- <=> UF_5^-$	27.01	Grenthe et al. (1992)
$U^{4+} + 6F^- <=> UF_6^{2-}$	29.08	Grenthe et al. (1992)

*1 For accurate thermodynamic model valid to high ionic strength, see Rai et al. (1997 and 1999b) for ion-interaction parameters for some of these species and for U^{4+} with chloride.

Table 2.1.4-4 log K values of Reactions Involving Solid Compounds of Uranium (VI)

Reaction	log K	Reference
α-UO_3 +2H^+ <=> UO_2^{2+} +H_2O	8.632*	Grenthe et al. (1992)
β-UO_3 +2H^+ <=> UO_2^{2+} +H_2O	8.302*	Grenthe et al. (1992)
γ-UO_3 +2H^+ <=> UO_2^{2+} +H_2O	7.702*	Grenthe et al. (1992)
α-UO_3•0.9H_2O +2H^+ <=> UO_2^{2+} +1.9H_2O	5.002*	Grenthe et al. (1992)
β-$UO_2(OH)_2$ +2H^+ <=> UO_2^{2+} +2H_2O	4.932*	Grenthe et al. (1992)
UO_3•2H_2O(cr)+2H^+<=> UO_2^{2+} +3H_2O	4.812*	Grenthe et al. (1992)
UF_6(cr) -4H^+ +2H_2O <=> UO_2^{2+} +6F^-	17.202*	Grenthe et al. (1992)
$UO_2(IO_3)_2$(cr) <=> UO_2^{2+} + 2IO_3^-	-7.880	Grenthe et al. (1992)
UO_2SO_4•3.5H_2O(cr) <=> UO_2^{2+} +SO_4^{2-} + 3.5H_2O	-1.585	Grenthe et al. (1992)
UO_2SO_4•2.5H_2O(cr) <=> UO_2^{2+} +SO_4^{2-} + 2.5H_2O	-1.589	Grenthe et al. (1992)
UO_2CO_3(cr) <=>UO_2^{2+} +CO_3^{2-}	-14.490	Silva et al. (1995)
$Na_4UO_2(CO_3)_3$(cr) <=> 4Na^+ +$UO_2(CO_3)_3^{4-}$	-5.340	Grenthe et al. (1992)

* log K value of the reaction based on Gibbs free energy $\Delta_f G$ in Grenthe et al. (1992)

Table 2.1.4-5 log K values of Reactions Involving Solution Species of Uranium (VI)

Reaction	log K	Reference
UO_2^{2+}+ H_2O <=> UO_2OH^+ + H^+	-5.200	Grenthe et al. (1992)
UO_2^{2+}+ 2H_2O <=> $UO_2(OH)_2$(aq)+ 2H^+	< -10.300 *1	Grenthe et al. (1992)
UO_2^{2+}+ 3H_2O <=> $UO_2(OH)_3^-$+3H^+	-19.200	Grenthe et al. (1992)
UO_2^{2+}+ 4H_2O <=> $UO_2(OH)_4^{2-}$+4H^+	-33.000	Grenthe et al. (1992)
2UO_2^{2+}+ H_2O <=> $(UO_2)_2OH^{3+}$ +H^+	-2.700	Grenthe et al. (1992)
2UO_2^{2+}+ 2H_2O <=> $(UO_2)_2(OH)_2^{2+}$ +2H^+	-5.620	Grenthe et al. (1992)
3UO_2^{2+}+ 4H_2O <=> $(UO_2)_3(OH)_4^{2+}$ +4H^+	-11.900	Grenthe et al. (1992)
3UO_2^{2+}+ 5H_2O <=> $(UO_2)_3(OH)_5^+$ +5H^+	-15.550	Grenthe et al. (1992)
3UO_2^{2+}+ 7H_2O <=> $(UO_2)_3(OH)_7^-$ +7H^+	-31.000	Grenthe et al. (1992)
4UO_2^{2+}+ 7H_2O <=> $(UO_2)_4(OH)_7^+$ +7H^+	-21.900	Grenthe et al. (1992)
UO_2^{2+}+ F^- <=> UO_2F^+	5.090	Grenthe et al. (1992)
UO_2^{2+}+ 2F^- <=> UO_2F_2(aq)	8.620	Grenthe et al. (1992)
UO_2^{2+}+ 3F^- <=> $UO_2F_3^-$	10.900	Grenthe et al. (1992)
UO_2^{2+}+ 4F^- <=> $UO_2F_4^{2-}$	11.700	Grenthe et al. (1992)
UO_2^{2+}+ Cl^- <=> UO_2Cl^+	0.170	Grenthe et al. (1992)
UO_2^{2+} +2Cl^- <=> UO_2Cl_2(aq)	-1.100	Grenthe et al. (1992)
UO_2^{2+} +ClO_3^- <=> $UO_2ClO_3^+$	0.500	Grenthe et al. (1992)
UO_2^{2+}+ Br^- <=> UO_2Br^+	0.220	Grenthe et al. (1992)
UO_2^{2+} +BrO_3^- <=> $UO_2BrO_3^+$	0.630	Grenthe et al. (1992)
UO_2^{2+} +IO_3^- <=> $UO_2IO_3^+$	2.000	Grenthe et al. (1992)
UO_2^{2+} +2IO_3^- <=> $UO_2(IO_3)_2$(aq)	3.590	Grenthe et al. (1992)
UO_2^{2+} +SO_3^{2-} <=> UO_2SO_3(aq)	6.600	Grenthe et al. (1992)
UO_2^{2+} +$S_2O_3^{2-}$ <=> $UO_2S_2O_3$(aq)	2.800	Grenthe et al. (1992)
UO_2^{2+} +SO_4^{2-} <=> UO_2SO_4(aq)	3.150	Grenthe et al. (1992)
UO_2^{2+} +2SO_4^{2-} <=> $UO_2(SO_4)_2^{2-}$	4.140	Grenthe et al. (1992)

continue to next page.

Table 2.1.4-5 log K values of Reactions Involving Solution Species of Uranium (VI) (continued)

$UO_2^{2+} + N_3^- <=> UO_2N_3^+$	2.580	Grenthe et al. (1992)
$UO_2^{2+} + 2N_3^- <=> UO_2(N_3)_2(aq)$	4.330	Grenthe et al. (1992)
$UO_2^{2+} + 3N_3^- <=> UO_2(N_3)_3^-$	5.740	Grenthe et al. (1992)
$UO_2^{2+} + 4N_3^- <=> UO_2(N_3)_4^{2-}$	4.920	Grenthe et al. (1992)
$UO_2^{2+} + NO_3^- <=> UO_2NO_3^+$	0.300	Grenthe et al. (1992)
$UO_2^{2+} + PO_4^{3-} <=> UO_2PO_4^-$	13.230	Grenthe et al. (1992)
$UO_2^{2+} + HPO_4^{2-} <=> UO_2HPO_4(aq)$	7.240	Grenthe et al. (1992)
$UO_2^{2+} + H_3PO_4(aq) <=> UO_2H_2PO_4^+ + H^+$	1.120	Grenthe et al. (1992)
$UO_2^{2+} + H_3PO_4(aq) <=> UO_2H_3PO_4^{2+}$	0.760	Grenthe et al. (1992)
$UO_2^{2+} + 2H_3PO_4(aq) <=> UO_2(H_2PO_4)_2(aq) + 2H^+$	0.640	Grenthe et al. (1992)
$UO_2^{2+} + 2H_3PO_4(aq) <=> UO_2(H_2PO_4)\ (H_3PO_4)^+ + H^+$	1.650	Grenthe et al. (1992)
$UO_2^{2+} + CO_3^{2-} <=> UO_2CO_3(aq)$	9.670	Silva et al. (1995)
$UO_2^{2+} + 2CO_3^{2-} <=> UO_2(CO_3)_2^{2-}$	16.940	Grenthe et al. (1992)
$UO_2^{2+} + 3CO_3^{2-} <=> UO_2(CO_3)_3^{4-}$	21.600	Grenthe et al. (1992)
$3UO_2^{2+} + 6CO_3^{2-} <=> (UO_2)_3(CO_3)_6^{6-}$	54.000	Grenthe et al. (1992)
$2UO_2(CO_3)_3^{4-} + PuO_2(CO_3)_3^{4-} <=> (UO_2)_2(PuO_2)(CO_3)_6^{6-} + 3CO_3^{2-}$	-8.200	Silva et al. (1995)
$2UO_2(CO_3)_3^{4-} + NpO_2(CO_3)_3^{4-} <=> (UO_2)_2(NpO_2)(CO_3)_6^{6-} + 3CO_3^{2-}$	-9.400	Silva et al. (1995)
$UO_2^{2+} + SCN^- <=> UO_2SCN^+$	1.400	Grenthe et al. (1992)
$UO_2^{2+} + 2SCN^- <=> UO_2(SCN)_2(aq)$	1.240	Grenthe et al. (1992)
$UO_2^{2+} + 3SCN^- <=> UO_2(SCN)_3^-$	2.100	Grenthe et al. (1992)
$2UO_2^{2+} + 3H_2O + CO_3^{2-} <=> (UO_2)_2CO_3(OH)_3^- + 3H^+$	-0.858*2	Grenthe et al. (1992)
$3UO_2^{2+} + 3H_2O + CO_3^{2-} <=> (UO_2)_3O(OH)_2(HCO_3)^+ + 3H^+$	0.652*2	Grenthe et al. (1992)
$11UO_2^{2+} + 12H_2O + 6CO_3^{2-} <=> (UO_2)_{11}(CO_3)_6(OH)_{12}^{2-} + 12H^+$	36.427*2	Grenthe et al. (1992)

*1 The log K value is a maximum value.

*2 log K value of the reaction based on Gibbs free energy $\Delta_f G$ in Grenthe et al. (1992)

2.1.5 Neptunium (Np)

The PNC-TDB_H-3 used thermodynamic data for Np reported by Cross et al. (1987). In the JNC-TDB development, Shibutani et al. (1998) compiled thermodynamic data for Np-OH^-, Np-CO_3^{2-}, Np-SO_4^{2-} and Np-Cl^- species, and recommended some data. Rai et al. (1999b) compiled thermodynamic data (equilibrium constants and Pitzer parameters) for Np(IV) in detail based on chemical analogy with other tetravalent actinides, and recent experimental data that were interpreted using the Pitzer model for activity corrections. In this compilation, thermodynamic data for Np(IV) complexes with OH^-, CO_3^{2-}, and SO_4^{2-} along with the solubility product for Np(IV)O_2(am) were discussed in detail. Rai et al. (1999d) measured solubility of NpO_2(am) in high carbonate concentrations to obtain thermodynamic data of Np(IV) carbonate and hydroxo-carbonate complex using Pitzer model. In this experiment, the solubilities of NpO_2(am) were measured in carbonate media under reducing conditions similar to the case of Eriksen et al. (1993), whose equilibrium constants for Np(IV) hydroxo-carbonate complexes were adopted by Shibutani et al. (1998). Choppin et al. (1999) discussed thermodynamic data for Np(V) hydroxide, sulfate, carbonate, phosphate complexes focused on the 1st step-wise complex formation. Thermodynamic data for redox reactions of Np were also discussed by Choppin et al. (1999).

Based on these reports, in the JNC-TDB development, the scientific advisory and review committee reviewed the thermodynamic data. From the view of experts, the committee consequently recommended:

1) thermodynamic data for redox reactions for Np adopted by Fuger and Oetting (1976) and selected by Choppin et al. (1999) should be adopted in the JNC-TDB;

2) thermodynamic data for Np(IV) recommend by Rai et al. (1999b) should be basically adopted in the JNC-TDB; those for Np(IV) carbonate and hydroxo-carbonate complexes determined by Rai et al. (1999d) should be adopted in the JNC-TDB;

and

3) thermodynamic data for Np(V) recommended by Choppin et al. (1999) should be basically adopted in the JNC-TDB.

On the other hand, the committee suggested the consideration of the recent data by Neck et al. (1992) and Neck et al. (1995) for Np(V)-OH^-, and Np(V)-CO_3^{2-} system. Shibutani et al. (1998) selected

thermodynamic data on solids and aqueous phase for Np(V)-OH^- and Np(V)-CO_3^{2-} system using the SIT model, including the data by Neck's group. However, in the derivation of data at I=0, molarity [mol/l] was used instead of molality [mol/kg]. In general, molality [mol/kg] should be used in the SIT model and chemical thermodynamics. Therefore, data determined by Shibutani et al. (1998) were not selected, and the data reported by Neck et al. (1992) were directly adopted for Np(V)-OH^- in the JNC-TDB. The datum recommended by Fuger et al. (1992) was adopted for $NpO_2CO_3^-$ tentatively following the recommendation by Choppin et al. (1999) (datum was adopted from the original reference), because Neck et al. (1995) is not reporting data at I=0.

In freezing, the dataset for Np was adopted in the JNC-TDB as shown in Tables 2.1.5-1, 2.1.5-2, 2.1.5-3, 2.1.5-4 and 2.1.5-5. The JNC-TDB development and the solubility estimation have been carried out in parallel for the last phase of the second progress report on the geological disposal research. For the solubility estimation, the dataset is shown in Appendix-2.

Table 2.1.5-1 log K values of Redox Reactions of Neptunium

Reaction	log K	Reference
$Np^{4+} + e^- <=> Np^{3+}$	2.49	Fuger and Oetting (1976)
$NpO_2^+ + e^- + 4H^+ <=> Np^{4+} + 2H_2O$	10.89	Fuger and Oetting (1976)
$NpO_2^{2+} + e^- <=> NpO_2^+$	20.89	Fuger and Oetting (1976)

Table 2.1.5-2 log K_{sp} values of Reactions Involving Solid Compounds of Neptunium (IV)

Reaction	log Ksp	Reference
$NpO_2(am) + 2H_2O <=> Np^{4+} + 4OH^-$	-54.5	Rai et al. (1987)
$NpO_2(am) + 2H_2O <=> Np(OH)_4(aq)$	< -8.5*	Rai and Ryan (1985)

* This value is the detection limit of literature.

Table 2.1.5-3 log K values of Reactions Involving Solution Species of Neptunium (IV) *1

Reaction	log K	Reference
$Np^{4+} + H_2O <=> NpOH^{3+} + H^+$	-0.5	Rai et al. (1999b)
$Np^{4+} + SO_4^{2-} <=> NpSO_4^{2+}$	9.0	Xia et al. (1999)
$Np^{4+} + 2SO_4^{2-} <=> Np(SO_4)_2(aq)$	11.7	Xia et al. (1999)
$Np^{4+} + 5CO_3^{2-} <=> Np(CO_3)_5^{6-}$	33.37	Rai et al. (1999d)
$Np^{4+} + 2CO_3^{2-} + 2OH^- <=> Np(OH)_2(CO_3)_2^{2-}$	42.75	Rai et al. (1999d)

*1 For accurate thermodynamic model valid to high ionic strength, involving these species, see Rai et al. (1999b) for associated ion-interaction parameters.

Table 2.1.5-4 log Ksp values of Reactions Involving Solid Compounds of Neptunium (V)

Reaction	log Ksp	Reference
$NpO_2OH(am) <=> NpO_2^+ + OH^-$	-8.79	Roberts et al. (1996)
$NaNpO_2CO_3(cr) <=> Na^+ + NpO_2^+ + CO_3^{2-}$	-11.00	Neck et al. (1995)
$Na_3NpO_2(CO_3)_2(cr) <=> 3Na^+ + NpO_2^+ + 2CO_3^{2-}$	-14.32	Neck et al (1995)

Table 2.1.5-5 log K values of Reactions Involving Solution Species of Neptunium (V)

Reaction	log K	Reference
$NpO_2^+ + OH^- <=> NpO_2OH(aq)$	2.70	Neck et al. (1992)
$NpO_2^+ + 2OH^- <=> NpO_2(OH)_2^-$	4.35	Neck et al. (1992)
$NpO_2^+ + CO_3^{2-} <=> NpO_2CO_3^-$	4.9	Fuger et al. (1992)
$NpO_2^+ + Cl^- <=> NpO_2Cl(aq)$	-0.07	Choppin et al. (1999)
$NpO_2^+ + NO_3^- <=> NpO_2NO_3$	1.1	Allard et al. (1978)
$NpO_2^+ + F^- <=> NpO_2F(aq)$	1.9	Fuger et al. (1992)
$NpO_2^+ + HPO_4^{2-} <=> NpO_2\ HPO_4^-$	3.4	Fuger et al. (1992)
$NpO_2^+ + H_2PO_4^- <=> NpO_2\ H_2PO_4(aq)$	1.5	Choppin et al. (1999)
$NpO_2^+ + SO_4^{2-} <=> NpO_2\ SO_4^-$	2	Wanner (1986)

2.1.6 Plutonium (Pu)

The PNC-TDB_H-3 used thermodynamic data for Pu reported by Cross et al. (1987). In the JNC-TDB development, Shibutani and Shibutani (1998b) compiled thermodynamic data of reactions for Pu(III to VI) complexes with OH^-, CO_3^{2-}, and SO_4^{2-} along with equilibrium constants for redox reactions involving different Pu oxidation studies. Rai et al. (1999a) and Rai et al. (1999b) compiled thermodynamic data (equilibrium constants and Pitzer parameters) for Pu(III) and Pu(IV) by using Pitzer model. In the Pu(III) compilations, the reliability of data for Pu(III) could not be confirmed enough, except for solubility of $Pu(OH)_3(s)$ as a function of pH. Recently, Rai et al. (1999c) obtained thermodynamic data for $Pu(OH)_2(CO_3)_2^{2-}$ and $Pu(CO_3)_5^{6-}$ based on their solubility measurements of $PuO_2(am)$ using Pitzer model. Choppin et al. (1999) compiled thermodynamic data of reactions for Pu(V) and Pu(VI) and redox reactions for Pu. However, the reliability of the data for Pu(V) and Pu(VI) are not enough discussed in their report.

In solubility estimation of Pu for the performance analysis of the geological disposal, the species of $Pu(IV)(OH)_2(CO_3)_2^{2-}$ is very important, because the bentonite porewater is assumed to include high carbonate concentrations ($\approx 10^{-2}$ mol/l). Shibutani and Shibutani (1998b) selected logK = 46.79 as the equilibrium constant at zero ionic strength for the reaction of $Pu^{4+} + 2OH^- + 2CO_3^{2-} <=> Pu(IV)(OH)_2(CO_3)_2^{2-}$ based on solubility measurements by Yamaguchi et al. (1994). On the other hand, Rai et al. (1999c) experimentally determined logK = 44.76 as the equilibrium constant for the same reaction. The former is about 2 orders of magnitude larger than the latter. This species is very important in case of high carbonate concentrations. The measurements by Yamaguchi et al. (1994) were carried out in the region of total carbonate concentrations, $10^{-4} - 10^{-1}$ mol/l. On the other hand, the measurements by Rai et al. (1999c) were carried out at total carbonate concentrations ranging from 0.01 to 6.2 mol/kg.

Based on these reports in the JNC-TDB development, the scientific advisory and review committee reviewed the thermodynamic data. From views of experts, the committee consequently recommended:

1) thermodynamic data of redox reactions for Pu selected by Choppin et al. (1999), which was referred from Fuger and Oetting (1976) for Pu(III)/Pu(IV) and Rai (1984) for Pu(IV)/Pu(V), Pu(IV)/Pu(VI), and Pu(V)/Pu(VI), would be adopted in the JNC-TDB;

2) thermodynamic data for Pu(III) based on chemical analogy with Am(III) as shown in Tables 2.1.1-1 and

2.1.1-2 should be adopted in the JNC-TDB;

3) thermodynamic data for Pu(IV) compiled by Rai et al. (1999b) should be adopted in the JNC-TDB;

4) thermodynamic data for $Pu(OH)_2(CO_3)_2^{2-}$ and $Pu(CO_3)_5^{6-}$ from Rai et al. (1999c) should be adopted in the JNC-TDB;

5) thermodynamic data for Pu(V) based on chemical analogy with Np(V) as shown in Tables 2.1.6-4 and 2.1.6-5 should be adopted in the JNC-TDB;

6) thermodynamic data for Pu(VI) solids were not considered, because the solids may not be formed in aquatic system;

and

7) thermodynamic data (first step-wise constants) for Pu(VI) aqueous species selected by Shibutani and Shibutani (1998b), in which chemical analogue to U(VI) was adopted for some species, should be adopted in the JNC-TDB.

In freezing, the dataset for Pu was adopted in the JNC-TDB as shown in Tables 2.1.6-1, 2.1.6-2, 2.1.6-3, 2.1.6-4 and 2.1.6-5. Based on chemical analogy with Am(III), thermodynamic data for Pu(III) shown in Tables 2.1.1-1 and 2.1.1-2 were adopted in the JNC-TDB. For the solubility estimation, the used dataset is shown in Appendix-2.

Table 2.1.6-1 log K values of Redox Reactions of Plutonium

Reaction	log K	Reference
$Pu^{4+} + e^- <=> Pu^{3+}$	16.99	Fuger and Oetting (1976)
$PuO_2^+ + e^- + 4H^+ <=> Pu^{4+} + 2H_2O$	18.60	Rai (1984)
$PuO_2^{2+} + e^- <=> PuO_2^+$	16.16	Rai (1984)

Table 2.1.6-2 log Ksp values of Reactions Involving Solid Compounds of Plutonium (IV)

Reaction	log Ksp	Reference
$PuO_2(am) + 2H_2O <=> Pu^{4+} + 4OH^-$	-56.85	Rai (1984)
$PuO_2(am) + 2H_2O <=> Pu(OH)_4(aq)$	< -10 *	Yamaguchi et al. (1994)

* This value is the detection limit in literature.

Table 2.1.6-3 log K values of Reactions Involving Solution Species of Plutonium (IV)

Reaction	log K	Reference
$Pu^{4+} + H_2O <=> PuOH^{3+} + H^+$	-0.50	Rai et al. (1999b)
$Pu^{4+} + SO_4^{2-} <=> PuSO_4^{2+}$	9.0	Rai et al. (1999b)
$Pu^{4+} + 2SO_4^{2-} <=> Pu(SO_4)_2(aq)$	11.7	Rai et al. (1999b)
$Pu^{4+} + 5CO_3^{2-} <=> Pu(CO_3)_5^{6-}$	34.18	Rai et al. (1999c)
$Pu^{4+} + 2CO_3^{2-} + 2OH^- <=> Pu(OH)_2(CO_3)_2^{2-}$	44.76	Rai et al. (1999c)

Table 2.1.6-4 log Ksp values of Reactions Involving Solid Compounds of Plutonium (V) *1

Reaction	log Ksp	Reference
$PuO_2OH(am) <=> PuO_2^+ + OH^-$	-8.79	see Table 2.1.5-4
$NaPuO_2CO_3(cr) <=> Na^+ + PuO_2^+ + CO_3^{2-}$	-11.00	see Table 2.1.5-4
$Na_3PuO_2(CO_3)_2(cr) <=> 3Na^+ + PuO_2^+ + 2CO_3^{2-}$	-14.32	see Table 2.1.5-4

*1 The scientific advisory and review committee recommended the log K value based on chemical analogy with Np(V).

Table 2.1.6-5 log K values of Reactions Involving Solution Species of Plutonium (V) *1

Reaction	log K	Reference
$PuO_2^+ + OH^- <=> PuO_2OH(aq)$	2.70	see Table 2.1.5-5
$PuO_2^+ + 2OH^- <=> PuO_2(OH)_2^-$	4.35	see Table 2.1.5-5
$PuO_2^+ + CO_3^{2-} <=> PuO_2CO_3^-$	4.9	see Table 2.1.5-5
$PuO_2^+ + Cl^- <=> PuO_2Cl(aq)$	0.7	see Table 2.1.5-5
$PuO_2^+ + NO_3^- <=> PuO_2NO_3$	1.1	see Table 2.1.5-5
$PuO_2^+ + F^- <=> PuO_2F(aq)$	1.9	see Table 2.1.5-5
$PuO_2^+ + HPO_4^{2-} <=> PuO_2HPO_4^-$	3.4	see Table 2.1.5-5
$PuO_2^+ + H_2PO_4^- <=> PuO_2H_2PO_4(aq)$	1.5	see Table 2.1.5-5
$PuO_2^+ + SO_4^{2-} <=> PuO_2SO_4^-$	2	see Table 2.1.5-5

*1 The scientific advisory and review committee recommended the log K value based on chemical analogy with Np(V).

Table 2.1.6-6 log K values of Reactions Involving Solution Species of Plutonium (VI)

Reaction	log K	Reference
$PuO_2^{2+} + Cl^- <=> PuO_2Cl^+$	0.1	Fuger et al. (1992)
$PuO_2^{2+} + F^- <=> PuO_2F^+$	4.57	Fuger et al. (1992)
$PuO_2^{2+} + 2F^- <=> PuO_2F_2(aq)$	8.24	Fuger et al. (1992)
$PuO_2^{2+} + 3F^- <=> PuO_2F_3^-$	9.80	Fuger et al. (1992)
$PuO_2^{2+} + H_2O <=> PuO_2OH^+ + H^+$	- 5.27	Shibutani and Shibutani (1998b)
$PuO_2^{2+} + 2H_2O <=> PuO_2(OH)_2(aq) + 2H^+$	- 12.46	Shibutani and Shibutani (1998b)
$PuO_2^{2+} + 3H_2O <=> PuO_2(OH)_3^- + 3H^+$	- 24.76	Shibutani and Shibutani (1998b)
$PuO_2^{2+} + NO_3^- <=> PuO_2NO_3^+$	0.3 *1	Choppin et al. (1999) / Shibutani and Shibutani (1998b)*2
$PuO_2^{2+} + CO_3^{2-} <=> PuO_2CO_3(aq)$	9.56	Pashaliddis et al. (1997)
$PuO_2^{2+} + 2CO_3^{2-} <=> PuO_2(CO_3)_2^{2-}$	15.0	Pashaliddis et al. (1997)
$PuO_2^{2+} + 3CO_3^{2-} <=> PuO_2(CO_3)_3^{4-}$	17.53	Pashaliddis et al. (1997)
$PuO_2^{2+} + HPO_4^{2-} <=> PuO_2HPO_4(aq)$	7.24 *1	Shibutani and Shibutani (1998b)
$PuO_2^{2+} + H_3PO_4(aq) <=> PuO_2H_2PO_4^+ + H^+$	1.12 *1	Shibutani and Shibutani (1998b)
$PuO_2^{2+} + SO_4^{2-} <=> PuO_2SO_4(aq)$	3.15 *1	Shibutani and Shibutani (1998b)
$PuO_2^{2+} + 2SO_4^{2-} <=> PuO_2(SO_4)_2^{2-}$	4.14 *1	Shibutani and Shibutani (1998b)

*1 The log K value was given by chemical analogy with U(VI).

*2 The estimated value by Choppin et al. (1999) is coincident with recommended value by Shibutani and Shibutani (1998b) considering chemical analogy with U(VI).

2.2 Non-actinide elements

This section shows the status and frozen thermodynamic data for non-actinide elements except for samarium(Sm) in the JNC-TDB development. Thermodynamic data for cesium (Cs), which are not included in the JNC-TDB, because this element is soluble.

2.2.1 Niobium (Nb)

The PNC-TDB_H-3 didn't include thermodynamic data for Nb. In the JNC-TDB development, Lothenbach et al. (1999) discussed thermodynamic data for Nb-OH^-, Nb-O, Nb-Cl^- and Nb-F^- systems. They consequently selected the data for Nb(V) based on solubility measurements of Nb_2O_5(s) by Yajima et al. (1992) and Yajima (1994) as shown in Table 2.2.1. That was recommended by the scientific advisory and review committee from the view of experts.

In freezing, the dataset of only two reactions for Nb was adopted in the JNC-TDB as shown in Table 2.2.1. At present, the thermodynamic data for other ligands could not be given in the JNC-TDB development.

Table 2.2.1 log K values of Niobium

Reaction	log K	Reference
$Nb(OH)_5(aq) + H_2O <=> Nb(OH)_6^- + H^+$	-6.6	Lothenbach et al. (1999)
$Nb_2O_5(s) + 5H_2O <=> 2Nb(OH)_5(aq)$	-16.0	Lothenbach et al. (1999)

2.2.2 Technetium (Tc)

The PNC-TDB_H-3 mainly included thermodynamic data for Tc of OECD/NEA (1989) which just compiled data by Rard (1983) and included those of Phillips et al. (1988) for a few reactions including solids. In the JNC-TDB development, the data were not revised. Hence, the data shown in Tables 2.2.2-1 and 2.2.2-2 were used for the solubility estimation for the performance analysis of geological disposal system.

Recently, Yamaguchi and Takeda (1999) discussed thermodynamic data for Tc based on original literature and several TDBs. In the near future, OECD/NEA will publish a thermodynamic database for Tc reviewed by experts similar to those for U and Am. Then, it will be necessary to discuss to adopt those in the JNC-TDB.

Table 2.2.2-1 log K Values of Involving Solid Compounds of Technetium

Reaction *	log K	Reference
$Tc(OH)_3(s) + H^+ <=> TcO^{2+} + 2H_2O + e^-$	-14.63	OECD/NEA (1989)
$Tc_2O_7(cr) <=> 2TcO_4^- + 5H_2O - 10H^+ - 6H^+$	13.11	OECD/NEA (1989)
$Tc_3O_4(s) + 2H^+ <=> 3TcO^{2+} + H_2O + 4e^-$	-56.89	OECD/NEA (1989)
$Tc_4O_7(s) + 6H^+ <=> 4TcO^{2+} + 3H_2O + 2e^-$	-36.79	OECD/NEA (1989)
$TcO_2 \cdot 2H_2O(am) + 2H^+ <=> TcO^{2+} + 3H_2O$	-4.23	OECD/NEA (1989)
$TcO_3(cr) + 4H^+ + 2e^- <=> TcO^{2+} + 2H_2O$	19.96	OECD/NEA (1989)
$NaTcO_4(cr) + 6H^+ + 3e^- <=> Na^+ + TcO^{2+} + 3H_2O$	35.54	OECD/NEA (1989)
$HTcO_4(pertechn) + 5H^+ + 3e^- <=> TcO^{2+} + 3H_2O$	38.97	OECD/NEA (1989)
$TcO_2(cr) + 2H^+ <=> TcO^{2+} + H_2O$	-19.76	Phillips et al. (1988)
$Tc(OH)_2(s) <=> TcO^{2+} + H_2O + 2e^-$	-21.63	Phillips et al. (1988)
$Tc(cr) + H_2O <=> TcO^{2+} + 2H^+ + 4e^-$	-23.94	Phillips et al. (1988)

* The reactions are described in PHREEQE format.

Table 2.2.2-2 log K values of Reaction Involving Solution Species of Technetium

Reaction*	log K	Reference
$2TcO^{2+} + 4H_2O <=> (TcO(OH)_2)_2(aq) + 4H^+$	-0.133	OECD/NEA (1989)
$TcO^{2+} + 3H_2O <=> H_2TcO_4(aq) + 4H^+ + 2e^-$	-34.310	OECD/NEA (1989)
$TcO^{2+} + 3H_2O <=> HTcO_4^- + 5H^+ + 2e^-$	-34.608	OECD/NEA (1989)
$TcO^{2+} + 2H + e^- <=> Tc^{3+} + H_2O$	5.391	OECD/NEA (1989)
$TcO^{2+} + 2H_2O <=> TcO(OH)_2(aq) + 2H^+$	-3.325	OECD/NEA (1989)
$TcO^{2+} + 3H_2O <=> TcO_4^- + 6H^+ + 3e^-$	-32.993	OECD/NEA (1989)
$TcO^{2+} + 3H_2O <=> TcO_4^{2-} + 6H^+ + 2e^-$	-43.315	OECD/NEA (1989)
$TcO^{2+} + 3H_2O <=> TcO_4^{3-} + 6H^+ + e^-$	-53.287	OECD/NEA (1989)
$TcO^{2+} + H_2O <=> TcOOH^+ + H^+$	-1.137	OECD/NEA (1989)

* The reactions are described in PHREEQE format.

2.2.3 Palladium (Pd)

The PNC-TDB_H-3 included thermodynamic data for Pd^{2+}, $PdOH^{+}$, $Pd(OH)_2(aq)$, PdO(s), $Pd(OH)_2(s)$ and Pd(cr) compiled by Phllips et al. (1988). In the JNC-TDB development, Lothenbach et al. (1999) discussed thermodynamic data for Pd-OH-, Pd-OH^--Cl^-, Pd-Cl^- and Pd-NH_3 systems by using SIT model. They consequently selected thermodynamic data for Pd-OH^--Cl^-, Pd-Cl^- and Pd-NH_3 aqueous species. For Pd-OH^- aqueous species, the reliable information could not be obtained enough to select the thermodynamic data. For Pd solids, they could have the reliable information only for Pd(cr). The data selection for Pd was recommended by the scientific advisory and review committee from view of experts.

In freezing, the dataset for Pd selected by Lothenbach et al. (1999) was adopted in the JNC-TDB shown in Table 2.2.3.

Table 2.2.3 log K values of Reactions of Palladium

Reaction	log K	Reference
$Pd(cr) <=> Pd^{2+} + 2e^-$	-32.9 *1	Lothenbach et al. (1999)
$Pd^{2+} + Cl^- <=> PdCl^+$	5.1	Lothenbach et al. (1999)
$Pd^{2+} + 2Cl^- <=> PdCl_2(aq)$	8.3	Lothenbach et al. (1999)
$Pd^{2+} + 3\ Cl^- <=> PdCl_3^-$	10.9	Lothenbach et al. (1999)
$Pd^{2+} + 4\ Cl^- <=> PdCl_4^{2-}$	11.7	Lothenbach et al. (1999)
$Pd^{2+} + 3Cl^- + H_2O <=> PdCl_3OH^{2-} + H^+$	2.5	Lothenbach et al. (1999)
$Pd^{2+} + 2Cl^- + 2H_2O <=> PdCl_2(OH)_2^{2-} + 2H^+$	-7.0 *1	Lothenbach et al. (1999)
$Pd^{2+} + NH_3(aq) <=> Pd\ NH_3^{2+}$	9.6	Lothenbach et al. (1999)
$Pd^{2+} + 2NH_3\ (aq) <=> Pd(NH_3)_2^{2+}$	18.5	Lothenbach et al. (1999)
$Pd^{2+} + 3NH_3\ (aq) <=> Pd(NH_3)_3^{2+}$	26.0	Lothenbach et al. (1999))
$Pd^{2+} + 4NH_3\ (aq) <=> Pd(NH_3)_4^{2+}$	32.8	Lothenbach et al. (1999)

*1 tentative values (refer to Lothenbach et al., 1999).

2.2.4 Tin (Sn)

The PNC-TDB_H-3 included thermodynamic data for Sn from the EQ3/6 data. In the JNC-TDB development, Lothenbach et al. (1999) selected thermodynamic data for Sn(II) -OH^-, Sn(IV)-OH^-, Sn(II)-Cl^-, Sn(II)-F^-, Sn(II)-NO_3^- and Sn(II)-SO_4^{2-} systems by using the SIT model based on the experimental measurements. These selections were recommended by the scientific advisory and review committee from the view of chemical approach.

In freezing, the dataset for Sn selected by Lothenbach et al. (1999) was adopted in the JNC-TDB as shown in Table 2.2.4-1, 2.2.4-2 and 2.2.4-3.

Table 2.2.4-1 log K Values of Redox Reactions of Tin

Reaction	log K	Reference
$Sn(cr) <=> Sn^{2+} + 2e^-$	4.63	Lothenbach et al. (1999)
$Sn^{2+} <=> Sn^{4+} + 2e^-$	-5 *1	Lothenbach et al. (1999)
$Sn^{2+} + 4H_2O <=> Sn(OH)_4(aq) + 4H^+ + 2e^-$	-5.4 *1	Lothenbach et al. (1999)

*1 tentative values (refer to Lothenbach et al., 1999).

Table 2.2.4-2 log K Values of Reactions of Tin (II)

Reaction	log K	Reference
$Sn(OH)_2(am) + 2H^+ <=> Sn^{2+} + 2H_2O$	2.82	Lothenbach et al. (1999)
$SnO(cr) + 2H^+ <=> Sn^{2+} + H_2O$	2.41	Lothenbach et al. (1999)
$SnOHCl(s) + H^+ <=> Sn^{2+} + Cl^- + H_2O$	-2.42	Lothenbach et al. (1999)
$Sn^{2+} + H_2O <=> SnOH^+ + H^+$	-3.75	Lothenbach et al. (1999)
$Sn^{2+} + 2H_2O <=> Sn(OH)_2(aq) + 2H^+$	-7.71	Lothenbach et al. (1999)
$Sn^{2+} + 3H_2O <=> Sn(OH)_3^- + 3H^+$	-17.54	Lothenbach et al. (1999)
$3Sn^{2+} + 4H_2O <=> Sn_3(OH)_4^{2+} + 4H^+$	-6.51 *1	Lothenbach et al. (1999)
$Sn^{2+} + Cl^- <=> SnCl^+$	1.65	Lothenbach et al. (1999)
$Sn^{2+} + 2Cl^- <=> SnCl_2(aq)$	2.31	Lothenbach et al. (1999)
$Sn^{2+} + 3Cl^- <=> SnCl_3^-$	2.09	Lothenbach et al. (1999)
$Sn^{2+} + Cl^- + H_2O <=> SnOHCl(aq) + H^+$	-2.27	Lothenbach et al. (1999)
$Sn^{2+} + F^- <=> SnF^+$	4.46 *1	Lothenbach et al. (1999)
$Sn^{2+} + 2F^- <=> SnF_2(aq)$	7.74 *1	Lothenbach et al. (1999)
$Sn^{2+} + 3F^- <=> SnF_3^-$	9.61 *1	Lothenbach et al. (1999)
$Sn^{2+} + NO_3^- <=> SnNO_3^+$	1.25	Lothenbach et al. (1999)
$Sn^{2+} + 2NO_3^- <=> Sn(NO_3)_2(aq)$	1.74	Lothenbach et al. (1999)
$Sn^{2+} + 3NO_3^- <=> Sn(NO_3)_3^-$	1.37	Lothenbach et al. (1999)
$Sn^{2+} + 4NO_3^- <=> Sn(NO_3)_4^{2-}$	0.30 *1	Lothenbach et al. (1999)
$Sn^{2+} + SO_4^{2-} <=> SnSO_4(aq)$	2.91 *1	Lothenbach et al. (1999)
$Sn^{2+} + 2SO_4^{2-} <=> Sn(SO_4)_2^{2-}$	2.83 *1	Lothenbach et al. (1999)

*1 tentative values (refer to Lothenbach et al., 1999).

Table 2.2.4-3 log K Values of Reactions of Tin (IV)

Reaction	log K	Reference
$SnO_2(am) <=> Sn(OH)_4(aq) - 2H_2O$	-7.46	Lothenbach et al. (1999)
$SnO_2(cassiterite) <=> Sn(OH)_4(aq) - 2H_2O$	-8	Lothenbach et al. (1999)
$Sn(OH)_4(aq) + 4H^+ <=> Sn^{4+} + 4H_2O$	0.4 *1	Lothenbach et al. (1999)
$Sn(OH)_4(aq) + H_2O <=> Sn(OH)_5^- + H^+$	-7.97	Lothenbach et al. (1999)
$Sn(OH)_4(aq) + 2H_2O <=> Sn(OH)_6^{2-} + 2H^+$	-18.40	Lothenbach et al. (1999)

*1 tentative values (refer to Lothenbach et al., 1999).

2.2.5 Antimony (Sb)

The PNC-TDB_H-3 included thermodynamic data for Sb from NBS-82 (Wagman et al., 1982). The data were given for SbO_2^- and a few oxide solids. In the JNC-TDB development, Lothenbach et al. (1999) selected thermodynamic data for Sb(III, V)-OH-, Sb(III)-Cl-, Sb(III)-F-, Sb(III)-O and Sb(III)-S systems by using the SIT model based on the experimental measurements. The scientific advisory and review committee recommended the data selections from view of experts.

In freezing, the dataset for Sb selected by Lothenbach et al. (1999) was adopted in the JNC-TDB as shown in Tables 2.2.5-1, 2.2.5-2 and 2.2.5-3.

Table 2.2.5-1 log K Values of Redox Reactions of Antimony

Reaction	log K	Reference
$Sb(cr) + 3H_2O <=> Sb(OH)_3(aq) + 3H^+ + 3e^-$	-11.99	Lothenbach et al. (1999)
$Sb(OH)_3(aq) + 2H_2O <=> Sb(OH)_5(aq) + 2H^+ + 2e^-$	-21.84	Lothenbach et al. (1999)

Table 2.2.5-2 log K values of Reactions of Antimony (III)

Reaction	log K	Reference
Sb_2O_3(valentinite) $+3H_2O <=> 2Sb(OH)3(aq)$	-8.72	Lothenbach et al. (1999)
Sb_2S_3(stibnite) $+6H_2O <=> 2Sb(OH)_3(aq) + 3H^+ + 3HS^-$	-55.14	Lothenbach et al. (1999)
$Sb(OH)_3(aq) + 3H^+ <=> Sb^{3+} + 3H_2O$	-0.73 *1	Lothenbach et al. (1999)
$Sb(OH)_3(aq) + 2H^+ <=> SbOH^{2+} + 2H_2O$	0.83 *1	Lothenbach et al. (1999)
$Sb(OH)_3(aq) + H^+ <=> Sb(OH)_2^+ + H_2O$	1.30	Lothenbach et al. (1999)
$Sb(OH)_3(aq) + H_2O <=> Sb(OH)_4^- + H^+$	-11.93	Lothenbach et al. (1999)
$2Sb(OH)_3(aq) <=> Sb_2(OH)_6(aq)$	0.08 *1	Lothenbach et al. (1999)
$Sb(OH)_3(aq) + 3H^+ + Cl^- <=> SbCl^{2+} + 3H_2O$	2.78 *1	Lothenbach et al. (1999)
$Sb(OH)_3(aq) + 3H^+ + 2Cl^- <=> Sb(Cl)_2^+ + 3H_2O$	3.27 *1	Lothenbach et al. (1999)
$Sb(OH)_3(aq) + 3H^+ + F^- <=> SbF^{2+} + 3H_2O$	6.48 *1	Lothenbach et al. (1999)
$Sb(OH)_3(aq) + 3H^+ + 2F^- <=> SbF_2^+ + 3H_2O$	12.65 *1	Lothenbach et al. (1999)
$Sb(OH)_3(aq) + 3H^+ + 3F^- <=> SbF_3(aq) + 3H_2O$	18.36 *1	Lothenbach et al. (1999)
$2Sb(OH)_3(aq) + 2H^+ + 4HS^- <=> Sb_2S_4^{2-} + 6H_2O$	42.53	Lothenbach et al. (1999)
$2Sb(OH)_3(aq) + 3H^+ + 4HS^- <=> HSb_2S_4^- + 6H_2O$	52.18	Lothenbach et al. (1999)
$2Sb(OH)_3(aq) + 4H^+ + 4HS^- <=> H_2Sb_2S_4(aq) + 6H_2O$	57.00	Lothenbach et al. (1999)

*1 tentative value (refer to Lothenbach et al., 1999)

Table 2.2.5-3 log K values of Reactions of Antimony (V)

Reaction	log K	Reference
$Sb_2O_5(am) + 5H_2O <=> 2Sb(OH)_5(aq)$	-7.40	Lothenbach et al. (1999)
$Sb(OH)_5(aq) + H_2O <=> Sb(OH)_6^- + H^+$	-2.72	Lothenbach et al. (1999)
$12Sb(OH)_5(aq) - 4H^+ + 4H_2O <=> Sb_{12}(OH)_{64}^{4-}$	20.34	Lothenbach et al. (1999)
$12Sb(OH)_5(aq) - 5H^+ + 5H_2O <=> Sb_{12}(OH)_{65}^{5-}$	16.72	Lothenbach et al. (1999)
$12Sb(OH)_5(aq) - 6H^+ + 6H_2O <=> Sb_{12}(OH)_{66}^{6-}$	11.89	Lothenbach et al. (1999)
$12Sb(OH)_5(aq) - 7H^+ + 7H_2O <=> Sb_{12}(OH)_{67}^{7-}$	6.07	Lothenbach et al. (1999)

2.2.6 Lead (Pb)

The PNC-TDB_H-3 included thermodynamic data for Pb from Harwell R12324 (Cross et al, 1987). In the JNC-TDB development, Lothenbach et al. (1999) selected thermodynamic data for Pb-OH^-, Pb-Cl^-, Pb-F^-, Pb-CO_3^{2-}, Pb-NO_3^-, Pb-PO_4^{3-}, Pb-SO_4^{2-} and Pb-HS^- systems using the SIT model based on the experimental measurements. The scientific advisory and review committee recommended these selections from the view of experts.

In freezing, the dataset for Pb selected by Lothenbach et al. (1999) was adopted in the JNC-TDB as shown in Tables 2.2.6-1, 2.2.6-2 and 2.2.6-3.

Table 2.2.6-1 log K Values of Redox Reactions of Lead

Reaction	log K	Reference
$Pb(cr) <=> Pb^{2+} + 2e^-$	4.25	Lothenbach et al. (1999)
$PbO_2(s) + 4H^+ + 2e^- <=> Pb^{2+} + 2H_2O$	48.98 *1	Lothenbach et al. (1999)
$Pb_3O_4(s) + 8H^+ + 2e^- <=> 3Pb^{2+} + 4H_2O$	70.98 *1	Lothenbach et al. (1999)

*1 tentative value (refer to Lothenbach et al, 1999)

Table 2.2.6-2 log K Values of Involving Solid Compounds of Lead

Reaction	log K	Reference
$PbO(red, litharge) + 2H^+ <=> Pb^{2+} + H_2O$	12.68	Lothenbach et al. (1999)
$PbO(yellow, massicot) + 2H^+ <=> Pb^{2+} + H_2O$	12.96	Lothenbach et al. (1999)
$Pb(OH)_2(am) + 2H^+ <=> Pb^{2+} + 2H_2O$	13.05	Lothenbach et al. (1999)
$PbCl_2(s) <=> Pb^{2+} + 2Cl^-$	-4.81	Lothenbach et al. (1999)
$PbOHCl(cr) + H^+ <=> Pb^{2+} + Cl^- + H_2O$	0.62	Lothenbach et al. (1999)
$PbF_2(s) <=> Pb^{2+} + 2F^-$	-7.52	Lothenbach et al. (1999)
$PbFCl(matlockite) <=> Pb^{2+} + F^- + Cl^-$	-8.82	Lothenbach et al. (1999)
$PbCO_3(cerrusite) <=> Pb^{2+} + CO_3^{2-}$	-13.23	Lothenbach et al. (1999)
$Pb_3(CO_3)_2(OH)_2(hydrocerrusite) + 2H^+ <=> 3Pb^{2+} + 2CO_3^{2-} + 2H_2O$	-17.64 *1	Lothenbach et al. (1999)
$Pb_{10}(CO_3)_6(OH)_6O(plumbonacrite) + 8H^+ <=> 10Pb^{2+} + 6CO_3^{2-} + 7H_2O$	-41.21 *1	Lothenbach et al. (1999)
$PbOHNO_3(cr) + H^+ <=> Pb^{2+} + NO_3^- + H_2O$	2.94	Lothenbach et al. (1999)
$PbHPO_4(s) <=> Pb^{2+} + H^+ + PO_4^{3-}$	-23.78 *1	Lothenbach et al. (1999)
$Pb_3(PO_4)_2(s) <=> 3Pb^{2+} + 2PO_4^{3-}$	-44.40 *1	Lothenbach et al. (1999)
$Pb_4(PO_4)_2O(s) + 2H^+ <=> 4Pb^{2+} + 2PO_4^{3-} + H_2O$	-37.09 *1	Lothenbach et al. (1999)
$Pb(H_2PO_4)_2(s) <=> Pb^{2+} + 2PO_4^{3-} + 4H^+$	-48.94 *1	Lothenbach et al. (1999)
$Pb_5(PO_4)_3OH$ (hydroxy pyromorphite) $+ H^+ <=> 5Pb^{2+} + 3PO_4^{3-} + H_2O$	-62.80 *1	Lothenbach et al. (1999)
$Pb_5(PO_4)_3Cl$(chloro pyromorphite) $<=> 5Pb^{2+} + 3PO_4^{3-} + Cl^-$	-84.40 *1	Lothenbach et al. (1999)
$Pb_5(PO_4)_3F$(fluoro pyromorphite) $<=> 5Pb^{2+} + 3PO_4^{3-} + F^-$	-71.60 *1	Lothenbach et al. (1999)
$PbSO_4(anglesite) <=> Pb^{2+} + SO_4^{2-}$	-7.81	Lothenbach et al. (1999)
$PbS(galena) + H^+ <=> Pb^{2+} + HS^-$	-12.17	Lothenbach et al. (1999)

*1 tentative value (refer to Lothenbach et al., 1999)

Table 2.2.6-3 log K Values of Involving Solution Species of Lead

Reaction	log K	Reference
$Pb^{2+} + H_2O <=> PbOH^+ + H^+$	-7.51	Lothenbach et al. (1999)
$Pb^{2+} + 2H_2O <=> Pb(OH)_2(aq) + 2H^+$	-16.95	Lothenbach et al. (1999)
$Pb^{2+} + 3H_2O <=> Pb(OH)_3^- + 3H^+$	-28.02	Lothenbach et al. (1999)
$2Pb^{2+} + H_2O <=> Pb_2OH^{3+} + H^+$	-7.18	Lothenbach et al. (1999)
$4Pb^{2+} + 4H_2O <=> Pb_4(OH)_4^{4+} + 4H^+$	-20.63	Lothenbach et al. (1999)
$3Pb^{2+} + 4H_2O <=> Pb_3(OH)_4^{2+} + 4H^+$	-22.48	Lothenbach et al. (1999)
$3Pb^{2+} + 5H_2O <=> Pb_3(OH)_5^+ + 5H^+$	-30.72	Lothenbach et al. (1999)
$6Pb^{2+} + 8H_2O <=> Pb_6(OH)_8^{4+} + 8H^+$	-42.68	Lothenbach et al. (1999)
$Pb^{2+} + Cl^- <=> PbCl^+$	1.55	Lothenbach et al. (1999)
$Pb^{2+} + 2Cl^- <=> PbCl_2(aq)$	2.00	Lothenbach et al. (1999)
$Pb^{2+} + 3Cl^- <=> PbCl_3^-$	2.01	Lothenbach et al. (1999)
$Pb^{2+} + 4Cl^- <=> PbCl_4^{2-}$	1.35	Lothenbach et al. (1999)
$Pb^{2+} + F^- <=> PbF^+$	2.27	Lothenbach et al. (1999)
$Pb^{2+} + 2F^- <=> PbF_2(aq)$	3.01	Lothenbach et al. (1999)
$Pb^{2+} + F^- + Cl^- <=> PbFCl(aq)$	3.55	Lothenbach et al. (1999)
$Pb^{2+} + CO_3^{2-} <=> PbCO_3(aq)$	7.30	Lothenbach et al. (1999)
$Pb^{2+} + 2CO_3^{2-} <=> Pb(CO_3)_2^{2-}$	10.13	Lothenbach et al. (1999)
$Pb^{2+} + NO_3^- <=> PbNO_3^+$	1.06	Lothenbach et al. (1999)
$Pb^{2+} + 2NO_3^- <=> Pb(NO_3)_2(aq)$	1.48	Lothenbach et al. (1999)
$Pb^{2+} + 3NO_3^- <=> Pb(NO_3)_3^-$	0.76 *1	Lothenbach et al. (1999)
$Pb^{2+} + H^+ + PO_4^{3-} <=> PbHPO_4(aq)$	15.45 *1	Lothenbach et al. (1999)
$Pb^{2+} + 2H^+ + PO_4^{3-} <=> PbH_2PO_4^+$	21.05 *1	Lothenbach et al. (1999)
$Pb^{2+} + SO_4^{2-} <=> PbSO_4(aq)$	2.82	Lothenbach et al. (1999)
$Pb^{2+} + 2SO_4^{2-} <=> Pb(SO_4)_2^{2-}$	2.37 *1	Lothenbach et al. (1999)
$Pb^{2+} + 2HS^- <=> Pb(HS)_2(aq)$	12.34 *1	Lothenbach et al. (1999)
$Pb^{2+} + 3HS^- <=> Pb(HS)_3^-$	13.59 *1	Lothenbach et al. (1999)

*1 tentative value (refer to Lothenbach et al., 1999)

2.2.7 Bismuth (Bi)

The PNC-TDB_H-3 only included an equilibrium constant of the reaction, $Bi_2O_3(s) <=> 2Bi^{2+} +3H_2O -6H^+$, from NBS-82 (Wagman et al., 1982). In the JNC-TDB development, Lothenbach et al. (1999) selected thermodynamic data for Bi-OH^-, Bi-Cl^-, Bi-NO_3^- systems using the SIT model based on the experimental measurements. The scientific advisory and review committee recommended these selections from the view of experts.

In freezing, the dataset for Bi selected by Lothenbach et al. (1999) was adopted in the JNC-TDB as shown in Tables 2.2.7-1 and 2.2.7-2.

Table 2.2.7-1 log K Values of Involving Solid Compounds of Bismuth

Reaction	log K	Reference
$\alpha-Bi_2O_3(cr) +6H^+ <=> 2Bi^{3+} +3H_2O$	0.76	Lothenbach et al. (1999)
$BiOCl(s) +2H^+ <=> Bi^{3+} +H_2O +Cl^-$	-8.47	Lothenbach et al. (1999)
$(BiO)_2CO_3(cr) +4H^+ <=> 2Bi^{3+} +2H_2O +CO_3^{2-}$	-14.27 *1	Lothenbach et al. (1999)
$(BiO)_4(OH)_2CO_3(cr) +10H^+ <=> 4Bi^{3+} +6H_2O + CO_3^{2-}$	-8.68 *1	Lothenbach et al. (1999)
$BiONO_3(s) +2H^+ <=> Bi^{3+} +H_2O +NO_3^-$	-2.75	Lothenbach et al. (1999)
$Bi(cr) <=> Bi^{3+} + 3e^-$	-16.74	Lothenbach et al. (1999)

*1 tentative value (refer to Lothenbach et al., 1999)

Table 2.2.7-2 log K Values of Involving Solution Species of Bismuth

Reaction	log K	Reference
$Bi^{3+} + H_2O <=> BiOH^{2+} + H^+$	-0.92	Lothenbach et al. (1999)
$Bi^{3+} + 2H_2O <=> Bi(OH)_2^+ + 2H^+$	-2.56	Lothenbach et al. (1999)
$Bi^{3+} + 3H_2O <=> Bi(OH)_3(aq) + 3H^+$	-5.31	Lothenbach et al. (1999)
$Bi^{3+} + 4H_2O <=> Bi(OH)_4^- + 4H^+$	-18.71	Lothenbach et al. (1999)
$6Bi^{3+} + 12H_2O <=> Bi_6(OH)_{12}^{6+} + 12H^+$	1.34	Lothenbach et al. (1999)
$9Bi^{3+} + 20H_2O <=> Bi_9(OH)_{20}^{7+} + 20H^+$	-1.36	Lothenbach et al. (1999)
$9Bi^{3+} + 21H_2O <=> Bi_9(OH)_{21}^{6+} + 21H^+$	-3.25	Lothenbach et al. (1999)
$9Bi^{3+} + 22H_2O <=> Bi_9(OH)_{22}^{5+} + 22H^+$	-4.86	Lothenbach et al. (1999)
$3Bi^{3+} + 4H_2O <=> Bi_3(OH)_4^{5+} + 4H^+$	-0.80 *1	Lothenbach et al. (1999)
$Bi^{3+} + Cl^- <=> BiCl^{2+}$	3.65	Lothenbach et al. (1999)
$Bi^{3+} + 2Cl^- <=> BiCl_2^+$	5.85	Lothenbach et al. (1999)
$Bi^{3+} + 3Cl^- <=> BiCl_3(aq)$	7.62	Lothenbach et al. (1999)
$Bi^{3+} + 4Cl^- <=> BiCl_4^-$	9.06	Lothenbach et al. (1999)
$Bi^{3+} + 5Cl^- <=> BiCl_5^{2-}$	8.33 *1	Lothenbach et al. (1999)
$Bi^{3+} + 6Cl^- <=> BiCl_6^{3-}$	7.64 *1	Lothenbach et al. (1999)
$Bi^{3+} + NO_3^- <=> BiNO_3^{2+}$	1.97	Lothenbach et al. (1999)
$Bi^{3+} + 2NO_3^- <=> Bi(NO_3)_2^+$	2.95	Lothenbach et al. (1999)
$Bi^{3+} + 3NO_3^- <=> Bi(NO_3)_3(aq)$	3.62	Lothenbach et al. (1999)
$Bi^{3+} + 4NO_3^- <=> Bi(NO_3)_4^-$	3.09	Lothenbach et al. (1999)
$Bi^{3+} + Cl^- + NO_3^- <=> BiClNO_3^+$	5.16	Lothenbach et al. (1999)
$Bi^{3+} + Cl^- + 2NO_3^- <=> BiCl(NO_3)_2(aq)$	5.28	Lothenbach et al. (1999)
$Bi^{3+} + 2Cl^- + NO_3^- <=> BiCl_2NO_3(aq)$	6.86	Lothenbach et al. (1999)
$Bi^{3+} + 2Cl^- + 2NO_3^- <=> BiCl_2(NO_3)_2^-$	5.75	Lothenbach et al. (1999)
$Bi^{3+} + 3Cl^- + NO_3^- <=> BiCl_3NO_3^-$	8.09	Lothenbach et al. (1999)

*1 tentative value (refer to Lothenbach et al., 1999)

2.2.8 Polonium (Po)

In general, the chemical property of polonium is analogous to Se and Te, and the physical property be to Bi and Pb. Many compounds of Po were reported in literatures, but their thermodynamic data or constants were not reported.

The PNC-TDB_H-3 included only thermodynamic data of the reaction, $Po(OH)_4(s) <=> Po^{4+} +4H_2O -4H^+$, from NBS-82 (Wagman et al., 1982). In the JNC-TDB development, thermodynamic data for the other reactions were investigated. PoO^{2+} in acidic range, PoO_3^{2-} in alkaline range are considered for polonium aqueous species. The standard potentials for the reaction are given by

$PoO_3 + 2e^- \rightarrow PoO_3^{2-}$: +1.47V, and $PoO_3^{2-} + 6H^+ + 4e^- \rightarrow Po +3H_2O$: 0.748V.

Stability constants of Po aqueous species were obtained by solvent extraction. The experimental procedure and analytical method were considered to be appropriate. However, the reported species did not agree with the above redox reaction. The experimental studies indicated $Po(OH)_4(aq)$ or Po-OH-Cl complexes as dominant (Mikheev,1978, Hataye et al., 1981a; 1981b, Suganuma and Hataye, 1981) in the neutral pH region.

Up to now, thermodynamic data for Po were not discussed enough to confirm the reliability based on experimental measurements. In freezing, the JNC-TDB included only thermodynamic data of the reaction, $Po(OH)_4(s) <=> Po^{4+} +4H_2O -4H^+$, from NBS-82 (Wagman et al., 1982) as shown in Table 2.2.8.

Table 2.2.8 log K value of Reaction of Polonium

Reaction	log K	Reference
$Po(OH)_4(s) +4H^+ <=> Po^{4+} + 4H_2O$	19.52	Wagman et al. (1982)

Polonium is considered to be less important from a viewpoint of the performance analysis of geological disposal system. Because, a half-life of the isotope of polonium ^{221}Po is 138.38 days. ^{210}Po is of the series of 4n+2, including ^{210}Pb(a half-life: 22.3 years), ^{226}Ra(a half-life: 1600 years) in its ancestor. ^{210}Po will be generated during these radionuclides migration, and decayed to the stable ^{206}Pb soon.

The scientific advisory and review committee recommended that solubility limit should not be given

by the thermodynamic data for Po.

2.2.9 Radium (Ra)

The PNC-TDB_H-3 included thermodynamic data for Ra from Harwell R12324 (Cross et al, 1987). In the JNC-TDB development, thermodynamic data for Ra could not be discussed enough to revise due to no data development.

In freezing, the dataset for Ra of the Harwell R12324 was adopted in the JNC-TDB as shown in Tables 2.2.9-1 and 2.2.9-2.

Table 2.2.9-1 log K values of Reactions Involving Solid Compounds of Radium

Reaction	log K	Reference
$RaSO_4(s) <=> Ra^{2+} + SO_4^{2-}$	-10.40	Cross et al. (1987)
$RaCO_3(s) <=> Ra^{2+} + CO_3^{2-}$	-7.00	Cross et al. (1987)

Table 2.2.9-2 log K values of Reactions Involving Solution Species of Radium

Reaction	log K	Reference
$Ra^{2+} + H_2O <=> RaOH^+ + H^+$	-13.6	Cross et al. (1987)
$Ra^{2+} + SO_4^{2-} <=> RaSO_4(aq)$	0.022	Cross et al. (1987)

The scientific advisory and review committee discussed the limiting solid for Ra in the solubility estimation of geological disposal system. It is considered that co-precipitation of Ra with Ba, Sr and Ca of alkaline metal elements takes place, because the chemical property of Ra is very analogous to those. The committee recommended that the solubility of Ra should be estimated using simple co-precipitation model like Kristallin-I (Berner, 1995).

2.2.10 Nickel (Ni)

The PNC-TDB_H-3 included thermodynamic data for Ni from Harwell R12324 (Cross et al., 1987). In the JNC-TDB development, the reliability of thermodynamic data for Ni were discussed, comparing with the solubility measurements in a bentonite water system (Shibutani, 1996b). Thermodynamic data for solids including Ni such as $Ni(OH)_2$(s), NiO(cr), NiS(millerite), Ni_3S_2(heazlewoodite), $NiCO_3$(s), etc. were selected from Nagra-TDB (Baeyens and McKinley, 1989) by Shibutani (1996b). In this selection, thermodynamic data for Ni-CO_3^{2-} complexes were not determined. Thermodynamic data for Ni were consequently selected as shown in Tables 2.2.12-1 and 2.2.12-2, where the log K value for $NiCO_3$(aq) was recommended by Berner (1998).

However, the reliability could not be confirmed in this selection. In the solubility measurements in the bentonite water system, solids and aqueous species were not identified, due to a complex water system with the bentonite. Sorption should be also considered in the bentonite-water system. Hence, a solubility measurement for an element in complex water system is not adequate to determine thermodynamic data, which was suggested by the scientific advisory and review committee.

In freezing, the JNC-TDB tentatively included the dataset for Ni shown in the following tables. In future, it will be necessary to investigate the data based on experimental measurements for Ni in simple water systems, considering the development procedure by the OECD/NEA.

Table 2.2.12-1 log K values of Reactions Involving Solid Compounds of Nickel

Reaction	log K	Reference
$Ni(OH)_2(s) + 2H^+ <=> Ni^{2+} + 2H_2O$	12.73	Baeyens and McKinley (1989)
$NiO(cr) + 2H^+ <=> Ni^{2+} + H_2O$	12.44	Baeyens and McKinley (1989)
$NiS(millerite) + 4H_2O <=> Ni^{2+} + SO_4^{2-} + 8H^+ + 8e^-$	-42.83	Baeyens and McKinley (1989)
$Ni_3S_2(heazlewoodite) + 8H_2O <=> 3Ni^{2+} + 2SO_4^{2-} + 16H^+ + 18e^-$	-82.00	Baeyens and McKinley (1989)
$NiCO_3(s) <=> Ni^{2+} + CO_3^{2-}$	-6.97	Baeyens and McKinley (1989)
$Ni_3(PO_4)_2(cr) <=> 3Ni^{2+} + 2PO_4^{3-}$	-29.59	Baeyens and McKinley (1989)
$Ni_2P_2O_7(cr) <=> 2Ni^{2+} + 2PO_4^{3-} - H_2O + 2H^+$	-33.57	Baeyens and McKinley (1989)
$Ni_2SiO_4(olivine) + 4H^+ <=> 2Ni^{2+} + H_4SiO_4(aq)$	18.84	Baeyens and McKinley (1989)
$Ni_2SiO_4(spinel) + 4H^+ <=> 2Ni^{2+} + H_4SiO_4(aq)$	20.24	Baeyens and McKinley (1989)
$NiSiO_3(cr) + H_2O + 2H^+ <=> Ni^{2+} + H_4SiO_4(aq)$	-2.28	Baeyens and McKinley (1989)

Table 2.2.12-2 log K values of Reactions Involving Solution Species of Nickel

Reaction	log K	Reference
$Ni^{2+} + H_2O <=> NiOH^+ + H^+$	-9.86	Cross et al. (1987)
$Ni^{2+} + 2H_2O <=> Ni(OH)_2(aq) + 2H^+$	-19.0	Cross et al. (1987)
$Ni^{2+} + 3H_2O <=> Ni(OH)_3^- + 3H^+$	-30.0	Cross et al. (1987)
$2Ni^{2+} + H_2O <=> Ni_2OH^{3+} + H^+$	-10.7	Cross et al. (1987)
$4Ni^{2+} + 4H_2O <=> Ni_4(OH)_4^{4+} + 4H^+$	-27.7	Cross et al. (1987)
$Ni^{2+} + CO_3^{2-} <=> NiCO_3(aq)$	4	Berner (1998)
$Ni^{2+} + SO_4^{2-} <=> NiSO_4(aq)$	2.32	Cross et al. (1987)

2.2.11 Selenium (Se)

The PNC-TDB_H-3 included thermodynamic data for Se from Harwell R12324 (Cross et al., 1987). In the JNC-TDB development, thermodynamic data for SeO_3^{2-}, $HSeO_3^-$, and H_2SeO_3(aq) were modified taking consideration of the OECD/NEA-TDB by Silva et al. (1995). However, Silva et al. (1995) only includes the standard molar Gibbs energy of formation for these species, and doesn't include the data for SeO_4^{2-}, which is a master species for Se in JNC-TDB. Therefore, to derive equilibrium constants, which are applicable in JNC-TDB, thermodynamic data for SeO_4^{2-} were needed and introduced from Wagman et al. (1982). Equilibrium constant for FeSe(cr) was also added. Thermodynamic data for FeSe(cr) were adopted from Mills (1974). In the derivation of equilibrium constant for FeSe(cr), thermodynamic data for SeO_4^{2-} and Fe^{2+} were adopted from Wagman et al. (1982) and Robie and Hemingway (1995), respectively. Silva et al. (1995) was used for the thermodynamic data of other compound.

Thermodynamic data for Se shown in Tables 2.2.11-1 and 2.2.11-2 were consequently selected in the JNC-TDB development. The scientific advisory and review committee recommended that the selected data were adequate to estimate the solubility in geological disposal in this stage. In freezing, the JNC-TDB included the dataset for Se, although the procedure, combining data from different database, may cause internal inconsistency and the reliability of the data had not been investigated in detail. In future, it will be necessary to discuss the data based on experiments for Se in detail, considering the development procedure by the OECD/NEA.

Table 2.2.11-1 log K values of Reactions Involving Solid Compounds of Selenium

Reaction*1	log K	Reference
$Se(cr) + 4H_2O <=> SeO_4^{2-} + 8H^+ + 6e^-$	-88.92	Cross et al. (1987)
$SeO_2(cr) + 2H_2O <=> SeO_4^{2-} + 4H^+ + 2e^-$	-35.82	Cross et al. (1987)
$SeO_3(cr) + H_2O <=> SeO_4^{2-} + 2H^+$	19.2	Cross et al. (1987)
$Se_2O_5(cr) + 3H_2O <=> 2SeO_4^{2-} + 6H^+ + 2e^-$	-19.6	Cross et al. (1987)
$FeSe_2(cr) + 8H_2O <=> 2SeO_4^{2-} + Fe^{2+} + 16H^+ + 14e^-$	-181.1	Cross et al. (1987)
$FeSe(cr) + 4H_2O <=> SeO_4^{2-} + Fe^{2+} + 8H^+ + 8e^-$	-84.78	Mills (1974), Silva et al. (1995), Wagman et al. (1982), and Robie and Hemingway (1995)

*1 These reactions are given by PHREEQE format.

Table 2.2.11-2 log K values of Reactions Involving Solution Species of Selenium

Reaction[*1]	log K	Reference
$SeO_4^{2-} + 2H^+ + 2e^- <=> SeO_3^{2-} + H_2O$	27.578[*2]	Silva et al. (1995) and Wagman et al. (1982)
$SeO_4^{2-} + 3H^+ + 2e^- <=> HSeO_3^- + H_2O$	35.978[*2]	Silva et al. (1995) and Wagman et al (1982)
$SeO_4^{2-} + 4H^+ + 2e^- <=> H_2SeO_3(aq) + H_2O$	38.783[*2]	Silva et al. (1995) and Wagman et al. (1982)
$SeO_4^{2-} + 8H^+ + 8e^- <=> Se^{2-} + 4H_2O$	66.26[*3]	Cross et al. (1987)
$SeO_4^{2-} + 9H^+ + 8e^- <=> HSe^- + 4H_2O$	81.16[*3]	Cross et al. (1987)
$SeO_4^{2-} + 10H^+ + 8e^- <=> H_2Se(aq) + 4H_2O$	85.1	Cross et al. (1987)
$SeO_4^{2-} + H^+ <=> HSeO_4^-$	1.91[*3]	Cross et al. (1987)

*1 These reactions are given by PHREEQE format.

*2 The log K value is calculated from the molar Gibbs free energy in the references.

*3 The last figure was rounded in the solubility calculations.

2.2.12 Zirconium (Zr)

The PNC-TDB_H-3 included thermodynamic data for Zr from Harwell R12324 (Cross et al., 1987). However, experimental data and natural analogue data for Zr did not agree with the thermodynamic estimation. In the JNC-TDB development, thermodynamic data for Zr were discussed, comparing with the solubility measurements in a bentonite-water system (Shibutani and Yui, 1998). The measured solubility varied widely, $10^{-9} - 10^{-6}$ mol/l, in the pH range 7 to 11. The large scattering of Zr concentrations were confirmed in natural water, and the following reactions were considered to be dominant processes based on the reports (Ellison and Navrotsky; 1992, Kulmura and Hakanen; 1993, Boswell and Elderfield; 1988).

$$ZrO_2(am) + 2H_2O \Leftrightarrow Zr(OH)_4(aq) \text{ --------(1)}$$

$$ZrO_2(am) + 3H_2O - H^+ \Leftrightarrow Zr(OH)_5^- \text{ ------(2)}$$

The Zr oxide (or hydrous oxide) solubilities calculated using the Zr data of HATCHES, the PNC-TDB_H-3 and Baes and Mesmer, were not in good agreement with the measured solubilities in the experimental pH range due to the scattered measurements. Shibutani and Yui (1998) didn't select thermodynamic data for Zr concretely.

Shibutani and Yui (1998) selected the data for ZrO_2(am), $Zr(OH)_4$(aq) and $Zr(OH)_5^-$ as shown in Table 2.2.13 based on the measured solubility by Shibutani and Yui (1998). However, the solubility measurement could not identify solids and aqueous species in bentonite-water system similar to the case of Ni. Hence, the solubility measurement in a complex water system is not adequate to determine thermodynamic data, which was suggested by the scientific advisory and review committee.

In freezing, the JNC-TDB tentatively included the dataset for Zr shown in Table 2.2.13. In future, it will be necessary to investigate the data based on experimental measurements for Zr in simple water systems in detail, considering the development procedure by the OECD/NEA.

Table 2.2.13 log K values of Reactions Involving Solid Compounds of Zirconium

Reaction	log K
$ZrO_2(am) + 2H_2O <=> Zr(OH)_4(aq)$	-8
$Zr(OH)_4(aq) + H_2O <=> Zr(OH)_5^- + H^+$	-10

3. CONCLUSION / FUTURE TASKS

The first progress report used thermodynamic database (PNC-TDB_H-3) compiled from other TDBs and related literature, (e.g., Cross et al. 1987, Grenthe et al. 1992). The JNC-TDB development has continued after the first progress report for geological disposal system of HLW in Japan (PNC, 1992). In the development, thermodynamic data (equilibrium constants at 25 °C, I=0) for important radioactive elements have been determined from the original experimental data by using the SIT, Pitzer models, etc. As a result, the reliability and traceability of thermodynamic data for the most important elements were improved. In the JNC-TDB development, it was necessary to investigate the data for the 22 radioactive elements. In future, it will be necessary to focus on important elements and realistic reactions in the geological disposal, for example, the data for iron, silicate, aluminosilicate, sulfide minerals including radioactive elements or the data at high carbonate concentrations. In the JNC-TDB development, besides the equilibrium constants, the activity correction parameters of the Pitzer and the SIT models have been partially compiled for the radioactive elements. In future, it will be necessary to develop these parameters when solubility in saline groundwater and bentonite porewater in the geological disposal system is estimated more accurately. The use of the JNC-TDB only provides solubility and speciation for radioactive elements at 25 °C, because reliable thermodynamic data at elevated temperatures are not available at this time. In future, it will be necessary to develop thermodynamic data to estimate solubilities at a high temperature. The data for complexes with the inorganic ligands, OH^-, CO_3^{2-}, SO_4^{2-}, PO_4^{3-}, etc., have not been sufficiently selected since the status of measurements, selections and activity correction methods were different. In future, it will be necessary to complement insufficient thermodynamic data for these complexes.

For actinides (III and IV), Rai et al. (1999a and 1999b) selected the thermodynamic data for the carbonate and hydroxo-carbonate complexes enough to improve the reliability of solubility estimation in high carbonate-concentrated water. In these selections, the Pitzer model was used for activity corrections. For actinides(III), the data were primarily selected based on the Am(III) data. Limited validation of the applicability of Am(III) data to other trivalent actinides will be required. The identification of actinide(IV)

hydroxo-carbonate complexes and other species that exist in low concentrations cannot at present be made using existing spectroscopic techniques. Therefore, in future, with the advancement of analytical tools, the identification of these species should be challenged.

For actinides (V and VI) and redox reactions, Choppin et al. (1999) and Shibutani and Shibutani (1998b) selected the thermodynamic data for the Pu(V) and Pu(VI) aqueous species based on the chemical analogy with Np(V) and U(VI), respectively. In future, it will be necessary to confirm the data given by the chemical analogy, comparing with the solubility measurements. In contrast, the data for Pa were not discussed in the selection, because the property is not chemically analogous to those of other actinides (V). Shibutani and Shibutani (1998a) investigated the data for Pa, but selected only those for Pa-OH^- species. In future, it will be necessary to carry out the solubility measurement in carbonate media.

For a lanthanide (III), that is Sm(III), Shibutani (1996a) experimentally selected the data for Sm-OH^- and Sm-CO_3^{2-} aqueous species in the JNC-TDB development. In freezing the JNC-TDB, however, the data were set on the basis of the chemical analogy with Am(III), because the data were not sufficient.

Lothenbach et al. (1999) selected the data for aqueous species of Nb, Pd, Sn, Sb, Pb and Bi using the SIT model for calculations. For Nb aqueous species, a few data only for Nb(V)-OH^- species were selected from a few experimental measurements. In future, it will be necessary to develop the data, considering how to confirm the solubility limit in geological disposal system. The scientific advisory and review committee recommended that a solubility limit for Nb should not be set for the performance analysis of geological disposal due to limited data. That will also be discussed in more detail. The reliable data for Pd-OH^- species could not be given in the JNC-TDB development due to lack of reliable data. In future, it will be necessary to carry out the solubility measurements related to PdO(cr) and Pd-OH^- species to obtain reliable data. In the development, the data for Pd-NH_3 complexes were given on the basis of the measurements. This ligand was not considered in the JNC-TDB development. Considering that ammonium species are dominant nitrogen (N) species under reducing conditions, if nitrogen concentration is high, it may be necessary to consider ammonium complexes in the future JNC-TDB development.

For Tc, Ra and Po aqueous species, the data were not discussed in the JNC-TDB development due to lack of new information. For Tc, OECD/NEA will publish the database in the near future as mentioned in

section 2.2.2. For Ra, the co-precipitation model with alkaline earth metals (Berner, 1995) was adopted in the solubility estimation in geological disposal system. In future, it will be necessary to study co-precipitation reactions of Ra with alkaline earth metals rather than pure phase solubility measurements. For Po, it will not be necessary to develop the data because of the shorter half-life.

For Ni and Zr, the data selections were discussed, comparing the calculated and measured solubility in bentonite-water system in the JNC-TDB development. In such a complex system, sorption must be considered. In future, it will be necessary to develop the data in a simple system, considering the TDB development procedure by the OECD/NEA.

For Se, the data selection was not discussed in detail in the JNC-TDB development. Finally, the JNC-TDB included the dataset in this stage. Se(-II) aqueous species are considered to be dominant under reducing conditions. Silva et al. (1995) recommended the data only for Se(IV) aqueous species. In future, it will be necessary to study the data for Se(-II) aqueous species and redox reactions of Se(-II)/Se(0)/Se(IV)/Se(VI) in detail. Besides, solubility measurements for Se will be necessary in iron-sulfur system under reducing conditions.

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Appendixes

Appendix-1

Guideline for critical review of thermodynamic data

- Experimental -

- Is the experimental procedure adequate?
- What is the accuracy of the measurement?
- Is the change in the measured parameter, compared with the error, sufficient to identify the chemical reaction proposed?
- Were the parameters such as ionic strength and temperature held constant? If not, is it possible to estimate the error caused by such variations?
- Were other experimental variables adequately controlled / measured?
  - Solid / liquid separation techniques (for solubility experiments).
  - Control of redox potentials (in redox-sensitive experiments).
  - Characterization of reactants (e.g., solid phase for solubility experiments).
  - Evidence of equilibrium (e.g., for experiments involving fixed partial pressure of CO_2 gas: Are the soluble carbonate species in equilibrium with CO_2 gas at the given partial pressure?)
  - Characterization of products (e.g., oxidation states for redox-sensitive species, spectroscopic evidence for the species).

- Data Interpretation -

- Verify that the chemical conditions of the experiments were chosen such that the species participating in the proposed reactions were all present in measurable quantities at equilibrium.
- How many experimental points are available for each of the proposed reactions?
- Are any secondary reactions (e.g., protonation, complexation with inert salt ions, hydrolysis, redox reactions, etc.) expected to take place under the experimental conditions chosen, and were they corrected for by the authors? If they were not corrected for, are the reported data sufficient to allow such corrections at this stage?
- Were the data correctly interpreted including the use of appropriate electrolyte theories and other auxiliary data? If not, are the experimental results available and reliable such that the data can be reinterpreted?

- Results -

- Do the resulting constants make sense? For example, would the resulting values have been anticipated based on common knowledge (e.g., $K_{n+1} < K_n$, etc.)?
- Have others judged this paper before (e.g., in later papers on a similar subject, or in reviews like NEA, IAEA and others)? If there are differences in the different expert judgments, an explanation should be given if possible.

Appendix-2

Used data for solubility and speciation calculation for the second progress report on the geological disposal research in Japan (H12)

JNC has used thermodynamic data to estimate solubility and speciation of radioactive elements in the safety assessment of high-level waste disposal system. The JNC-TDB has been developed for this objective. However, unfortunately, the JNC-TDB development and the solubility estimation have been carried out in parallel for the last phase for the second progress report (H12), due to delay of the JNC-TDB development project. Some parts of the selected and frozen datasets were not consequently used for the solubility estimation in the second progress report. In such cases, the datasets for the solubility estimation shown in the following tables were used. The datasets for Am, Np, Pu, and U were used in the following tables.

A-2.1 Americium (Am)

The dataset for Am compiled by Silva et al. (1995) was used for the solubility estimation. The used data are shown in Tables A-2.1-1 and A-2.1-2. For Sm, Ac, Pu(III), and Cm, the dataset for Am shown in the tables was used for the solubility estimation.

Table A-2.1-1 log Ksp values of Reactions Involving Solid Compounds of Americium(III)

Reaction	log Ksp	Reference
$Am(OH)_3(am) + 3H^+ <=> Am^{3+} + 3H_2O$	17.0	Silva et al. (1995)
$Am(OH)_3(cr) + 3H^+ <=> Am^{3+} + 3H_2O$	15.2	Silva et al. (1995)
$Am_2(CO_3)_3(cr) <=> 2Am^{3+} + 3CO_3^{2-}$	-33.4	Silva et al. (1995)
$AmOHCO_3(cr) <=> Am^{3+} + OH^- + CO_3^{2-}$	-21.2	Silva et al. (1995)
$AmPO_4(am) <=> Am^{3+} + PO_4^{3-}$	-24.79	Rai et al. (1992)

Table A-2.1-2 log K values of Reactions Involving Solution Species of Americium (III)

Reaction	log K	Reference
$Am^{3+} + H_2O <=> AmOH^{2+} + H^+$	-6.4	Silva et al. (1995)
$Am^{3+} + 2\ H_2O <=> Am(OH)_2^+ + 2H^+$	-14.1	Silva et al. (1995)
$Am^{3+} + 3\ H_2O <=> Am(OH)_3(aq) + 3H^+$	-25.7	Silva et al. (1995)
$Am^{3+} + F^- <=> AmF^{2+}$	3.4	Silva et al. (1995)
$Am^{3+} + 2F^- <=> AmF_2^+$	5.8	Silva et al. (1995)
$Am^{3+} + CO_3^{2-} <=> AmCO_3^+$	7.8	Silva et al. (1995)
$Am^{3+} + 2CO_3^{2-} <=> Am(CO_3)_2^-$	12.3	Silva et al. (1995)
$Am^{3+} + 3CO_3^{2-} <=> Am(CO_3)_3^{3-}$	15.2	Silva et al. (1995)
$Am^{3+} + NO_3^- <=> AmNO_3^{2+}$	1.33	Silva et al. (1995)
$Am^{3+} + Cl^- <=> AmCl^{2+}$	1.05	Silva et al. (1995)
$Am^{3+} + SO_4^{2-} <=> AmSO_4^+$	3.85	Silva et al. (1995)
$Am^{3+} + 2SO_4^{2-} <=> Am(SO_4)_2^-$	5.40	Silva et al. (1995)
$Am^{3+} + H_2PO_4^- <=> AmH_2PO_4^{2+}$	3.00	Silva et al. (1995)

A-2.2 Neptunium (Np)

The data of reactions including Np(III), Np(V) and Np(VI) compiled by Shibutani et al. (1998) were used for the solubility estimation as shown in Tables A-2.2-1, A-2.2-2, A-2.2-3, A-2.2-5, A-2.2-6 and A-2.2-7. For the solubility estimation, the data for Np(IV) shown in Table A-2.2-4 were used in addition to the frozen data shown in Tables 2.1.5-2 and 2.1.5-3 in section 2.1.5.

Table A-2.2-1 log K values of Redox Reactions of Neptunium

Reaction	log K	Reference
$Np^{4+} + e^- <=> Np^{3+}$	3.03	Cross et al. (1987)
$NpO_2^+ + e^- + 4H^+ <=> Np^{4+} + 2H_2O$	10.89	Fuger and Oetting (1976)
$NpO_2^{2+} + e^- <=> NpO_2^+$	21.40	Cross et al. (1987)

Table A-2.2-2 log K values of Reactions Involving Solid Compounds of Neptunium (III)

Reaction	log K	Reference
$Np(OH)_3(s) + 3H^+ <=> Np^{4+} + e^- + 3H_2O$	15.93	Cross et al. (1987)

Table A-2.2-3 log K values of Reactions Involving Solution Species of Neptunium (III)

Reaction	log K	Reference
$Np^{4+} + e^- + H_2O <=> NpOH^{2+} + H^+$	-4.37	Cross et al. (1987)
$Np^{4+} + e^- + 2H_2O <=> Np(OH)_2^+ + 2H^+$	-13.97	Cross et al. (1987)
$Np^{4+} + e^- + 3H_2O <=> Np(OH)_3(aq) + 3H^+$	-23.97	Cross et al. (1987)
$Np^{4+} + e^- + 4H_2O <=> Np(OH)_4^- + 4H^+$	-34.97	Cross et al. (1987)
$2Np^{4+} + 2e^- + 2H_2O <=> Np_2(OH)_2^{4+} + 2H^+$	-7.43	Cross et al. (1987)
$Np^{4+} + e^- + CO_3^{2-} <=> NpCO_3^+$	9.53	Cross et al. (1987)
$Np^{4+} + e^- + 2CO_3^{2-} <=> Np(CO_3)_2^-$	14.03	Cross et al. (1987)
$Np^{4+} + e^- + 3CO_3^{2-} <=> Np(CO_3)_3^{3-}$	17.53	Cross et al. (1987)
$Np^{4+} + e^- + Cl^- <=> NpCl^{2+}$	0.63	Cross et al. (1987)
$Np^{4+} + e^- + 2Cl^- <=> NpCl_2^+$	-2.35	Cross et al. (1987)

Table A-2.2-4 log K values of Reactions Involving Solution Species of Neptunium (IV)

Reaction	log K	Reference
$Np^{4+} + Cl^- <=> NpCl^{3+}$	1.80	Shibutani et al. (1998)
$Np^{4+} + 2Cl^- <=> NpCl_2^{2+}$	2.11	Shibutani et al. (1998)
$Np^{4+} + F^- <=> NpF^{3+}$	8.33	Cross et al. (1987)
$Np^{4+} + 2F^- <=> NpF_2^{2+}$	14.59	Cross et al. (1987)
$Np^{4+} + 3F^- <=> NpF_3^+$	20.3	Cross et al. (1987)
$Np^{4+} + 4F^- <=> NpF_4(aq)$	25.1	Cross et al. (1987)

Table A-2.2-5 log Ksp values of Reactions Involving Solid Compounds of Neptunium (V)

Reaction	log Ksp	Reference
$NpO_2OH(am) <=> NpO_2^+ + OH^-$	-8.76 *1	Shibutani et al. (1998)
$NaNpO_2CO_3(cr) <=> Na^+ + NpO_2^+ + CO_3^{2-}$	-11.0 *1	Shibutani et al. (1998)
$Na_3NpO_2(CO_3)_2(cr) <=> 3Na^+ + NpO_2^+ + 2CO_3^{2-}$	-14.3 *1	Shibutani et al. (1998)

*1 Ion strength in molarity [mol/l] was used in SIT activity correction.

Table A-2.2-6 log K values of Reactions Involving Solution Species of Neptunium (V)

Reaction	log K	Reference
$NpO_2^+ + OH^- <=> NpO_2OH(aq)$	3.31 *1	Shibutani et al. (1998)
$NpO_2^+ + 2OH^- <=> NpO_2(OH)_2^-$	5.39 *1	Shibutani et al. (1998)
$NpO_2^+ + CO_3^{2-} <=> NpO_2CO_3^-$	4.79 *1	Shibutani et al. (1998)
$NpO_2^+ + 2CO_3^{2-} <=> NpO_2(CO_3)_2^{3-}$	6.65 *1	Shibutani et al. (1998)
$NpO_2^+ + 3CO_3^{2-} <=> NpO_2(CO_3)_3^{5-}$	5.51 *1	Shibutani et al. (1998)
$NpO_2^+ + Cl^- <=> NpO_2Cl(aq)$	-0.29	Neck et al. (1995)
$Np^{4+} + 2H_2O - 4H^+ - e^- + F^- = NpO_2F(aq)$	-10.38	Cross et al. (1987)
$NpO_2^+ + SO_4^{2-} <=> NpO_2SO_4^-$	0.6 *2	Fuger et al. (1992)

*1 Ion strength in molarity [mol/l] was used in SIT activity correction.

*2 The log K value was given at ionic strength I=1 [mol/l].

Note that an equilibrium constant for $Np(V)O_2HCO_3(aq)$ compiled by Shibutani et al. (1998) was not used for the solubility estimation, because the constant was not experimentally confirmed.

Table A-2.2-7 log K values of Reactions Involving Solution Species of Neptunium (VI)

Reaction	log K	Reference
$Np^{4+} + 3H_2O - 5H^+ - 2e^- <=> NpO_2OH^+$	- 37.39	Cross et al. (1987)
$Np^{4+} + 4H_2O - 6H^+ - 2e^- <=> NpO_2(OH)_2(aq)$	- 43.81	Cross et al. (1987)
$Np^{4+} + 5H_2O - 7H^+ - 2e^- <=> NpO_2(OH)_3^-$	- 53.99	Cross et al. (1987)
$2Np^{4+} + 6H_2O - 10H^+ - 4e^- <=> (NpO_2)_2(OH)_2^{2+}$	- 70.98	Cross et al. (1987)
$3Np^{4+} + 11H_2O - 17H^+ - 6e^- <=> (NpO_2)_3(OH)_5^+$	- 114.37	Cross et al. (1987)
$2Np^{4+} + 5H_2O - 9H^+ - 4e^- <=> (NpO_2)_2OH^{3+}$	- 68.58	Cross et al. (1987)
$Np^{4+} + 2H_2O - 4H^+ - 2e^- + Cl^- <=> NpO_2Cl^+$	- 32.59	Cross et al. (1987)
$Np^{4+} + 2H_2O - 4H^+ - 2e^- + 2Cl^- <=> NpO_2Cl_2(aq)$	- 31.29	Cross et al. (1987)
$Np^{4+} + 2H_2O - 4H^+ - 2e^- + SO_4^{2-} <=> NpO_2SO_4(aq)$	- 29.02	Cross et al. (1987)
$Np^{4+} + 2H_2O - 4H^+ - 2e^- + 2SO_4^{2-} <=> NpO_2(SO_4)_2^{2-}$	- 28.19	Cross et al. (1987)
$Np^{4+} + 2H_2O - 4H^+ - 2e^- + 3SO_4^{2-} <=> NpO_2(SO_4)_3^{4-}$	- 27.29	Cross et al. (1987)

A-2.3 Plutonium (Pu)

For Pu(III), based on chemical analogy the data for Am shown in Table A-2.1-2 and A-2.1-2 were adopted in the solubility estimation. The data for redox reaction are basically same as the finally frozen data shown in Tables 2.1.6-1. However, there was a mistake in deriving the data of the redox reaction of Pu(IV)/Pu(III). The log K values used in the solubility estimation are shown in Table A-2.3-1. The value in Table 2.1.6-1 was correctly calculated. Log K values for Pu(IV) shown in Table A-2.3-2 were used for the solubility estimation besides the frozen data as shown in Tables 2.1.6-2 and 2.1.6-3. For Pu(IV) fluoride complexes, data of U(IV) selected by Grenthe et al. (1992) were used as analogue data considering the discussion in Shibutani and Shibutani (1998b). For Pu(V), the data compiled by Shibutani and Shibutani (1998b) shown in Tables A-2.3-3, and A-2.3-4 were used instead of Tables 2.1.6-4 and 2.1.6-5. For Pu(VI), the used data were the same as the frozen data in Table 2.1.6-6 besides the data shown in Tables A-2.3-5 and 2.3-6.

Table A-2.3-1 log K values of Redox Reactions of Plutonium

Reaction	log K	Reference
$Pu^{4+} + e^- <=> Pu^{3+}$	17.01	Fuger and Oetting (1976)
$PuO_2^+ + e^- + 4H^+ <=> Pu^{4+} + 2H_2O$	18.60	Rai (1984)
$PuO_2^{2+} + e^- <=> PuO_2^+$	16.16	Rai (1984)

Table A-2.3-2 log K values of Reactions Involving Solution Species of Plutonium (IV)

Reaction	log K	Reference
$Pu^{4+} + Cl^- <=> PuCl^{3+}$	2.00	Fuger et al.(1992)
$Pu^{4+} + NO_3^- <=> PuNO_3^{3+}$	2.60	Fuger et al.(1992)
$Pu^{4+} + F^- <=> PuF^{3+}$	9.28 *1	Grenthe et al.(1992)
$Pu^{4+} + 2F^- <=> PuF_2^{2+}$	16.23 *1	Grenthe et al.(1992)
$Pu^{4+} + 3F^- <=> PuF_3^+$	21.6 *1	Grenthe et al.(1992)
$Pu^{4+} + 4F^- <=> PuF_4(aq)$	25.6 *1	Grenthe et al.(1992)
$Pu^{4+} + 5F^- <=> PuF_5^-$	27.01 *1	Grenthe et al.(1992)
$Pu^{4+} + 6F^- <=> PuF_6^{2-}$	29.08*1	Grenthe et al.(1992)

*1 The log K value was given by chemical analogy with U(IV)

Table A-2.3-3 log Ksp values of Reactions Involving Solid Compounds of Plutonium (V)

Reaction	log Ksp	Reference
$PuO_2OH(s) + H^+ <=> PuO_2^{2+} + H_2O$	4.83	Shibutani and Shibutani (1998b)

Table A-2.3-4 log K values of Reactions Involving Solution Species of Plutonium (V)

Reaction	log K	Reference
$PuO_2^+ + H_2O <=> PuO_2OH(aq) + H^+$	-9.73	Bennett et al.(1992)
$PuO_2^+ + CO_3^{2-} <=> PuO_2CO_3^-$	5.12	Bennett et al.(1992)

Table A-2.3-5 log Ksp values of Reactions Involving Solid Compounds of Plutonium (VI)

Reaction	log Ksp	Reference
$PuO_2(OH)_2(s) + 2H^+ <=> PuO_2^{2+} + 2H_2O$	4.4	Lierse and Kim (1986)
$PuO_2CO_3(s) <=> PuO_2^{2+} + CO_3^{2-}$	-14.85	Pashalidis et al. (1997)

Table A-2.3-6 log K values of Reactions Involving Solution Species of Plutonium (VI)

Reaction	log K	Reference
$2PuO_2^{2+} + 2H_2O <=> (PuO_2)_2(OH)_2^{2+} + 2H^+$	-5.620 *1	Grenthe et al. (1992)
$3PuO_2^{2+} + 5H_2O <=> (PuO_2)_3(OH)_5^+ + 5H^+$	-15.550 *1	Grenthe et al. (1992)
$2PuO_2^{2+} + 3OH^- + CO_3^{2-} <=> (PuO_2)_2(OH)_3CO_3^-$	41	Allard (1983)
$3PuO_2^{2+} + 3OH^- + CO_3^{2-} <=> (PuO_2)_3(OH)_3CO_3^+$	43	Allard (1983)

*1 The log K value was given by chemical analogy with U(VI)

A-2.4 Uranium (U)

For the solubility estimation, the data for U(IV) shown in Table A-2.5.1 were used in addition to the frozen data shown in Tables 2.1.4-2 and 2.1.4-3 in section 2.1.4. A log K value for $U(V)O_2(CO_3)_3^{5-}$ compiled by Grenthe et al. (1992) was included in the database used for the solubility estimation (see Table A-2.5.2). The data for U(VI) thiocyanate (SCN^-) complexes in Table 2.1.4-5 are not included in calculation because thiocyanate is unlikely to exist in the repository conditions. $(UO_2)_2(NpO_2)(CO_3)_6^{6-}$ is neither included due to lack of the data of $Np(VI)O_2(CO_3)_3^{4-}$.

Table A-2.5-1 log K values of Reactions Involving Solution Species of Uranium (IV)

Reaction	log K	Reference
$U^{4+} + Cl^- <=> UCl^{3+}$	1.720	Grenthe et al. (1992)
$U^{4+} + Br^- <=> UBr^{3+}$	1.460	Grenthe et al. (1992)
$U^{4+} + I^- <=> UI^{3+}$	1.250	Grenthe et al. (1992)

Table A-2.5-2 log K values of Reactions Involving Solution Species of Uranium (V)

Reaction	log K	Reference
$UO_2^+ + 3CO_3^{2-} <=> UO_2(CO_3)_3^{5-}$	7.406 *1	Grenthe et al. (1992)

*1 log K value of the reaction based on Gibbs free energy $\Delta_f G$ in Grenthe et al. (1992)

Appendix-3

PHREEQE format database used for solubility and speciation calculation for H12

The database prepared for use in a geochemical calculation code (PHREEQE: Parkhurst, 1980) is given in the following pages. This database contains a number of aqueous species, gases and compounds in addition to the radioactive elements discussed in this report. For these auxiliary data, the selected auxiliary data by OECD/NEA Thermodynamic Database Project (i.e. Silva et al., 1995) were primarily adopted. For the species, which were not covered by Silva et al. (1995), the data in PHREEQE original database were used. An additional database of minerals compiled by OECD/NEA (e.g., Muller, 1985), which was adopted in PNC-TDB_H-3 (Yui et al., 1992), was also included.

The equilibrium constants (log K) at 25℃ are stored, however, the other parameter related to the activity coefficient model and temperature dependency are not included. This database is prepared for the use with Davis equation as an activity coefficient model.

Detailed discussion for the solubility and speciation calculation is described in Azuma et al. (1999).

```
ELEMENTS
CA          4          40.      CA+2
MG          5          24.      MG+2
NA          6          23.      NA+
K           7          39.      K+
FE          8          56.      FE+2
MN          9          55.      MN+2
AL         10          27.      AL+3
BA         11         137.      BA+2
SR         12          88.      SR+2
SI         13          96.      H4SIO4(AQ)
CL         14          35.      CL-
C          15          60.      CO3-2
S          16          96.      SO4-2
N          17          62.      NO3-
B          18          62.      B(OH)3(A
P          19          95.      PO4-3
F          20          19.      F-
LI         21           7.      LI+
BR         22          80.      BR-
I          23         127.      I-
TC         24         115.      TCO+2
U          25         238.      U+4
CO         27          59.      CO+2
AM         28         243.      AM+3
PU         29         239.      PU+4
CS         30         133.      CS+
NI         31          59.      NI+2
SE         32         143.      SEO4-2
ZR         33         159.      ZR(OH)4
SN         34         119.      SN(OH)4
SM         35         150.      SM+3
PB         36         207.      PB+2
RA         37         226.      RA+2
TH         38         232.      TH+4
PA         39         231.      PA+4
NP         40         237.      NP+4
NB         41         178.      NB(OH)5
PD         42         106.      PD+2
ND         44         144.      ND+3
SB         46         173.      SB(OH)3
BI         47         209.      BI+3
PO         48         209.      PO+4
AC         49         227.      AC+3
CM         50         247.      CM+3

SPECIES
  1
H+            100     1.000     0.000     9.000     0.000     0.000     0.
 0.0          0.0
  1  1.000
  2
E-            100    -1.000     0.000     0.000     0.000     0.000     0.
 0.0          0.0
  2  1.000
  3
H2O(L)        100     0.000     0.000     0.000     0.000     0.000     0.
 0.0          0.0
  3  1.000
  4
CA+2          101     2.000     0.000     6.000     5.000     0.165     0.
 0.0          0.0
  4  1.000
  5
MG+2          101     2.000     0.000     8.000     5.500     0.200     0.
0.0          0.0
  5  1.000
  6
NA+           101     1.000     0.000     4.000     4.000     0.075     0.
0.0          0.0
  6  1.000
  7
K+            101     1.000     0.000     3.000     3.500     0.015     0.
0.0          0.0
  7  1.000
  8
FE+2          100     2.000     2.000     6.000     0.000     0.000     0.
```

```
0.0       0.0
  8  1.000
  9
MN+2          100     2.000     2.000     6.000     0.000     0.000     0.
 0.0       0.0
  9  1.000
 10
AL+3          100     3.000     0.000     9.000     0.000     0.000     0.
 0.0       0.0
 10  1.000
 11
BA+2          100     2.000     0.000     5.000     0.000     0.000     0.
 0.0       0.0
 11  1.000
 12
SR+2          101     2.000     0.000     5.000     5.260     0.121     0.
 0.0       0.0
 12  1.000
 13
H4SIO4(A      100     0.000     0.000     0.000     0.000     0.000     0.
 0.0       0.0
 13  1.000
 14
CL-           101    -1.000     0.000     3.000     3.500     0.015     0.
 0.0       0.0
 14  1.000
 15
CO3-2         101    -2.000     4.000     4.500     5.400     0.000     2.
 0.0       0.0
 15  1.000
 16
SO4-2         101    -2.000     6.000     4.000     5.000    -0.040     0.
 0.0       0.0
 16  1.000
 17
NO3-          100    -1.000     5.000     3.000     0.000     0.000     0.
 0.0       0.0
 17  1.000
 18
B(OH)3(A      100     0.000     0.000     0.000     0.000     0.000     0.
0.0       0.0
 18  1.000
 19
PO4-3         100    -3.000     0.000     4.000     0.000     0.000     2.
 0.0       0.0
 19  1.000
 20
F-            100    -1.000     0.000     3.500     0.000     0.000     0.
 0.0       0.0
 20  1.000
 21
LI+           100     1.000     0.000     6.000     0.000     0.000     0.
0.0       0.0
 21  1.000
 22
BR-           100    -1.000     0.000     3.000     0.000     0.000     0.
0.0       0.0
 22  1.000
 23
I-            100    -1.000    -1.000     0.000     0.000     0.000     0.
0.0       0.0
 23  1.000
 24  FOR TCO+2
TCO+2         100     2.000     4.000     0.000     0.000     0.000     0.
0.0       0.0
 24  1.000
 25  FOR U+4
U+4           100     4.000     4.000     0.000     0.000     0.000     0.
0.0       0.0
 25  1.000
 27
CO+2          100     2.000     2.000     0.000     0.000     0.000     0.
0.0       0.0
 27  1.000
 28  FOR AM+3
AM+3          100     3.000     3.000     0.000     0.000     0.000     0.
0.0       0.0
```

```
 28  1.000
 29  FOR PU+4
PU+4          100      4.000      4.000      0.000      0.000      0.000      0.
0.0         0.0
 29  1.000
 30  FOR CS+
CS+           100      1.000      0.000      0.000      0.000      0.000      0.
0.0         0.0
 30  1.000
 31
NI+2          100      2.000      0.0        0.0        0.0        0.0        0.
     0.0         0.0
 31  1.000
 32  FOR SE04-2
SE04-2        100     -2.000      6.0        0.0        0.0        0.0        0.
     0.0         0.0
 32  1.000
 33  FOR ZR(OH)4(aq)
ZR(OH)4       100      0.000      0.0        0.0        0.0        0.0        0.
     0.0         0.0
 33  1.000
 34  FOR SN(OH)4
SN(OH)4       100      0.000      0.0        0.0        0.0        0.0        0.
     0.0         1.0
 34  1.000
 35
SM+3          100      3.000      0.0        0.0        0.0        0.0        0.
     0.0         0.0
 35  1.000
 36
PB+2          100      2.000      2.0        0.0        0.0        0.0        0.
     0.0         0.0
 36  1.000
 37  FOR RA+2
RA+2          100      2.000      0.0        0.0        0.0        0.0        0.
     0.0         0.0
 37  1.000
 38  FOR TH+4
TH+4          100      4.000      0.0        0.0        0.0        0.0        0.
     0.0         0.0
 38  1.000
 39  FOR PA+4
PA+4          100      4.000      4.0        0.0        0.0        0.0        0.
     0.0         0.0
 39  1.000
 40  FOR NP+4
NP+4          100      4.000      4.0        0.0        0.0        0.0        0.
     0.0         0.0
 40  1.000
 41   FOR NB(OH)5(aq)
NB(OH)5       100      0.000      0.0        0.0        0.0        0.0        0.
     0.0         0.0
 41  1.000
 42 FOR PD+2
PD+2          100      2.000      2.0        0.0        0.0        0.0        0.
     0.0         0.0
 42  1.000
 44
ND+3          100      3.000      3.0        0.0        0.0        0.0        0.
     0.0         0.0
 44  1.000
 46  FOR SB(OH)3(AQ)
SB(OH)3       100  0.0       3.0        0.0                              0.0
0.0         0.0
 46  1.000
 47
BI+3          100  3.0       0.0        0.0                              0.0
0.0         0.0
 47  1.000
 48
PO+4          100  4.0       4.0        0.0                              0.0
0.0         0.0
 48  1.000
 49 FOR AC+3
AC+3          100  3.0       0.0        0.0                              0.0
0.0         0.0
 49  1.000
```

```
 50
CM+3          100  3.0       3.0        0.0                                  0.0
0.0         0.0
 50  1.000
 61  FROM ORIGINAL
H2 AQ         200      0.000     -2.000      0.000      0.000      0.000      0.
-3.15         0.000
  1  2.000  2  2.000
 62   FOR OH- FROM [NEA95]
OH-           200     -1.000      0.000      3.500      0.000      0.000      1.
   -14.002       0.000
  3  1.000  1 -1.000
 63  FROM ORIGINAL
O2 AQ         300      0.000      4.000      0.000      0.000      0.000      0.
-86.08        0.00
  3  2.000  1 -4.000  2 -4.000
 64  FROM ORIGINAL
CAOH+         300      1.000      0.000      0.000      0.000      0.000      1.
 -12.598    0.000
  4  1.000  3  1.000  1 -1.000
 65  FROM ORIGINAL
MGOH+         300      1.000      0.000      0.000      0.000      0.000      1.
-11.794     0.000
  5  1.000  3  1.000  1 -1.000
 66  FROM ORIGINAL
FEOH+         300      1.000      2.000      0.000      0.000      0.000      1.
-9.500       0.0
  8  1.000  3  1.000  1 -1.000
 67  FROM ORIGINAL
FEOH2         300      0.000      2.000      0.000      0.000      0.000      2.
-20.570      0.000
  8  1.000  3  2.000  1 -2.000
 68  FROM ORIGINAL
FEOH3-        300     -1.000      2.000      0.000      0.000      0.000      3.
-31.000      0.000
  8  1.000  3  3.000  1 -3.000
 69  FROM ORIGINAL
FE+3          200      3.000      3.000      9.000      0.000      0.000      0.
-13.032      0.0
  8  1.000  2 -1.000
 70  FROM ORIGINAL
FEOH+2        400      2.000      3.000      0.000      0.000      0.000      0.
-15.22       0.0
  8  1.000  3  1.000  2 -1.000  1 -1.000
 71  FROM ORIGINAL
FEOH2+        400      1.000      3.000      0.000      0.000      0.000      0.
-18.70       0.0
  8  1.000  3  2.000  1 -2.000  2 -1.000
 72  FROM ORIGINAL
FEOH3         400      0.000      3.000      0.000      0.000      0.000      1.
-26.63       0.0
  8  1.000  3  3.000  1 -3.000  2 -1.000
 73  FROM ORIGINAL
FEOH4-        400     -1.000      3.000      0.000      0.000      0.000      2.
-34.63       0.0
  8  1.000  3  4.000  1 -4.000  2 -1.000
 74  FROM ORIGINAL
FE2OH2+4      400      4.000      6.000      0.000      0.000      0.000      0.
-29.01       0.0
  8  2.000  3  2.000  1 -2.000  2 -2.000
 75  FROM ORIGINAL
FE3OH4+5      400      5.000      9.000      0.000      0.000      0.000      0.
-45.4        0.0
  8  3.000  3  4.000  1 -4.000  2 -3.000
 76  FROM ORIGINAL
MNOH+         300      1.000      2.000      0.000      0.000      0.000      1.
-10.59       0.00
  9  1.000  3  1.000  1 -1.000
 77  FROM ORIGINAL
MNOH3-        300     -1.000      2.000      0.000      0.000      0.000      3.
-34.80     0.0
  9  1.000  3  3.000  1 -3.000
 78  FROM ORIGINAL
MN+3          200      3.000      3.000      0.000      0.000      0.000      0.
 -25.507     0.0
  9  1.000  2 -1.000
 79  FROM ORIGINAL
```

```
MNO4-2      400    -2.000     6.000     0.000     0.000     0.000     0.
 -118.440    0.0
  9  1.000  3  4.000  1 -8.000  2 -4.000
 80  FROM ORIGINAL
MNO4-       400    -1.000     7.000     3.500     0.000     0.000     0.
 -127.824    0.0
  9  1.000  3  4.000  1 -8.000  2 -5.000
 81  FROM ORIGINAL
ALOH+2      300     2.000     0.000     0.000     0.000     0.000     0.
-4.99      0.0
 10  1.000  3  1.000  1 -1.000
 82  FROM ORIGINAL
ALOH2+      300     1.000     0.000     0.000     0.000     0.000     0.
-10.1     0.0
 10  1.000  3  2.000  1 -2.000
 83  FROM ORIGINAL
ALOH3       300     0.000     0.000     0.000     0.000     0.000     1.
-16.0     0.0
 10  1.000  3  3.000  1 -3.000
 84  FROM ORIGINAL
ALOH4-      300    -1.000     0.000     0.000     0.000     0.000     2.
-23.000    0.0
 10  1.000  3  4.000  1 -4.000
 85  FROM ORIGINAL
BAOH+       300     1.000     0.000     0.000     0.000     0.000     1.
 -13.358    0.0
 11  1.000  3  1.000  1 -1.000
 86  FROM ORIGINAL
SROH+       300     1.000     0.000     5.000     0.000     0.000     1.
 -13.178    0.0
 12  1.000  3  1.000  1 -1.000
 87 FOR SR(OH)2 FROM [CROSS87]
SR(OH)2     300     0.000     0.0       0.0       0.0       0.0       0.
   -28.5       0.0
 12  1.000  3  2.000  1 -2.000
 88   FOR SIO2(OH)2-2 FROM [NEA95]
SIO2(OH)    200    -2.000     0.000     0.000     0.000     0.000     0.
   -23.141     0.000 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.0
 13  1.000  1 -2.000
 89   FOR SIO(OH)3- FROM [NEA95]
SIO(OH)3    200    -1.000     0.000     0.000     0.000     0.000     0.
    -9.810     0.000 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.0
 13  1.000  1 -1.000
 90   FOR SI203(OH)4-2 FROM [NEA95]
SI203(OH    300    -2.000     0.000     0.000     0.000     0.000     0.
   -19.000     0.000 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.0
 13  2.000  3 -1.000  1 -2.000
 91   FOR SI202(OH)5- FROM [NEA95]
SI202(OH    300    -1.000     0.000     0.000     0.000     0.000     0.
    -8.100     0.000 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.0
 13  2.000  3 -1.000  1 -1.000
 92   FOR SI306(OH)3-3 FROM [NEA95]
SI306(OH    300    -3.000     0.000     0.000     0.000     0.000     0.
   -28.601     0.000 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.0
 13  3.000  3 -3.000  1 -3.000
 93   FOR SI305(OH)5-3 FROM [NEA95]
SI305(OH    300    -3.000     0.000     0.000     0.000     0.000     0.
   -27.501     0.000 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.0
 13  3.000  3 -2.000  1 -3.000
 94   FOR SI408(OH)4-4 FROM [NEA95]
SI408(OH    300    -4.000     0.000     0.000     0.000     0.000     0.
   -36.301     0.000
 13  4.000  3 -4.000  1 -4.000
 95   FOR SI407(OH)5-3 FROM [NEA95]
SI407(OH    300    -3.000     0.000     0.000     0.000     0.000     0.
   -25.500     0.000 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.0
 13  4.000  3 -4.000  1 -3.000
 96 FOR SI403(OH)13-3
SI403(OH    200    -3.000     0.000     0.000     0.000     0.000     0.
   -34.901     0.000 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.0
 13  4.000  1 -3.000
 97   FOR CLO- FROM [NEA95]
CLO-        400    -1.000     2.000     0.000     0.000     0.000     0.
   -57.935     0.000 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.0
 14  1.000  3  1.000  1 -2.000  2 -2.000
 98   FOR CLO2- FROM [NEA95]
CLO2-       400    -1.000     4.000     0.000     0.000     0.000     0.
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  -107.877      0.000 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.0
 14  1.000  3  2.000  1 -4.000  2 -4.000
 99   FOR CLO3- FROM [NEA95]
CLO3-         400     -1.000      6.000      0.000      0.000      0.000      0.
  -146.242      0.0    0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.0
 14  1.000  3  3.000  1 -6.000  2 -6.000
100   FOR CLO4- FROM [NEA95]
CLO4-         400     -1.000      8.000      0.000      0.000      0.000      0.
  -187.791      0.0    0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.0
 14  1.000  3  4.000  1 -8.000  2 -8.000
101   FOR HCLO(aq) FROM [NEA95]
HCLO(AQ)      400      0.000      2.000      0.000      0.000      0.000      0.
   -50.515      0.000 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.0
 14  1.000  3  1.000  1 -1.000  2 -2.000
102   FOR HCLO2(aq) FROM [NEA95]
HCLO2(AQ      400      0.000      4.000      0.000      0.000      0.000      0.
  -105.916      0.000 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.0
 14  1.000  3  2.000  1 -3.000  2 -4.000
103  FROM ORIGINAL
FECL+2        300      2.000      3.000      0.000      0.000      0.000      0.
-11.55      0.0
  8  1.000 14  1.000  2 -1.000
104  FROM ORIGINAL
FECL2+        300      1.000      3.000      0.000      0.000      0.000      0.
-10.90      0.0
  8  1.000 14  2.000  2 -1.000
105  FROM ORIGINAL
FECL3         300      0.000      3.000      0.000      0.000      0.000      0.
-11.90      0.0
  8  1.000 14  3.000  2 -1.000
106  FROM ORIGINAL
MNCL+         200      1.000      2.000      0.000      0.000      0.000      0.
 0.607      0.0
  9  1.000 14  1.000
107  FROM ORIGINAL
MNCL2         200      0.000      2.000      0.000      0.000      0.000      0.
 0.041      0.0
  9  1.000 14  2.000
108  FROM ORIGINAL
MNCL3-        200     -1.000      2.000      0.000      0.000      0.000      0.
 -0.305     0.0
  9  1.000 14  3.000
109 FOR SRCL+1 FROM [CROSS87]
SRCL+1        200      1.000      0.0        0.0        0.0        0.0        0.
    -0.2        0.0
 12  1.000 14  1.000
110 FOR SRCL2 FROM [CROSS87]
SRCL2         200      0.000      0.0        0.0        0.0        0.0        0.
     0.0        0.0
 12  1.000 14  2.000
111   FOR HCO3- FROM [NEA95]
HCO3-         211     -1.000      4.000      4.500      5.400      0.000      1.
    10.327      0.000 107.8871     0.03252849  -5151.79     -38.92561   563713.9
 15  1.000  1  1.000
112   FOR CO2(aq) FROM [NEA95]
CO2(AQ)       300      0.000      4.000      0.000      0.000      0.000      0.
    16.681      0.000 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.0
 15  1.000  3 -1.000  1  2.000
113  FROM ORIGINAL
CH4 AQ        400      0.000     -4.000      0.000      0.000      0.000      0.
 41.071       0.000
 15  1.000  1 10.000  2  8.000  3 -3.000
114  FROM ORIGINAL
CACO3         210      0.000      4.000      0.000      0.000      0.000      2.
3.225      0.000      -1228.732    -0.299440    35512.75      485.818
  4  1.000 15  1.000
115  FROM ORIGINAL
CAHCO3+       311      1.000      4.000      0.000      5.400      0.000      1.
11.435      0.000      1317.0071    0.34546894  -39916.84     -517.70761   563713.9
  4  1.000 15  1.000  1  1.000
116  FROM ORIGINAL
MGCO3         210      0.000      4.000      0.000      0.000      0.000      2.
2.981      0.000      -32.172      0.0            1093.486     12.72433
  5  1.000 15  1.000
117  FROM ORIGINAL
MGHCO3+       310      1.000      4.000      0.000      0.000      0.000      1.
11.397      0.000      48.6721      0.03252849  -2614.335      -18.00263   563713.9
```

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  5  1.000  1  1.000 15  1.000
118  FROM ORIGINAL
NACO3-       200     -1.000      4.000      0.000      0.000      0.000      2.
1.268      0.000
  6  1.000 15  1.000
119  FROM ORIGINAL
NAHCO3       300      0.000      4.000      0.000      0.000      0.000      1.
10.080      0.000
  6  1.000  1  1.000 15  1.000
120  FROM ORIGINAL
MNHCO3+      300      1.000      6.000      0.000      0.000      0.000      1.
 11.60      0.000
  9  1.000 15  1.000  1  1.000
121  FROM ORIGINAL
SRHCO3+      310      1.000      4.000      5.400      0.000      0.000      1.
 11.513     0.000     104.6389     0.04739549  -5151.79     -38.92561    563713.9
 12  1.000 15  1.000  1  1.000
122  FROM ORIGINAL
SRCO3        210      0.000      4.000      0.000      0.000      0.000      2.
 2.805      0.000     -1.019       0.012826
 12  1.000 15  1.000
123   FOR S-2 FROM [NEA95]
S-2          400     -2.000     -2.000      5.000      0.000      0.000      2.
    14.692      0.000
 16  1.000  3 -4.000  1  8.000  2  8.000
124   FOR SO3-2 FROM [NEA95]
SO3-2        400     -2.000      4.000      0.000      0.000      0.000      0.
    -3.397      0.000 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.0
 16  1.000  3 -1.000  1  2.000  2  2.000
125   FOR S2O3-2 FROM [NEA95]
S2O3-2       400     -2.000      4.000      0.000      0.000      0.000      0.
    38.015      0.000 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.0
 16  2.000  3 -5.000  1 10.000  2  8.000
126   FOR HS- FROM [NEA95]
HS-          400     -1.000     -2.000      3.500      0.000      0.000      1.
    33.693      0.000
 16  1.000  3 -4.000  1  9.000  2  8.000
127   FOR H2S(aq) FROM [NEA95]
H2S(AQ)      400      0.000     -2.000      0.000      0.000      0.000      0.
    40.681      0.000 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.0
 16  1.000  3 -4.000  1 10.000  2  8.000
128   FOR HSO3- FROM [NEA95]
HSO3-        400     -1.000      4.000      0.000      0.000      0.000      0.
     3.823      0.000 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.0
 16  1.000  3 -1.000  1  3.000  2  2.000
129   FOR HS2O3- FROM [NEA95]
HS2O3-       400     -1.000      4.000      0.000      0.000      0.000      0.
    39.605      0.000 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.0
 16  2.000  3 -5.000  1 11.000  2  8.000
130   FOR H2SO3(aq) FROM [NEA95]
H2SO3(AQ     400      0.000      4.000      0.000      0.000      0.000      0.
     5.663      0.000 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.0
 16  1.000  3 -1.000  1  4.000  2  2.000
131   FOR HSO4- FROM [NEA95]
HSO4-        210     -1.000      6.000      0.000      0.000      0.000      0.
     1.982      0.000 -5.3505      0.0183412    557.2461
 16  1.000  1  1.000
132  FROM ORIGINAL
CASO4        200      0.000      6.000      0.000      0.000      0.000      0.
2.309      0.000
  4  1.000 16  1.000
133  FROM ORIGINAL
MGSO4        200      0.000      6.000      0.000      0.000      0.000      0.
2.250      0.0
  5  1.000 16  1.000
134  FROM ORIGINAL
NASO4-       200     -1.000      6.000      0.000      0.000      0.000      0.
0.700      0.000
  6  1.000 16  1.000
135  FROM ORIGINAL
KSO4-        200     -1.000      6.000      0.000      0.000      0.000      0.
0.85       0.00
  7  1.000 16  1.000
136  FROM ORIGINAL
FESO4        200      0.000      8.000      0.000      0.000      0.000      0.
2.25       0.00
  8  1.000 16  1.000
```

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137  FROM ORIGINAL
FE(HS)2      500      0.000     -2.000      0.000      0.000      0.000      2.
76.250         0.000
  8  1.000 16  2.000  1 18.000  2 16.000  3 -8.000
138  FROM ORIGINAL
FE(HS)3-     500     -1.000     -4.000      0.000      0.000      0.000      3.
111.937        0.000
  8  1.000 16  3.000  1 27.000  2 24.000  3-12.000
139  FROM ORIGINAL
FESO4+       300      1.000      9.000      0.000      0.000      0.000      0.
-9.11        0.00
  8  1.000 16  1.000  2 -1.000
140  FROM ORIGINAL
FESO42-      300     -1.000     15.000      0.000      0.000      0.000      0.
-7.61        0.00
  8  1.000 16  2.000  2 -1.000
141  FROM ORIGINAL
MNSO4        200      0.000      8.000      0.000      0.000      0.000      0.
 2.26      0.00
  9  1.000 16  1.000
142  FROM ORIGINAL
ALSO4+       200      1.000      6.000      0.000      0.000      0.000      0.
 3.02        0.00
 10  1.000 16  1.000
143  FROM ORIGINAL
ALSO42-      200     -1.000     12.000      0.000      0.000      0.000      0.
 4.92        0.00
 10  1.000 16  2.000
144  FROM ORIGINAL
SRSO4        200      0.000      6.000      0.000      0.000      0.000      0.
 2.55        0.0
 12  1.000 16  1.000
147   FOR NH3(aq) FROM [NEA95]
NH3(AQ)      400      0.000     -3.000      0.000      0.000      0.000      1.
   109.901        0.000
 17  1.000  3 -3.000  1  9.000  2  8.000
148   FOR NH4+ FROM [NEA95]
NH4+         400      1.000     -3.000      2.500      0.000      0.000      0.
   119.138        0.000
 17  1.000  3 -3.000  1 10.000  2  8.000
150  FROM ORIGINAL
NO2-         400     -1.000      3.000      3.000      0.000      0.000      0.
 28.57         0.00
 17  1.000  1  2.000  2  2.000  3 -1.000
151  FROM ORIGINAL
N2 AQ        400      0.000      0.000      0.000      0.000      0.000      0.
 207.08         0.00
 17  2.000  1 12.000  2 10.000  3 -6.000
152  FROM ORIGINAL
NH4SO4-      500     -1.000      3.000      0.000      0.000      0.000      0.
 120.19        0.000
 17  1.000  1 10.000  2  8.000 16  1.000  3 -3.000
153  FROM ORIGINAL
MN(NO3)2     200      0.000     12.000      0.000      0.000      0.000      0.
0.6          0.000
  9  1.000 17  2.000
154 FOR SRNO3+ FROM [CROSS87]
SRNO3+       200      1.000      5.0        0.0        0.0        0.0        0.
     0.8         0.0
 12  1.000 17  1.000
155  FROM ORIGINAL
H2BO3-       200     -1.000      0.000      0.000      0.000      0.000      1.
-9.240     0.000
 18  1.000  1 -1.000
156   FOR P2O7-4 FROM [NEA95]
P2O7-4       300     -4.000      0.000      0.000      0.000      0.000      0.
    21.315        0.000
 19  2.000  3 -1.000  1  2.000
157   FOR HPO4-2 FROM [NEA95]
HPO4-2       200     -2.000      0.000      4.000      0.000      0.000      1.
    12.350        0.000
 19  1.000  1  1.000
158   FOR H2PO4- FROM [NEA95]
H2PO4-       200     -1.000      0.000      4.500      0.000      0.000      0.
    19.563        0.000
 19  1.000  1  2.000
159   FOR H3PO4(aq) FROM [NEA95]
```

```
H3PO4(AQ    200     0.000     0.000     0.000     0.000     0.000     0.
    21.703     0.000
 19  1.000  1  3.000
160   FOR HP2O7-3 FROM [NEA95]
HP2O7-3     300    -3.000     0.000     0.000     0.000     0.000     0.
    30.715     0.000
 19  2.000  3 -1.000  1  3.000
161   FOR H2P2O7-2 FROM [NEA95]
H2P2O7-2    300    -2.000     0.000     0.000     0.000     0.000     0.
    37.365     0.000
 19  2.000  3 -1.000  1  4.000
162   FOR H3P2O7- FROM [NEA95]
H3P2O7-     300    -1.000     0.000     0.000     0.000     0.000     0.
    39.615     0.000
 19  2.000  3 -1.000  1  5.000
163   FOR H4P2O7(aq) FROM [NEA95]
H4P2O7(A    300     0.000     0.000     0.000     0.000     0.000     0.
    40.615     0.000
 19  2.000  3 -1.000  1  6.000
164  FROM ORIGINAL
CAPO4-      200    -1.000     0.000     0.000     0.000     0.000     2.
6.459     0.000
  4  1.000 19  1.000
165  FROM ORIGINAL
CAHPO4      300     0.000     0.000     0.000     0.000     0.000     1.
15.085     0.000
  4  1.000  1  1.000 19  1.000
166  FROM ORIGINAL
CAH2PO4+    300     1.000     0.000     0.000     0.000     0.000     0.
20.961     0.000
  4  1.000  1  2.000 19  1.000
167  FROM ORIGINAL
MGPO4-      200    -1.000     0.000     0.000     0.000     0.000     2.
6.589     0.000
  5  1.000 19  1.000
168  FROM ORIGINAL
MGHPO4      300     0.000     0.000     0.000     0.000     0.000     1.
15.216     0.000
  5  1.000  1  1.000 19  1.000
169  FROM ORIGINAL
MGH2PO4+    300     1.000     0.000     0.000     0.000     0.000     0.
21.066     0.000
  5  1.000  1  2.000 19  1.000
170  FROM ORIGINAL
NAHPO4-     300    -1.000     0.000     0.000     0.000     0.000     1.
12.636     0.000
  6  1.000  1  1.000 19  1.000
171  FROM ORIGINAL
KHPO4-      300    -1.000     0.000     0.000     0.000     0.000     1.
12.636    - 0.00
  7  1.000  1  1.000 19  1.000
172  FROM ORIGINAL
FEHPO4      300     0.000     2.000     0.000     0.000     0.000     1.
15.946     0.000
  8  1.000  1  1.000 19  1.000
173  FROM ORIGINAL
FEH2PO4+    300     1.000     2.000     0.000     0.000     0.000     0.
22.253     0.00
  8  1.000  1  2.000 19  1.000
174  FROM ORIGINAL
FEHPO4+     400     1.000     3.000     0.000     0.000     0.000     1.
 4.74      0.00
  8  1.000  1  1.000 19  1.000  2 -1.000
175  FROM ORIGINAL
FEH2P+2     400     2.000     3.000     0.000     0.000     0.000     0.
 11.95     0.00
  8  1.000  1  2.000 19  1.000  2 -1.000
176 FOR SRPO4- FROM [CROSS87]
SRPO4-      200    -1.000     0.0       0.0       0.0       0.0       0.
     4.2       0.0
 12  1.000 19  1.000
177   FOR HF(aq) FROM [NEA95]
HF(AQ)      200     0.000     0.000     0.000     0.000     0.000     0.
     3.180     0.000
 20  1.000  1  1.000
178   FOR HF2- FROM [NEA95]
HF2-        200    -1.000     0.000     0.000     0.000     0.000     0.
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     3.620      0.000
 20  2.000  1  1.000
179  FROM ORIGINAL
BF0H3-        200     -1.000      0.000      0.000      0.000      0.000      0.
-0.40      0.00
 18  1.000 20  1.000
180  FROM ORIGINAL
BF20H2-       400     -1.000      0.000      0.000      0.000      0.000      0.
7.628      0.000
 18  1.000 20  2.000  1  1.000  3 -1.000
181  FROM ORIGINAL
BF30H-        400     -1.000      0.000      0.000      0.000      0.000      0.
13.666      0.00
 18  1.000  1  2.000 20  3.000  3 -2.000
182  FROM ORIGINAL
BF4-          400     -1.000      0.000      0.000      0.000      0.000      0.
20.274      0.000
 18  1.000  1  3.000 20  4.000  3 -3.000
183  FROM ORIGINAL
HF AQ         200      0.000      0.000      0.000      0.000      0.000      0.
 3.170      0.00
  1  1.000 20  1.000
184  FROM ORIGINAL
HF2-          200     -1.000      0.000      0.000      0.000      0.000      0.
 3.749      0.00
  1  1.000 20  2.000
185  FROM ORIGINAL
CAF+          200      1.000      0.000      0.000      0.000      0.000      0.
0.940      0.000
  4  1.000 20  1.000
186  FROM ORIGINAL
MGF+          200      1.000      0.000      0.000      0.000      0.000      0.
1.820      0.000
  5  1.000 20  1.000
187  FROM ORIGINAL
FEF+2         300      2.000      3.000      0.000      0.000      0.000      0.
-6.8         0.0
  8  1.000 20  1.000  2 -1.000
188  FROM ORIGINAL
FEF2+         300      1.000      3.000      0.000      0.000      0.000      0.
-2.2         0.0
  8  1.000 20  2.000  2 -1.000
189  FROM ORIGINAL
FEF3          300      0.000      3.000      0.000      0.000      0.000      0.
0.97         0.0
  8  1.000 20  3.000  2 -1.000
190  FROM ORIGINAL
MNF+          200      1.000      2.000      0.000      0.000      0.000      0.
 0.85        0.0
  9  1.000 20  1.000
191  FROM ORIGINAL
ALF+2         200      2.000      0.000      0.000      0.000      0.000      0.
 7.01        0.0
 10  1.000 20  1.000
192  FROM ORIGINAL
ALF2+         200      1.000      0.000      0.000      0.000      0.000      0.
 12.75       0.0
 10  1.000 20  2.000
193  FROM ORIGINAL
ALF3          200      0.000      0.000      0.000      0.000      0.000      0.
 17.02      0.00
 10  1.000 20  3.000
194  FROM ORIGINAL
ALF4-         200     -1.000      0.000      0.000      0.000      0.000      0.
 19.72       0.0
 10  1.000 20  4.000
195  FROM ORIGINAL
SIF6-2        400     -2.000      0.000      0.000      0.000      0.000      0.
 30.18        0.0
 13  1.000  1  4.000 20  6.000  3 -4.000
196  FROM ORIGINAL
LIS04-        200     -1.000      6.000      0.000      0.000      0.000      0.
0.640      0.0
 21  1.000 16  1.000
197   FOR BR2(aq) FROM [NEA95]
BR2(AQ)       200      0.000      2.000      0.000      0.000      0.000      0.
   -37.247      0.000
```

```
 22  2.000  2 -2.000
198   FOR BR2(l) FROM [NEA95]
BR2(L)        200     0.000     2.000     0.000     0.000     0.000     0.
     0.000     0.000
 22  2.000  2 -2.000
199   FOR BRO- FROM [NEA95]
BRO-          400    -1.000     2.000     0.000     0.000     0.000     0.
   -54.109     0.000
 22  1.000  3  1.000  1 -2.000  2 -2.000
200   FOR BRO3- FROM [NEA95]
BRO3-         400    -1.000     6.000     0.000     0.000     0.000     0.
  -146.173     0.000
 22  1.000  3  3.000  1 -6.000  2 -6.000
201   FOR HBRO(aq) FROM [NEA95]
HBRO(AQ)      400     0.000     2.000     0.000     0.000     0.000     0.
   -45.487     0.000
 22  1.000  3  1.000  1 -1.000  2 -2.000
202   FOR IO3- FROM [NEA95]
IO3-          400    -1.000     5.000     0.000     0.000     0.000     0.
  -111.566     0.000
 23  1.000  3  3.000  1 -6.000  2 -6.000
203   FOR HIO3(aq) FROM [NEA95]
HIO3(AQ)      400     0.000     5.000     0.000     0.000     0.000     0.
  -110.778     0.000
 23  1.000  3  3.000  1 -5.000  2 -6.000
204 FOR I3- FROM [CROSS87]
I3-           200    -1.000    -1.0       0.0       0.0       0.0       0.
   -18.3       0.0
 23  3.000  2 -2.000
205 FOR HI FROM [CROSS87]
HI            200     0.000    -1.0       0.0       0.0       0.0       0.
    -0.051     0.00
 23  1.000  1  1.000
206 FOR IO- FROM [CROSS87]
IO-           400    -1.000     1.0       0.0       0.0       0.0       0.
   -44.0       0.0
 23  1.000  3  1.000  1 -2.000  2 -2.000
207 FOR IO4- FROM [CROSS87]
IO4-          400    -1.000     7.0       0.0       0.0       0.0       0.
  -165.0       0.0
 23  1.000  3  4.000  1 -8.000  2 -8.000
208 FOR I2O-2 FROM [CROSS87]
I2O-2         400    -2.000     0.0       0.0       0.0       0.0       0.
   -45.30      0.0
 23  2.000  3  1.000  1 -2.000  2 -2.000
209 FOR HIO FROM [CROSS87]
HIO           400     0.000     1.0       0.0       0.0       0.0       0.
   -33.3       0.0
 23  1.000  3  1.000  1 -1.000  2 -2.000
210 FOR H2OI- FROM [CROSS87]
H2OI-         200    -1.000    -1.0       0.0       0.0       0.0       0.
   -32.10      0.0
 23  1.000  3  1.000
211 FOR I2OH- FROM [CROSS87]
I2OH-         400    -1.000     0.0       0.0       0.0       0.0       1.
   -19.4       0.0
 23  2.000  3  1.000  1 -1.000  2 -2.000
212 FOR HIO3 FROM [CROSS87]
HIO3          400     0.000     5.0       0.0       0.0       0.0       0.
  -111.0       0.0
 23  1.000  3  3.000  1 -5.000  2 -6.000
213 FOR I2CL- FROM [CROSS87]
I2CL-         300    -1.000     0.0       0.0       0.0       0.0       0.
   -20.8       0.0
 23  2.000 14  1.000  2 -2.000
214 FOR ICL- FROM [CROSS87]
ICL-          300    -1.000     0.0       0.0       0.0       0.0       0.
   -29.0       0.0
 23  1.000 14  1.000  2 -1.000
215 FOR ICL2- FROM [CROSS87]
ICL2-         300    -1.000     1.0       0.0       0.0       0.0       0.
   -26.9       0.0
 23  1.000 14  2.000  2 -2.000
216 FOR I2 FROM [CROSS87]
I2            200     0.000     0.0       0.0       0.0       0.0       0.
   -18.18      0.0
 23  2.000  2 -2.000
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300 FOR NI(OH)2 FROM [CROSS87]
NI(OH)2      300      0.000      0.0        0.0        0.0        0.0        2.
   -19.0         0.0
 31  1.000  3  2.000  1 -2.000
301 FOR NI(OH)3- FROM [CROSS87]
NI(OH)3-     300     -1.000      0.0        0.0        0.0        0.0        3.
   -30.0         0.0
 31  1.000  3  3.000  1 -3.000
302 FOR NIOH+ FROM [CROSS87]
NIOH+        300      1.000      0.0        0.0        0.0        0.0        1.
    -9.9         0.0
 31  1.000  3  1.000  1 -1.000
303 FOR NI2(OH)+3 FROM [CROSS87]
NI2(OH)+     300      3.000      0.0        0.0        0.0        0.0        1.
   -10.7         0.0
 31  2.000  3  1.000  1 -1.000
304 FOR NI4(OH)4+4 FROM [CROSS87]
NI4(OH)+     300      4.000      0.0        0.0        0.0        0.0        4.
   -27.7         0.0
 31  4.000  3  4.000  1 -4.000
305 FOR NISO4 FROM [CROSS87]
NISO4(AQ     200      0.000      6.0        0.0        0.0        0.0        2.
     2.3         0.0
 31  1.000 16  1.000
306 FOR NICO3 FROM [BERNER98]
NICO3(AQ     200      0.000      4.0        0.0        0.0        0.0        2.
     4.0         0.0
 31  1.000 15  1.000
400 FOR SE-2 FROM [CROSS87]
SE-2         400     -2.000     -2.0        0.0        0.0        0.0        2.
    66.3         0.0
 32  1.000  1  8.000  2  8.000  3 -4.000
401 FOR HSE- FROM [CORSS87]
HSE-         400     -1.000     -2.0        0.0        0.0        0.0        1.
    81.2         0.0
 32  1.000  1  9.000  2  8.000  3 -4.000
402 FOR H2SE FROM [CROSS87]
H2SE         400      0.000     -2.0        0.0        0.0        0.0        0.
    85.1         0.0
 32  1.000  1 10.000  2  8.000  3 -4.000
403   FOR SEO3-2 FROM [YUI99]
SEO3-2       400     -2.000      4.000      0.0        0.0        0.0        2.
    27.578       0.000
 32  1.000  3 -1.000  1  2.000  2  2.000
404   FOR HSEO3- FROM [YUI99]
HSEO3-       400     -1.000      4.000      0.0        0.0        0.0        1.
    35.978       0.000
 32  1.000  3 -1.000  1  3.000  2  2.000
405   FOR H2SEO3(aq) FROM [YUI99]
H2SEO3(A     400      0.000      4.000      0.000      0.000      0.000      0.
    38.783       0.000
 32  1.000  3 -1.000  1  4.000  2  2.000
406 FOR HSEO4- FROM [CROSS87]
HSEO4-       200     -1.000      6.0        0.0        0.0        0.0        1.
     1.9         0.0
 32  1.000  1  1.000
500 FOR ZR(OH)5-  FROM [YUI99]
ZR(OH)5-     300     -1.000      0.0        0.0        0.0        0.0        0.
   -10.0         0.0
 33  1.000  1 -1.000  3  1.000
600  FOR NB(OH)6-1 FROM [LOTHE99]
NB(OH)6-     300     -1.000      0.0        0.0        0.0        0.0        0.
    -6.60        0.0
 41  1.000  1 -1.000  3  1.000
700 FOR TC+3  FROM [NEA89]
TC+3         400      3.000      3.000      0.000      0.000      0.000      0.
     5.391       0.000 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.0
 24  1.000  1  2.000  3 -1.000  2  1.000
701 FOR (TCO(OH)2)2(AQ) FROM [NEA89]
(TCO(OH)     300      0.000      8.000      0.000      0.000      0.000      0.
    -0.133       0.000 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.0
 24  2.000  1 -4.000  3  4.000
702 FOR TCO(OH)2(AQ) FROM [NEA89]
TCO(OH)2     300      0.000      4.000      0.000      0.000      0.000      0.
    -3.325       0.000 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.0
 24  1.000  1 -2.000  3  2.000
703 FOR TCOOH+ FROM [NEA89]
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TCOOH+      300     1.000     4.000     0.000     0.000     0.000     0.
   -1.137     0.000 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.0
 24  1.000  3  1.000  1 -1.000
704 FOR TCO4-3 FROM [NEA89]
TCO4-3      400    -3.000     5.000     0.000     0.000     0.000     0.
  -53.287     0.000 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.0
 24  1.000  1 -6.000  3  3.000  2 -1.000
705 FOR H2TCO4(AQ) FROM [NEA89]
H2TCO4(A    400     0.000     6.000     0.000     0.000     0.000     0.
  -34.310     0.000 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.0
 24  1.000  1 -4.000  3  3.000  2 -2.000
706 FOR HTCO4- FROM [NEA89]
HTCO4-      400    -1.000     6.000     0.000     0.000     0.000     0.
  -34.608     0.000 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.0
 24  1.000  1 -5.000  3  3.000  2 -2.000
707 FOR TCO4-2 FROM [NEA89]
TCO4-2      400    -2.000     6.000     0.000     0.000     0.000     0.
  -43.315     0.000 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.0
 24  1.000  1 -6.000  3  3.000  2 -2.000
708 FOR TCO4- FROM [NEA89]
TCO4-       400    -1.000     7.000     0.000     0.000     0.000     0.
  -32.993     0.000 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.0
 24  1.000  1 -6.000  3  3.000  2 -3.000
800 FOR PDCL+1 FROM [LOTHE99]
PDCL+1      200     1.000     2.0       0.0       0.0       0.0       0.
    5.1       0.0
 42  1.000 14  1.000
801 FOR PDCL2(AQ) FROM [LOTHE99]
PDCL2(AQ    200     0.000     2.0       0.0       0.0       0.0       0.
    8.3       0.0
 42  1.000 14  2.000
802 FOR PDCL3-1 FROM [LOTHE99]
PDCL3-1     200    -1.000     2.0       0.0       0.0       0.0       0.
   10.9       0.0
 42  1.000 14  3.000
803 FOR PDCL4-2 FROM [LOTHE99]
PDCL4-2     200    -2.000     2.0       0.0       0.0       0.0       0.
   11.7       0.0
 42  1.000 14  4.000
804 FOR PDCL3OH-2 FROM [LOTHE99]
PDCL3OH-    400    -2.000     2.0       0.0       0.0       0.0       0.
    2.5       0.0
 42  1.000 14  3.000  3  1.000  1 -1.000
805 FOR PDCL2(OH)2-2 FROM [LOTHE99]
PDCL2OH2    400    -2.000     2.0       0.0       0.0       0.0       0.
   -7.0       0.0
 42  1.000 14  2.000  3  2.000  1 -2.000
806 FOR PD(NH3)+2 FROM [LOTHE99]
PDNH3+2     500     2.000    -1.0       0.0       0.0       0.0       0.
  119.501     0.0
 42  1.000 17  1.000  3 -3.000  1  9.000  2  8.000
807 FOR PD(NH3)2+2 FROM [LOTHE99]
PDNH32+2    500     2.000    -4.0       0.0       0.0       0.0       0.
  238.302     0.0
 42  1.000 17  2.000  3 -6.000  1 18.000  2 16.000
808 FOR PD(NH3)3+2 FROM [LOTHE99]
PDNH33+2    500     2.000    -7.0       0.0       0.0       0.0       0.
  355.703     0.0
 42  1.000 17  3.000  3 -9.000  1 27.000  2 24.000
809 FOR PD(NH3)4+2 FROM [LOTHE99]
PDNH34+2    500     2.000   -10.0       0.0       0.0       0.0       0.
  472.404     0.0
 42  1.000 17  4.000  3-12.000  1 36.000  2 32.000
901 FOR SNOH+ FROM [LOTHE99]
SNOH+       400     1.000    -2.0       0.0       0.0       0.0       0.
    1.65      0.0
 34  1.000  1  3.000  3 -3.000  2  2.000
902 FOR SN(OH)2(AQ) FROM [LOTHE99]
SN(OH)2     400     0.000    -2.0       0.0       0.0       0.0       0.
   -2.31      0.0
 34  1.000  1  2.000  3 -2.000  2  2.000
903 FOR SN(OH)3-1 FROM [LOTHE99]
SN(OH)3-    400    -1.000    -2.0       0.0       0.0       0.0       0.
  -12.14      0.0
 34  1.000  1  1.000  3 -1.000  2  2.000
904 FOR SN3(OH)4+2 FROM [LOTHE99]
SN3OH4+2    400     2.000    -6.0       0.0       0.0       0.0       0.
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      9.69      0.0
 34  3.000  1  8.000  3 -8.000  2  6.000
905 FOR SNCL+ FROM [LOTHE99]
SNCL+         500      1.000     -2.0        0.0        0.0        0.0        0.
      7.05      0.0
 34  1.000  1  4.000  3 -4.000 14  1.000  2  2.000
906 FOR SNCL2(AQ) FROM [LOTHE99]
SNCL2(AQ      500      0.000     -2.0        0.0        0.0        0.0        0.
      7.71      0.0
 34  1.000  1  4.000  3 -4.000 14  2.000  2  2.000
907 FOR SNCL3- FROM [LOTHE99]
SNCL3-        500     -1.000     -2.0        0.0        0.0        0.0        0.
      7.49      0.0
 34  1.000  1  4.000  3 -4.000 14  3.000  2  2.000
908 FOR SNOHCL(AQ) FROM [LOTHE99]
SNOHCLAQ      500      0.000     -2.0        0.0        0.0        0.0        0.
      3.13      0.0
 34  1.000  1  3.000  3 -3.000 14  1.000  2  2.000
909 FOR SNF+ FROM [LOTHE99]
SNF+          500      1.000     -2.0        0.0        0.0        0.0        0.
      9.86      0.0
 34  1.000  1  4.000  3 -4.000 20  1.000  2  2.000
910 FOR SNF2(AQ) FROM [LOTHE99]
SNF2          500      0.000     -2.0        0.0        0.0        0.0        0.
     13.14      0.0
 34  1.000  1  4.000  3 -4.000 20  2.000  2  2.000
911 FOR SNF3-1 FROM [LOTHE99]
SNF3-1        500     -1.000     -2.0        0.0        0.0        0.0        0.
     15.01      0.0
 34  1.000  1  4.000  3 -4.000 20  3.000  2  2.000
912 FOR SNNO3+1 FROM [LOTHE99]
SNNO3+1       500      1.000      3.0        0.0        0.0        0.0        0.
      6.65      0.0
 34  1.000  1  4.000  3 -4.000 17  1.000  2  2.000
913 FOR SN(NO3)2(AQ) FROM [LOTHE99]
SNNO32AQ      500      0.000      8.0        0.0        0.0        0.0        0.
      7.14      0.0
 34  1.000  1  4.000  3 -4.000 17  2.000  2  2.000
914 FOR SN(NO3)3- FROM [LOTHE99]
SNNO33-1      500     -1.000     13.0        0.0        0.0        0.0        0.
      6.77      0.0
 34  1.000  1  4.000  3 -4.000 17  3.000  2  2.000
915 FOR SN(NO3)4-2 FROM [LOTHE99]
SNNO34-2      500     -2.000     18.0        0.0        0.0        0.0        0.
      5.70      0.0
 34  1.000  1  4.000  3 -4.000 17  4.000  2  2.000
916 FOR SN(SO4)(AQ) FROM [LOTHE99]
SNSO4(AQ      500      0.000      4.0        0.0        0.0        0.0        0.
      8.31      0.0
 34  1.000  1  4.000  3 -4.000 16  1.000  2  2.000
917 FOR SN(SO4)2-2 FROM [LOTHE99]
SNSO42-2      500     -2.000     10.0        0.0        0.0        0.0        0.
      8.23      0.0
 34  1.000  1  4.000  3 -4.000 16  2.000  2  2.000
918 FOR SN+2 FROM [LOTHE99]
SN+2          400      2.000     -2.0        0.0        0.0        0.0        0.
      5.40      0.0
 34  1.000  1  4.000  3 -4.000  2  2.000
950 FOR SN(OH)5-1 FROM [LOTHE99]
SN(OH)5-      300     -1.000      0.0        0.0        0.0        0.0        0.
     -7.97      0.0
 34  1.000  3  1.000  1 -1.000
951 FOR SN(OH)6-2 FROM [LOTHE99]
SN(OH)6-      300     -2.000      0.0        0.0        0.0        0.0        0.
    -18.40      0.0
 34  1.000  3  2.000  1 -2.000
952 FOR SN+4 FROM [LOTHE99]
SN+4          300      4.000      0.0        0.0        0.0        0.0        0.
      0.40      0.0
 34  1.000  1  4.000  3 -4.000
1000 FOR SB+3 FROM [LOTHE99]
SB+3          300      3.000      3.0        0.0        0.0        0.0        0.
     -0.73      0.0
 46  1.000  3 -3.000  1  3.000
1001 FOR SBOH+2 FROM [LOTHE99]
SBOH+2        300      2.000      3.0        0.0        0.0        0.0        0.
      0.83      0.0
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 46  1.000  3 -2.000  1  2.000
1002 FOR SB(OH)2+ FROM [LOTHE99]
SB(OH)2+     300     1.000     3.0       0.0       0.0       0.0       0.
     1.30      0.0
 46  1.000  3 -1.000  1  1.000
1003 FOR SB(OH)4- FROM [LOTHE99]
SB(OH)4-     300    -1.000     3.0       0.0       0.0       0.0       0.
   -11.93      0.0
 46  1.000  3  1.000  1 -1.000
1004 FOR SB2S4-2 FROM [LOTHE99]
SB2S4-2      500    -2.000    -2.0       0.0       0.0       0.0       0.
   177.302     0.0
 46  2.000  3-22.000  1 38.000  2 32.000 16  4.000
1005 FOR HSB2S4- FROM [LOTHE99]
HSB2S4-      500    -1.000    -2.0       0.0       0.0       0.0       0.
   186.952     0.0
 46  2.000  3-22.000  1 39.000  2 32.000 16  4.000
1006 FOR H2SB2S4(AQ) FROM [LOTHE99]
H2SB2S4A     500     0.000    -2.0       0.0       0.0       0.0       0.
   191.772     0.0
 46  2.000  3-22.000  1 40.000  2 32.000 16  4.000
1007 FOR SB2(OH)6(AQ) FROM [LOTHE99]
SB2(OH)6     100     0.000     6.0       0.0       0.0       0.0       0.
     0.08      0.0
 46  2.000
1008 FOR SBCL+2 FROM [LOTHE99]
SBCL+2       400     2.000     3.00      0.0       0.0       0.0       0.
     2.78      0.0
 46  1.000  1  3.000  3 -3.000 14  1.000
1009 FOR SBCL2+ FROM [LOTHE99]
SBCL2+       400     1.000     3.00      0.0       0.0       0.0       0.
     3.27      0.0
 46  1.000  1  3.000  3 -3.000 14  2.000
1010 FOR SBF+2 FROM [LOTHE99]
SBF+2        400     2.000     3.00      0.0       0.0       0.0       0.
     6.48      0.0
 46  1.000  1  3.000  3 -3.000 20  1.000
1011 FOR SBF2+ FROM [LOTHE99]
SBF2+        400     1.000     3.00      0.0       0.0       0.0       0.
    12.65      0.0
 46  1.000  1  3.000  3 -3.000 20  2.000
1012 FOR SBF3 FROM [LOTHE99]
SBF3         400     0.000     3.00      0.0       0.0       0.0       0.
    18.36      0.0
 46  1.000  1  3.000  3 -3.000 20  3.000
1050 FOR SB(OH)5(AQ) FROM [LOTHE99]
SB(OH)5      400     0.000     5.00      0.0       0.0       0.0       0.
   -21.84      0.0
 46  1.000  3  2.000  1 -2.000  2 -2.000
1051 FOR SB(OH)6- FROM [LOTHE99]
SB(OH)6-     400    -1.000     5.00      0.0       0.0       0.0       0.
   -24.56      0.0
 46  1.000  3  3.000  1 -3.000  2 -2.000
1052 FOR SB12(OH)64-4 FROM [LOTHE99]
SB12OH64     400    -4.000    60.00      0.0       0.0       0.0       0.
  -241.74      0.0
 46 12.000  3 28.000  1-28.000  2-24.000
1053 FOR SB12(OH)65-5 FROM [LOTHE99]
SB12OH65     400    -5.000    60.00      0.0       0.0       0.0       0.
  -245.36      0.0
 46 12.000  3 29.000  1-29.000  2-24.000
1054 FOR SB12(OH)66-6 FROM [LOTHE99]
SB12OH66     400    -6.000    60.00      0.0       0.0       0.0       0.
  -250.19      0.0
 46 12.000  3 30.000  1-30.000  2-24.000
1055 FOR SB12(OH)67-7 FROM [LOTHE99]
SB12OH67     400    -7.000    60.00      0.0       0.0       0.0       0.
  -256.01          0.0
 46 12.000  3 31.000  1-31.000  2-24.000
1300 FOR SMOH+2 FROM [YU199]
SMOH+2       300     2.000     0.000     0.000     0.000     0.000     0.
    -6.4       0.0
 35  1.000  3  1.000  1 -1.000
1301 FOR SM(OH)2+ FROM [YU199]
SM(OH)2+     300     1.000     0.000     0.000     0.000     0.000     0.
   -14.1       0.0
 35  1.000  3  2.000  1 -2.000
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```
1302 FOR SM(OH)3  FROM [YUI99]
SM(OH)3      300      0.000      0.000      0.000      0.000      0.000      0.
   -25.7         0.0
 35  1.000  3  3.000  1 -3.000
1303 FOR SMCO3+ FROM [YUI99]
SMCO3+       200      1.000      4.0        0.0        0.0        0.0        0.
     7.80        0.0
 35  1.000 15  1.000
1304 FOR SM(CO3)2- FROM [YUI99]
SMCO32-      200     -1.000      8.0        0.0        0.0        0.0        0.
    12.30        0.0
 35  1.000 15  2.000
1305 FOR SM(CO3)3-3 FROM [YUI99]
SMCO33-3     200     -3.000     12.0        0.0        0.0        0.0        0.
    15.2         0.0
 35  1.000 15  3.000
1306 FOR SMF+2  FROM [YUI99]
SMF+2        200      2.000      0.000      0.000      0.000      0.000      0.
     3.4         0.0
 35  1.000 20  1.000
1307 FOR SMF2+  FROM [YUI99]
SMF2+        200      1.000      0.000      0.000      0.000      0.000      0.
     5.800       0.0
 35  1.000 20  2.000
1308 FOR SMNO3+2 FROM [YUI99]
SMNO3+2      200      2.000      5.000      0.000      0.000      0.000      0.
    1.330        0.0
 35  1.000 17  1.000
1400 FOR PBOH+ FROM [LOTHE99]
PBOH+        300      1.000      2.0        0.0        0.0        0.0        1.
   -7.51         0.0
 36  1.000  3  1.000  1 -1.000
1401 FOR PB(OH)2 FROM [LOTHE99]
PB(OH)2      300      0.000      2.0        0.0        0.0        0.0        2.
   -16.95        0.0
 36  1.000  3  2.000  1 -2.000
1402 FOR PB(OH)3- FROM [LOTHE99]
PB(OH)3-     300     -1.000      2.0        0.0        0.0        0.0        3.
   -28.02        0.0
 36  1.000  3  3.000  1 -3.000
1403 FOR PB2(OH)+3 FROM [LOTHE99]
PB2(OH)+     300      3.000      4.0        0.0        0.0        0.0        1.
   -7.18         0.0
 36  2.000  3  1.000  1 -1.000
1404 FOR PB4(OH)4+4 FROM [LOTHE99]
PB4OH4+4     300      4.000      8.0        0.0        0.0        0.0        4.
   -20.63        0.0
 36  4.000  3  4.000  1 -4.000
1405 FOR PB3(OH)4+2 FROM [LOTHE99]
PB3OH4+2     300      2.000      6.0        0.0        0.0        0.0        4.
   -22.48        0.0
 36  3.000  3  4.000  1 -4.000
1406 FOR PB3(OH)5+  FROM [LOTHE99]
PB3OH5+1     300      1.000      6.0        0.0        0.0        0.0        4.
   -30.72        0.0
 36  3.000  3  5.000  1 -5.000
1407 FOR PB6(OH)8+4 FROM [LOTHE99]
PB6OH8+4     300      4.000     12.0        0.0        0.0        0.0        8.
   -42.68        0.0
 36  6.000  3  8.000  1 -8.000
1408 FOR PBCO3 FROM [LOTHE99]
PBCO3        200      0.000      6.0        0.0        0.0        0.0        2.
     7.30        0.0
 36  1.000 15  1.000
1409 FOR PB(CO3)2-2 FROM [LOTHE99]
PBCO32-2     200     -2.000     10.0        0.0        0.0        0.0        4.
    10.13        0.0
 36  1.000 15  2.000
1410 FOR PBNO3+ FROM [LOTHE99]
PBNO3+       200      1.000      7.0        0.0        0.0        0.0        2.
     1.06        0.0
 36  1.000 17  1.000
1411 FOR PB(NO3)2(AQ) FROM [LOTHE99]
PB(NO3)2     200      0.000     12.0        0.0        0.0        0.0        4.
     1.48        0.0
 36  1.000 17  2.000
1412 FOR PB(NO3)3- FROM [LOTHE99]
```

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PBNO33-      200    -1.000    17.0       0.0       0.0       0.0       2.
     0.76       0.0
 36  1.000 17  3.000
1413 FOR PBHPO4(AQ) FROM [LOTHE99]
PBHPO4(A     300      0.000     2.0       0.0       0.0       0.0       2.
    15.45       0.0
 36  1.000 19  1.000  1  1.000
1414 FOR PBH2PO4+ FROM [LOTHE99]
PBH2PO4+     300      1.000     2.0       0.0       0.0       0.0       2.
    21.05       0.0
 36  1.000 19  1.000  1  2.000
1415 FOR PBSO4(AQ) FROM [LOTHE99]
PBSO4        200      0.000     8.0       0.0       0.0       0.0       0.
     2.82       0.0
 36  1.000 16  1.000
1416 FOR PB(SO4)2-2 FROM [LOTHE99]
PBSO42-2     200     -2.000    14.0       0.0       0.0       0.0       0.
     2.37       0.0
 36  1.000 16  2.000
1417 FOR PB(HS)2(AQ) FROM [LOTHE99]
PB(HS)2      500      0.000    -2.0       0.0       0.0       0.0       0.
    79.726      0.0
 36  1.000 16  2.000  3 -8.000  1 18.000  2 16.000
1418 FOR PB(HS)3- FROM [LOTHE99]
PB(HS)3-     500     -1.000    -4.0       0.0       0.0       0.0       0.
   114.669      0.0
 36  1.000 16  3.000  3-12.000  1 27.000  2 24.000
1419 FOR PBCL+ FROM [LOTHE99]
PBCL+        200      1.000     2.0       0.0       0.0       0.0       0.
     1.55       0.0
 36  1.000 14  1.000
1420 FOR PBCL2 FROM [LOTHE99]
PBCL2        200      0.000     2.0       0.0       0.0       0.0       0.
     2.00       0.0
 36  1.000 14  2.000
1421 FOR PBCL3- FROM [LOTHE99]
PBCL3-       200     -1.000     2.0       0.0       0.0       0.0       0.
     2.01       0.0
 36  1.000 14  3.000
1422 FOR PBCL4-2 FROM [LOTHE99]
PBCL4-2      200     -2.000     2.0       0.0       0.0       0.0       0.
     1.35       0.0
 36  1.000 14  4.000
1423 FOR PBF+ FROM [LOTHE99]
PBF+         200      1.000     2.0       0.0       0.0       0.0       0.
     2.27       0.0
 36  1.000 20  1.000
1424 FOR PBF2(AQ) FROM [LOTHE99]
PBF2(A)      200      0.000     2.0       0.0       0.0       0.0       0.
     3.01       0.0
 36  1.000 20  2.000
1425 FOR PBFCL(AQ) FROM [LOTHE99]
PBFCL(AQ     300      0.000     2.0       0.0       0.0       0.0       0.
     3.55       0.0
 36  1.000 20  1.000 14  1.000
1500 FOR BIOH+2 FROM [LOTHE99]
BIOH+2       300      2.000     0.0       0.0       0.0       0.0       0.
    -0.92       0.0
 47  1.000  3  1.000  1 -1.000
1501 FOR BI(OH)2+ FROM [LOTHE99]
BI(OH)2+     300      1.000     0.0       0.0       0.0       0.0       0.
    -2.56       0.0
 47  1.000  3  2.000  1 -2.000
1502 FOR BI(OH)3(AQ) FROM [LOTHE99]
BI(OH)3(     300      0.000     0.0       0.0       0.0       0.0       0.
    -5.31       0.0
 47  1.000  3  3.000  1 -3.000
1503 FOR BI(OH)4- FROM [LOTHE99]
BI(OH)4-     300     -1.000     0.0       0.0       0.0       0.0       0.
   -18.71       0.0
 47  1.000  3  4.000  1 -4.000
1504 FOR BI6(OH)12+6 FROM [LOTHE99]
BI6OH12+     300      6.000     0.0       0.0       0.0       0.0       0.
     1.34       0.0
 47  6.000  3 12.000  1-12.000
1505 FOR BI9(OH)20+7 FROM [LOTHE99]
BI9OH20+     300      7.000     0.0       0.0       0.0       0.0       0.
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    -1.36       0.0
 47  9.000  3 20.000  1-20.000
1506 FOR BI9(OH)21+6 FROM [LOTHE99]
BI9OH21+     300      6.000      0.0        0.0        0.0        0.0        0.
    -3.25       0.0
 47  9.000  3 21.000  1-21.000
1507 FOR BI9(OH)22+5 FROM [LOTHE99]
BI9OH22+     300      5.000      0.0        0.0        0.0        0.0        0.
    -4.86       0.0
 47  9.000  3 22.000  1-22.000
1508 FOR BI3(OH)4+5 FROM [LOTHE99]
BI3OH4+5     300      5.000      0.0        0.0        0.0        0.0        0.
    -0.80       0.0
 47  3.000  3  4.000  1 -4.000
1509 FOR BICL+2 FROM [LOTHE99]
BICL+2       200      2.000      0.0        0.0        0.0        0.0        0.
     3.65       0.0
 47  1.000 14  1.000
1510 FOR BICL2+ FROM [LOTHE99]
BICL2+       200      1.000      0.0        0.0        0.0        0.0        0.
     5.85       0.0
 47  1.000 14  2.000
1511 FOR BICL3(AQ) FROM [LOTHE99]
BICL3(A)     200      0.000      0.0        0.0        0.0        0.0        0.
     7.62       0.0
 47  1.000 14  3.000
1512 FOR BICL4- FROM [LOTHE99]
BICL4-       200     -1.000      0.0        0.0        0.0        0.0        0.
     9.06       0.0
 47  1.000 14  4.000
1513 FOR BICL5-2 FROM [LOTHE99]
BICL5-2      200     -2.000      0.0        0.0        0.0        0.0        0.
     8.33       0.0
 47  1.000 14  5.000
1514 FOR BICL6-3 FROM [LOTHE99]
BICL6-3      200     -3.000      0.0        0.0        0.0        0.0        0.
     7.64       0.0
 47  1.000 14  6.000
1515 FOR BINO3+2 FROM [LOTHE99]
BINO3+2      200      2.000      5.0        0.0        0.0        0.0        0.
     1.97       0.0
 47  1.000 17  1.000
1516 FOR BI(NO3)2+ FROM [LOTHE99]
BINO32+1     200      1.000     10.0        0.0        0.0        0.0        0.
     2.95       0.0
 47  1.000 17  2.000
1517 FOR BI(NO3)3(AQ) FROM [LOTHE99]
BI(NO3)3     200      0.000     15.0        0.0        0.0        0.0        0.
     3.62       0.0
 47  1.000 17  3.000
1518 FOR BI(NO3)4- FROM [LOTHE99]
BINO34-1     200     -1.000     20.0        0.0        0.0        0.0        0.
     3.09       0.0
 47  1.000 17  4.000
1519 FOR BICLNO3+ FROM [LOTHE99]
BICLNO3+     300      1.000      5.0        0.0        0.0        0.0        0.
     5.16       0.0
 47  1.000 14  1.000 17  1.000
1520 FOR BICL(NO3)2(AQ) FROM [LOTHE99]
BICLNO32     300      0.000     10.0        0.0        0.0        0.0        0.
     5.28       0.0
 47  1.000 14  1.000 17  2.000
1521 FOR BICL2NO3(AQ) FROM [LOTHE99]
BICL2NO3     300      0.000      5.0        0.0        0.0        0.0        0.
     6.86       0.0
 47  1.000 14  2.000 17  1.000
1522 FOR BICL2(NO3)2- FROM [LOTHE99]
BINO32CL     300     -1.000     10.0        0.0        0.0        0.0        0.
     5.75       0.0
 47  1.000 14  2.000 17  2.000
1523 FOR BICL3NO3- FROM [LOTHE99]
BICL3NO3     300     -1.000      5.0        0.0        0.0        0.0        0.
     8.09       0.0
 47  1.000 14  3.000 17  1.000
1700 FOR RAOH+ FROM [CROSS87]
RAOH+        300      1.000      0.0        0.0        0.0        0.0        1.
   -13.6        0.0
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 37  1.000  3  1.000  1 -1.000
1701 FOR RAS04 FROM [CROSS87]
RAS04        200      0.000      6.0        0.0        0.0        0.0        0.
     0.022       0.0
 37  1.000 16  1.000
1800 FOR ACOH+2 FROM [YUI99]
ACOH+2       300      2.000      0.000      0.000      0.000      0.000      0.
    -6.4         0.0
 49  1.000  3  1.000  1 -1.000
1801 FOR AC(OH)2+ FROM [YUI99]
AC(OH)2+     300      1.000      0.000      0.000      0.000      0.000      0.
   -14.1         0.0
 49  1.000  3  2.000  1 -2.000
1802 FOR AC(OH)3 FROM [YUI99]
AC(OH)3      300      0.000      0.000      0.000      0.000      0.000      0.
   -25.7         0.0
 49  1.000  3  3.000  1 -3.000
1803 FOR ACCO3+ FROM [YUI99]
ACCO3+       200      1.000      4.0        0.0        0.0        0.0        0.
     7.80        0.0
 49  1.000 15  1.000
1804 FOR AC(CO3)2- FROM [YUI99]
ACCO32-      200     -1.000      8.0        0.0        0.0        0.0        0.
    12.30        0.0
 49  1.000 15  2.000
1805 FOR AC(CO3)3-3 FROM [YUI99]
ACCO33-3     200     -3.000     12.0        0.0        0.0        0.0        0.
    15.2         0.0
 49  1.000 15  3.000
1806 FOR ACF+2  FROM [YUI99]
ACF+2        200      2.000      0.000      0.000      0.000      0.000      0.
     3.4         0.0
 49  1.000 20  1.000
1807 FOR ACF2+  FROM [YUI99]
ACF2+        200      1.000      0.000      0.000      0.000      0.000      0.
     5.800       0.0
 49  1.000 20  2.000
1808 FOR ACNO3+2 FROM [YUI99]
ACNO3+2      200      2.000      5.000      0.000      0.000      0.000      0.
     1.330       0.0
 49  1.000 17  1.000
1900 FOR TH(OH)3CO3- FROM [OSTH94]
THOH3CO3     400     -1.000      4.0        0.0        0.0        0.0        0.
    -3.72        0.0
 38  1.000 15  1.000  3  3.000  1 -3.000
1901 FOR TH(CO3)5-6 FROM [FELM97]
THCO35-6     200     -6.000     20.0        0.0        0.0        0.0        0.
    27.1         0.0
 38  1.000 15  5.000
1902 FOR TH(OH)4 FROM [RYAN87]
TH(OH)4      300      0.000      0.0        0.0        0.0        0.0        4.
   -19.7         0.00
 38  1.000  3  4.000  1 -4.000
1903 FOR TH(SO4)3-2 FROM [FELM92]
THSO43-2     200     -2.000     18.0        0.0        0.0        0.0        6.
    12.42        0.0
 38  1.000 16  3.000
1904 FOR THF3+ FROM [FELM93]
THF3+        200      1.000      0.0        0.0        0.0        0.0        0.
    18.89        0.0
 38  1.000 20  3.000
1905 FOR THF4 FROM [FELM93]
THF4         200      0.000      0.0        0.0        0.0        0.0        0.
    22.33        0.0
 38  1.000 20  4.000
1906 FOR THF5- FROM [FELM93]
THF5-        200     -1.000      0.0        0.0        0.0        0.0        0.
    24.76        0.0
 38  1.000 20  5.000
1907 FOR THF6-2 FROM [FELM93]
THF6-2       200     -2.000      0.0        0.0        0.0        0.0        0.
    25.56        0.0
 38  1.000 20  6.000
1908 FOR TH(NO3)+3 FROM [RAI99B]
THNO3+3      200      3.000      5.0        0.0        0.0        0.0        0.
     2.5         0.0
 38  1.000 17  1.000
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2001 FOR PAOH+3 FROM [BAES 76]
PA(OH)+3     300      3.000      4.0        0.0        0.0        0.0        1.
      0.84       0.0
 39  1.000  3  1.000  1 -1.000
2002 FOR PA(OH)2+2 FROM [BAES 76]
PA(OH)2+     300      2.000      4.0        0.0        0.0        0.0        2.
     -0.02       0.0
 39  1.000  3  2.000  1 -2.000
2003 FOR PA(OH)3+ FROM [BAES 76]
PA(OH)3+     300      1.000      4.0        0.0        0.0        0.0        3.
     -1.5        0.0
 39  1.000  3  3.000  1 -3.000
2004 FOR PAO(OH)3(aq) FROM [SHIB98A]
PAO(OH)3     400      0.000      5.0        0.0        0.0        0.0        0.
     -3.60       0.0
 39  1.000  2 -1.000  3  4.000  1 -5.000
2005 FOR PAO(OH)2+ FROM [SHIB98A]
PAO(OH)2     400      1.000      5.0        0.0        0.0        0.0        0.
      0.85       0.0
 39  1.000  3  3.000  1 -4.000  2 -1.000
2006 FOR PAOOH+2 FROM [FUGER76]
PAO(OH)+     400      2.000      5.0        0.0        0.0        0.0        1.
      1.86       0.0
 39  1.000  3  2.000  2 -1.000  1 -3.000
2100 FOR U+3 FROM [NEA92]
U+3          200      3.000      3.000      0.000      0.000      0.000      0.
    -9.353      0.000 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.0
 25  1.000  2  1.000
2130 FOR UOH+3 FROM [RAI 90]
UOH+3        300      3.000      4.0        0.0        0.0        0.0        4.
    -0.5
 25  1.000  3  1.000  1 -1.000
2131 FOR U(OH)4 FROM [YAJI95]
U(OH)4       300      0.000      4.0        0.0        0.0        0.0        4.
   -11.300
 25  1.000  3  4.000  1 -4.000
2132 FOR USO4+2 FROM [RAI99B]
USO4+2       200      2.000     10.0        0.0        0.0        0.0        6.
      9.00       0.0
 25  1.000 16  1.000
2133 FOR U(SO4)2(AQ) FROM [RAI99B]
USO42AQ      200      0.000     16.0        0.0        0.0        0.0        6.
     11.70       0.0
 25  1.000 16  2.000
2134 FOR UF+3 FROM [NEA 92]
UF+3         200      3.000      4.0        0.0        0.0        0.0        0.
      9.28       0.0
 25  1.000 20  1.000
2135 FOR UF2+2 FROM [NEA 92]
UF2+2        200      2.000      4.0        0.0        0.0        0.0        0.
     16.23       0.0
 25  1.000 20  2.000
2136 FOR UF3+ FROM [NEA 92]
UF3+         200      1.000      4.0        0.0        0.0        0.0        0.
     21.60       0.0
 25  1.000 20  3.000
2137 FOR UF4 FROM [NEA 92]
UF4          200      0.000      4.0        0.0        0.0        0.0        0.
     25.60       0.0
 25  1.000 20  4.000
2138 FOR UF5- FROM [NEA 92]
UF5-         200     -1.000      4.0        0.0        0.0        0.0        0.
     27.01        0.0
 25  1.000 20  5.000
2139 FOR UF6-2 FROM [NEA 92]
UF6-2        200     -2.000      4.0        0.0        0.0        0.0        0.
     29.08       0.0
 25  1.000 20  6.000
2140 FOR U(NO3)+3 FROM [NEA 92]
UNO3+3       200      3.000      9.0        0.0        0.0        0.0        0.
      1.47       0.0
 25  1.000 17  1.000
2141 FOR U(NO3)2+2 FROM [NEA 92]
UNO32+2      200      2.000     14.0        0.0        0.0        0.0        0.
      2.30       0.0
 25  1.000 17  2.000
2142 FOR U(OH)2(CO3)2-2 FROM [RAI 98]
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```
UOH2CO32    400    -2.000    12.0       0.0       0.0       0.0       0.
   13.33       0.0
 25  1.000 15  2.000  3  2.000  1 -2.000
2143 FOR U(CO3)5-6 FROM [RAI 98]
UCO35-6     200    -6.000    24.0       0.0       0.0       0.0       0.
   31.290      0.0
 25  1.000 15  5.000
2144  FOR UCl+3 FROM [NEA92]
UCL+3       200     3.000     4.000     0.000     0.000     0.000     0.
    1.720   -19.000 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.0
 14  1.000 25  1.000
2145  FOR UBr+3 FROM [NEA92]
UBR+3       200     3.000     4.000     0.000     0.000     0.000     0.
    1.460     0.000
 22  1.000 25  1.000
2146  FOR UI+3 FROM [NEA92]
UI+3        200     3.000     3.000     0.000     0.000     0.000     0.
    1.250     0.000
 23  1.000 25  1.000
2160 FOR UO2+ FROM [NEA92]
UO2+        400     1.000     5.000     0.000     0.000     0.000     0.
   -7.554     0.000 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.0
 25  1.000  3  2.000  1 -4.000  2 -1.000
2161  FOR UO2(CO3)3-5 FROM [NEA92]
UO2CO335    500    -5.000    17.000     0.000     0.000     0.000     0.
   -0.148     0.000 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.0
 15  3.000 25  1.000  3  2.000  1 -4.000  2 -1.000
2190 FOR UO2+2 FROM [NEA92]
UO2+2       400     2.000     6.000     0.000     0.000     0.000     0.
   -9.038     0.000 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.0
 25  1.000  3  2.000  1 -4.000  2 -2.000
2191  FOR UO2(OH)3- FROM [NEA92]
UO2(OH)3    400    -1.000     6.000     0.000     0.000     0.000     0.
  -28.239     0.000 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.0
 25  1.000  3  5.000  1 -7.000  2 -2.000
2192  FOR UO2(OH)4-2 FROM [NEA92]
UO2(OH)4    400    -2.000     6.000     0.000     0.000     0.000     0.
  -42.039     0.000 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.0
 25  1.000  3  6.000  1 -8.000  2 -2.000
2193  FOR (UO2)2OH+3 FROM [NEA92]
(UO2)2OH    400     3.000    12.000     0.000     0.000     0.000     0.
  -20.777     0.000 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.0
 25  2.000  3  5.000  1 -9.000  2 -4.000
2194  FOR (UO2)2(OH)2+2 FROM [NEA92]
(UO2)2(O    400     2.000    12.000     0.000     0.000     0.000     0.
  -23.697     0.000 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.0
 25  2.000  3  6.000  1-10.000  2 -4.000
2195  FOR (UO2)3(OH)4+2 FROM [NEA92]
(UO2)3(O    400     2.000    18.000     0.000     0.000     0.000     0.
  -39.015     0.000 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.0
 25  3.000  3 10.000  1-16.000  2 -6.000
2196  FOR (UO2)3(OH)5+ FROM [NEA92]
(UO2)3(O    400     1.000    18.000     0.000     0.000     0.000     0.
  -42.665     0.000 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.0
 25  3.000  3 11.000  1-17.000  2 -6.000
2197  FOR (UO2)3(OH)7- FROM [NEA92]
(UO2)3(O    400    -1.000    18.000     0.000     0.000     0.000     0.
  -58.115     0.000 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.0
 25  3.000  3 13.000  1-19.000  2 -6.000
2198  FOR (UO2)4(OH)7+ FROM [NEA92]
(UO2)4(O    400     1.000    24.000     0.000     0.000     0.000     0.
  -58.053     0.000 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.0
 25  4.000  3 15.000  1-23.000  2 -8.000
2199  FOR UO2F+ FROM [NEA92]
UO2F+       500     1.000     6.000     0.000     0.000     0.000     0.
   -3.948     0.000 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.0
 20  1.000 25  1.000  3  2.000  1 -4.000  2 -2.000
2200  FOR UO2F2(aq) FROM [NEA92]
UO2F2(AQ    500     0.000     6.000     0.000     0.000     0.000     0.
   -0.418     0.000 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.0
 20  2.000 25  1.000  3  2.000  1 -4.000  2 -2.000
2201  FOR UO2F3- FROM [NEA92]
UO2F3-      500    -1.000     6.000     0.000     0.000     0.000     0.
    1.862     0.000 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.0
 20  3.000 25  1.000  3  2.000  1 -4.000  2 -2.000
2202  FOR UO2F4-2 FROM [NEA92]
UO2F4-2     500    -2.000     6.000     0.000     0.000     0.000     0.
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     2.662      0.000 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.0
 20  4.000 25  1.000  3  2.000  1 -4.000  2 -2.000
2203  FOR UO2Cl+ FROM [NEA92]
UO2CL+       500      1.000      6.000      0.000      0.000      0.000      0.
    -8.868      0.000 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.0
 14  1.000 25  1.000  3  2.000  1 -4.000  2 -2.000
2204  FOR UO2Cl2(aq) FROM [NEA92]
UO2CL2(A     500      0.000      6.000      0.000      0.000      0.000      0.
   -10.138      0.000 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.0
 14  2.000 25  1.000  3  2.000  1 -4.000  2 -2.000
2205  FOR UO2ClO3+ FROM [NEA92]
UO2CLO3+     500      1.000     12.000      0.000      0.000      0.000      0.
  -154.781      0.000 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.0
 14  1.000 25  1.000  3  5.000  1-10.000  2 -8.000
2206  FOR UO2Br+ FROM [NEA92]
UO2BR+       500      1.000      6.000      0.000      0.000      0.000      0.
    -8.818      0.000
 22  1.000 25  1.000  3  2.000  1 -4.000  2 -2.000
2207  FOR UO2BrO3+ FROM [NEA92]
UO2BRO3+     500      1.000     12.000      0.000      0.000      0.000      0.
  -154.582      0.000
 22  1.000 25  1.000  3  5.000  1-10.000  2 -8.000
2208  FOR UO2IO3+ FROM [NEA92]
UO2IO3+      500      1.000     11.000      0.000      0.000      0.000      0.
  -118.604      0.000
 23  1.000 25  1.000  3  5.000  1-10.000  2 -8.000
2209  FOR UO2(IO3)2(aq) FROM [NEA92]
UO2(IO3)     500      0.000     16.000      0.000      0.000      0.000      0.
  -228.581      0.000
 23  2.000 25  1.000  3  8.000  1-16.000  2-14.000
2210  FOR UO2SO3(aq) FROM [NEA92]
UO2SO3(A     400      0.000     10.000      0.000      0.000      0.000      0.
    -5.835      0.000 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.0
 16  1.000 25  1.000  3  1.000  1 -2.000
2211  FOR UO2S2O3(aq) FROM [NEA92]
UO2S2O3(     500      0.000     10.000      0.000      0.000      0.000      0.
    31.776      0.000 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.0
 16  2.000 25  1.000  3 -3.000  1  6.000  2  6.000
2212  FOR UO2SO4(aq) FROM [NEA92]
UO2SO4(A     500      0.000     12.000      0.000      0.000      0.000      0.
    -5.888      0.000 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.0
 16  1.000 25  1.000  3  2.000  1 -4.000  2 -2.000
2213  FOR UO2(SO4)2-2 FROM [NEA92]
UO2(SO4)     500     -2.000     18.000      0.000      0.000      0.000      0.
    -4.898      0.000 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.0
 16  2.000 25  1.000  3  2.000  1 -4.000  2 -2.000
2214  FOR UO2NO3+ FROM [NEA92]
UO2NO3+      500      1.000     11.000      0.000      0.000      0.000      0.
    -8.738      0.000
 17  1.000 25  1.000  3  2.000  1 -4.000  2 -2.000
2215  FOR UO2PO4- FROM [NEA92]
UO2PO4-      500     -1.000      6.000      0.000      0.000      0.000      0.
     4.192      0.000
 19  1.000 25  1.000  3  2.000  1 -4.000  2 -2.000
2216  FOR UO2HPO4(aq) FROM [NEA92]
UO2HPO4(     500      0.000      6.000      0.000      0.000      0.000      0.
    10.552      0.000
 19  1.000 25  1.000  3  2.000  1 -3.000  2 -2.000
2217  FOR UO2H2PO4+ FROM [NEA92]
UO2H2PO4     500      1.000      6.000      0.000      0.000      0.000      0.
    13.784      0.000
 19  1.000 25  1.000  3  2.000  1 -2.000  2 -2.000
2218  FOR UO2H3PO4+2 FROM [NEA92]
UO2H3PO4     500      2.000      6.000      0.000      0.000      0.000      0.
    13.424      0.000
 19  1.000 25  1.000  3  2.000  1 -1.000  2 -2.000
2219  FOR UO2(H2PO4)2(aq) FROM [NEA92]
UO2(H2PO     400      0.000      6.000      0.000      0.000      0.000      0.
    35.007      0.000
 19  2.000 25  1.000  3  2.000  2 -2.000
2220  FOR UO2(H2PO4)(H3PO FROM [NEA92]
UO2(H2PO     500      1.000      6.000      0.000      0.000      0.000      0.
    36.017      0.000
 19  2.000 25  1.000  3  2.000  1  1.000  2 -2.000
2221  FOR UO2CO3(aq) FROM [NEA95]
UO2CO3(A     500      0.000     10.000      0.000      0.000      0.000      0.
     0.632      0.000 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.0
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 15  1.000 25  1.000  3  2.000  1 -4.000  2 -2.000
2222  FOR UO2(CO3)2-2 FROM [NEA92]
UO2CO32-     500    -2.000     14.000      0.000      0.000      0.000      0.
     7.902      0.000 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.0
 15  2.000 25  1.000  3  2.000  1 -4.000  2 -2.000
2223  FOR UO2(CO3)3-4 FROM [NEA92]
UO2CO33-     500    -4.000     18.000      0.000      0.000      0.000      0.
    12.563      0.000 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.0
 15  3.000 25  1.000  3  2.000  1 -4.000  2 -2.000
2224  FOR (UO2)3(CO3)6-6  FROM [NEA92]
(UO2)3(C     500    -6.000     42.000      0.000      0.000      0.000      0.
    26.888      0.000 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.0
 15  6.000 25  3.000  3  6.000  1-12.000  2 -6.000
2225  FOR (UO2)2CO3(OH)3- FROM [NEA92]
(UO2)2CO     500    -1.000     16.000      0.000      0.000      0.000      0.
   -18.934      0.000
 15  1.000 25  2.000  3  7.000  1-11.000  2 -4.000
2226  FOR (UO2)3O(OH)2(HC FROM [NEA92]
(UO2)3O(     500     1.000     22.000      0.000      0.000      0.000      0.
   -26.462      0.000
 15  1.000 25  3.000  3  9.000  1-15.000  2 -6.000
2227  FOR (UO2)11(CO3)6(OH)12-2 FROM [NEA92]
(UO2)11(     500    -2.000     90.000      0.000      0.000      0.000      0.
   -62.991      0.000
 15  6.000 25 11.000  3 34.000  1-56.000  2-22.000
2228  FOR UO2OH+           FROM [NEA92]
UO2OH+       400     1.000      6.000      0.000      0.000      0.000      0.
   -14.238    187.033 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.0
 25  1.000  3  3.000  1 -5.000  2 -2.000
2229  FOR UO2(OH)2(aq)     FROM [NEA92]
UO2(OH)2     400     0.000      6.000      0.000      0.000      0.000      0.
   -19.339      0.000 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.0
 25  1.000  3  4.000  1 -6.000  2 -2.000
2240  FOR UO2N3+ FROM [NEA92]
UO2N3+       500     1.000      5.000      0.000      0.000      0.000      0.
   248.221      0.000
 17  3.000 25  1.000  3 -7.000  1 14.000  2 14.000
2241  FOR UO2(N3)2(aq) FROM [NEA92]
UO2(N3)2     500     0.000      4.000      0.000      0.000      0.000      0.
   504.650      0.000
 17  6.000 25  1.000  3-16.000  1 32.000  2 30.000
2242  FOR UO2(N3)3- FROM [NEA92]
UO2(N3)3     500    -1.000      3.000      0.000      0.000      0.000      0.
   760.740      0.000
 17  9.000 25  1.000  3-25.000  1 50.000  2 46.000
2243  FOR UO2(N3)4-2 FROM [NEA92]
UO2(N3)4     500    -2.000      2.000      0.000      0.000      0.000      0.
  1014.599      0.000
 17 12.000 25  1.000  3-34.000  1 68.000  2 62.000
2244  FOR (UO2)2(PUO2)(CO3)6-6 FROM [NEA95]
U-PUO2(C     600    -6.000     30.000      0.000      0.000      0.000      0.
   -0.304      0.000
 29  1.000 25  2.000 15  6.000  3  6.000  2 -6.000  1 -12.00
2300 FOR NP+3 FROM [CROSS87]
NP+3         200     3.000      3.0        0.0        0.0        0.0        0.
     3.03       0.0
 40  1.000  2  1.000
2301FOR NPOH+2 FROM [CROSS87]
NPOH+2       400     2.000      3.0        0.0        0.0        0.0        0.
    -4.37       0.0
 40  1.000  3  1.000  1 -1.000  2  1.000
2302FOR NP(OH)2+ FROM [CROSS87]
NP(OH)2+     400     1.000      3.0        0.0        0.0        0.0        0.
   -13.97       0.0
 40  1.000  1 -2.000  2  1.000  3  2.000
2303FOR NP(OH)3 FROM [CROSS87]
NP(OH)3      400     0.000      3.0        0.0        0.0        0.0        0.
   -23.97       0.0
 40  1.000  1 -3.000  2  1.000  3  3.000
2304FOR NP(OH)4- FROM [CROSS87]
NP(OH)4-     400    -1.000      3.0        0.0        0.0        0.0        0.
   -34.97       0.0
 40  1.000  1 -4.000  2  1.000  3  4.000
2305FOR NP2(OH)2+4 FROM [CROSS87]
NP2(OH)2     400     4.000      6.0        0.0        0.0        0.0        0.
    -7.43       0.0
 40  2.000  1 -2.000  2  2.000  3  2.000
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2306FOR NPCO3+ FROM [CROSS87]
NPCO3+       300      1.000      7.0        0.0        0.0        0.0        0.
      9.53       0.0
 40  1.000  2  1.000 15  1.000
2307FOR NP(CO3)2- FROM [CROSS87]
NP(CO3)2     300     -1.000     11.0        0.0        0.0        0.0        0.
     14.03       0.0
 40  1.000  2  1.000 15  2.000
2308FOR NP(CO3)3-3 FROM [CROSS87]
NP(CO3)3     300     -3.000     15.0        0.0        0.0        0.0        0.
     17.53       0.0
 40  1.000  2  1.000 15  3.000
2309FOR NPCL+2 FROM [CROSS87]
NPCL+2       300      2.000      3.0        0.0        0.0        0.0        0.
      0.63       0.0
 40  1.000  2  1.000 14  1.000
2310FOR NPCL2+ FROM [CROSS87]
NPCL2+       300      1.000      3.0        0.0        0.0        0.0        0.
     -2.35       0.0
 40  1.000  2  1.000 14  2.000
2330 FOR NP(OH)4 FROM [RAI 85]
NP(OH)4      300      0.000      4.0        0.0        0.0        0.0        4.
   -10.01
 40  1.000  3  4.000  1 -4.000
2331 FOR NPOH+3 FROM [RAI99B]
NPOH+3       300      3.000      4.0        0.0        0.0        0.0        4.
     -0.50
 40  1.000  3  1.000  1 -1.000
2332 FOR NPSO4+2 FROM [XIA 99]
NPSO4+2      200      2.000     10.0        0.0        0.0        0.0        6.
      9.00       0.0
 40  1.000 16  1.000
2333 FOR NP(SO4)2(AQ) FROM [XIA 99]
NPSO42AQ     200      0.000     16.0        0.0        0.0        0.0        6.
     11.70       0.0
 40  1.000 16  2.000
2334 FOR NP(OH)2(CO3)2-2 FROM [RAI 99D]
NPOH2CO3     400     -2.000     12.0        0.0        0.0        0.0        0.
     14.75       0.0
 40  1.000 15  2.000  3  2.000  1 -2.000
2335 FOR NP(CO3)5-6 FROM [RAI 99D]
NPCO35-6     200     -6.000     24.0        0.0        0.0        0.0        0.
     33.370      0.0
 40  1.000 15  5.000
2336FOR NPCL+3 FROM [SHIB98B]
NPCL+3       200      3.000      4.0        0.0        0.0        0.0        0.
      1.80       0.0
 40  1.000 14  1.000
2337FOR NPCL2+2 FROM [SHIB98B]
NPCL2+2      200      2.000      4.0        0.0        0.0        0.0        0.
      2.11       0.0
 40  1.000 14  2.000
2338FOR NPF+3 FROM [CROSS87]
NPF+3        200      3.000      4.0        0.0        0.0        0.0        0.
      8.33       0.0
 40  1.000 20  1.000
2339FOR NPF2+2 FROM [CROSS87]
NPF2+2       200      2.000      4.0        0.0        0.0        0.0        0.
     14.59       0.0
 40  1.000 20  2.000
2340FOR NPF3+1 FROM [CROSS87]
NPF3+        200      1.000      4.0        0.0        0.0        0.0        0.
     20.3        0.0
 40  1.000 20  3.000
2341FOR NPF4(AQ) FROM [CROSS87]
NPF4(AQ)     200      0.000      4.0        0.0        0.0        0.0        0.
     25.1        0.0
 40  1.000 20  4.000
2360 FOR NPO2+ FROM [FUGER76]
NPO2+        400      1.000      5.0        0.0        0.0        0.0        0.
    -10.89       0.00
 40  1.000  3  2.000  1 -4.000  2 -1.000
2361FOR NPO2OH FROM [SHIB98B]
NPO2OH       400      0.000      5.0        0.0        0.0        0.0        1.
    -21.58       0.0
 40  1.000  1 -5.000  2 -1.000  3  3.000
2362FOR NPO2(OH)2- FROM [SHIB98B]
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NPO2OH2-    400    -1.000     5.0       0.0       0.0       0.0       2.
   -33.50       0.0
 40  1.000  1 -6.000  2 -1.000  3  4.000
2363FOR NPO2CL(AQ) FROM [NECK95]
NPO2CL      500     0.000     5.0       0.0       0.0       0.0       0.
   -11.18       0.0
 40  1.000  1 -4.000  2 -1.000  3  2.000 14  1.000
2364FOR NPO2SO4- FROM [FUGER92]
NPO2SO4-    500    -1.000    11.0       0.0       0.0       0.0       0.
   -10.29       0.0
 40  1.000  1 -4.000  2 -1.000  3  2.000 16  1.000
2365FOR NPO2F(AQ) FROM [CROSS87]
NPO2F(A     500     0.000     5.0       0.0       0.0       0.0       0.
   -10.38       0.0
 40  1.000  3  2.000  1 -4.000  2 -1.000 20  1.000
2366FOR NPO2CO3- FROM [SHIB98B]
NPO2CO3-    500    -1.000     9.0       0.0       0.0       0.0       0.
    -6.10       0.0
 40  1.000  1 -4.000  2 -1.000  3  2.000 15  1.000
2367FOR NPO2(CO3)2-3 FROM [SHIB98B]
NPO2CO32    500    -3.000    13.0       0.0       0.0       0.0       0.
    -4.24       0.0
 40  1.000  1 -4.000  2 -1.000  3  2.000 15  2.000
2368FOR NPO2(CO3)3-5 FROM [SHIB98B]
NPO2CO33    500    -5.000    17.0       0.0       0.0       0.0       0.
    -5.38       0.0
 40  1.000  1 -4.000  2 -1.000  3  2.000 15  3.000
2390 FOR NPO2+2 FROM [CROSS87]
NPO2+2      400     2.000     6.0       0.0       0.0       0.0       0.
   -32.29       0.0
 40  1.000  1 -4.000  2 -2.000  3  2.000
2391FOR NPO2OH+ FROM [CROSS87]
NPO2OH      400     1.000     6.0       0.0       0.0       0.0       0.
   -37.39       0.0
 40  1.000  1 -5.000  2 -2.000  3  3.000
2392FOR NPO2(OH)2(AQ) FROM [CROSS87]
NPO2OH2     400     0.000     6.0       0.0       0.0       0.0       0.
   -43.81       0.0
 40  1.000  1 -6.000  2 -2.000  3  4.000
2393FOR NPO2(OH)3- FROM [CROSS87]
NPO2OH3-    400    -1.000     6.0       0.0       0.0       0.0       0.
   -53.99       0.0
 40  1.000  1 -7.000  2 -2.000  3  5.000
2394FOR (NPO)2(OH)2+2 FROM [CROSS87]
NPO22OH2    400     2.000    12.0       0.0       0.0       0.0       0.
   -70.98       0.0
 40  2.000  1-10.000  2 -4.000  3  6.000
2395FOR (NPO2)3(OH)5+ FROM [CROSS87]
NPO23OH5    400     1.000    18.0       0.0       0.0       0.0       0.
  -114.37       0.0
 40  3.000  1-17.000  2 -6.000  3 11.000
2396FOR (NPO2)2OH+3 FROM [CROSS87]
NPO22OH+    400     3.000    12.0       0.0       0.0       0.0       0.
   -68.58       0.0
 40  2.000  1 -9.000  2 -4.000  3  5.000
2397FOR NPO2SO4 FROM [CROSS87]
NPO2SO4     500     0.000    12.0       0.0       0.0       0.0       0.
   -29.02       0.0
 40  1.000  1 -4.000  2 -2.000  3  2.000 16  1.000
2398FOR NPO2(SO4)2-2 FROM [CROSS87]
NPO2SO42    500    -2.000    18.0       0.0       0.0       0.0       0.
   -28.19       0.0
 40  1.000  1 -4.000  2 -2.000  3  2.000 16  2.000
2399FOR NPO2(SO4)3-4 FROM [CROSS87]
NPO2SO43    500    -4.000    24.0       0.0       0.0       0.0       0.
   -27.29       0.0
 40  1.000  1 -4.000  2 -2.000  3  2.000 16  3.000
2400FOR NPO2CL+ FROM [CROSS87]
NPO2CL+     500     1.000     6.0       0.0       0.0       0.0       0.
   -32.59       0.0
 40  1.000  1 -4.000  2 -2.000  3  2.000 14  1.000
2401FOR NPO2CL2 FROM [CROSS87]
NPO2CL2     500     0.000     6.0       0.0       0.0       0.0       0.
   -31.29       0.0
 40  1.000  1 -4.000  2 -2.000  3  2.000 14  2.000
2500 FOR PU+3 FROM [FUGER76]
PU+3        200     3.000     3.000     0.000     0.000     0.000     0.
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    17.01       0.000 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.0
 29  1.000  2  1.000
2501 FOR PUOH+2 FROM [YUI99]
PUOH+2       400      2.000      3.000      0.000      0.000      0.000      0.
    10.61       0.0
 29  1.000  1 -1.000  2  1.000  3  1.000
2502 FOR PUOH2+ FROM [YUI99]
PUOH2+       400      1.000      3.000      0.000      0.000      0.000      0.
     2.910      0.0
 29  1.000  1 -2.000  2  1.000  3  2.000
2503 FOR PU(OH)3 FROM [YUI99]
PU(OH)3      400      0.000      3.000      0.000      0.000      0.000      0.
    -8.69       0.0
 29  1.000  1 -3.000  2  1.000  3  3.000
2504 FOR PUCO3+ FROM [YUI99]
PUCO3+       300      1.000      7.0        0.0        0.0        0.0        0.
    24.81       0.0
 29  1.000  2  1.000 15  1.000
2505 FOR PU(CO3)2- FROM [YUI99]
PUCO32-      300     -1.000     11.0        0.0        0.0        0.0        0.
    29.31       0.0
 29  1.000  2  1.000 15  2.000
2506 FOR PU(CO3)3-3 FROM [YUI99]
PUCO33-3     300     -3.000     15.0        0.0        0.0        0.0        0.
    32.21       0.0
 29  1.000  2  1.000 15  3.000
2507 FOR PUF+2 FROM [YUI99]
PUF+2        300      2.000      3.0        0.0        0.0        0.0        0.
    20.41       0.0
 29  1.000 20  1.000  2  1.000
2508 FOR PUF2+ FROM [YUI99]
PUF2+        300      1.000      3.0        0.0        0.0        0.0        0.
    22.81       0.0
 29  1.000 20  2.000  2  1.000
2509 FOR PUCL+2 FROM [YUI99]
PUCL+2       300      2.000      3.0        0.0        0.0        0.0        0.
    18.06       0.0
 29  1.000  2  1.000 14  1.000
2510 FOR PUSO4+ FROM [YUI99]
PUSO4+       300      1.000      9.0        0.0        0.0        0.0        0.
    20.86       0.0
 29  1.000  2  1.000 16  1.000
2511 FOR PU(SO4)2- FROM [YUI99]
PUSO42-      300     -1.000     15.0        0.0        0.0        0.0        0.
    22.41       0.0
 29  1.000  2  1.000 16  2.000
2512 FOR PUF3(AQ) FROM [YUI99]
PUF3         300      0.000      3.0        0.0        0.0        0.0        0.
    28.21       0.0
 29  1.000 20  3.000  2  1.000
2530 FOR PU(OH)4 FROM [YAMA94]
PU(OH)4      300      0.000      4.0        0.0        0.0        0.0        4.
    -9.16       0.00
 29  1.000  3  4.000  1 -4.000
2531 FOR PUOH+3 FROM [RAI99B]
PUOH+3       300      3.000      4.0        0.0        0.0        0.0        4.
    -0.500
 29  1.000  3  1.000  1 -1.000
2532 FOR PUSO4+2 FROM [RAI99B]
PUSO4+2      200      2.000     10.0        0.0        0.0        0.0        6.
     9.00       0.0
 29  1.000 16  1.000
2533 FOR PU(SO4)2(AQ) FROM [RAI99B]
PUSO42AQ     200      0.000     16.0        0.0        0.0        0.0        6.
    11.70       0.0
 29  1.000 16  2.000
2534 FOR PU(OH)2(CO3)2-2 FROM [RAI99C]
PUOH2CO3     400     -2.000     12.0        0.0        0.0        0.0        0.
    16.76       0.0
 29  1.000 15  2.000  3  2.000  1 -2.000
2535 FOR PU(CO3)5-6 FROM [RAI99C]
PUCO35-6     200     -6.000     24.0        0.0        0.0        0.0        0.
    34.18       0.0
 29  1.000 15  5.000
2536FOR PUCL+3 FROM [FUGER92]
PUCL+3       200      3.000      4.0        0.0        0.0        0.0        0.
     2.00       0.0
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 29  1.000 14  1.000
2537FOR PUNO3+3 FROM [FUGER92]
PUNO3+3      200      3.000      9.0        0.0        0.0        0.0        0.
     2.60       0.0
 29  1.000 17  1.000
2538FOR PUF+3 FROM [NEA 92]
PUF+3        200      3.000      4.0        0.0        0.0        0.0        0.
     9.28       0.0
 29  1.000 20  1.000
2539FOR PUF2+2 FROM [NEA 92]
PUF2+2       200      2.000      4.0        0.0        0.0        0.0        0.
    16.23       0.0
 29  1.000 20  2.000
2540FOR PUF3+ FROM [NEA 92]
PUF3+        200      1.000      4.0        0.0        0.0        0.0        0.
    21.6        0.0
 29  1.000 20  3.000
2541FOR PUF4 FROM [NEA 92]
PUF4         200      0.000      4.0        0.0        0.0        0.0        0.
    25.60       0.0
 29  1.000 20  4.000
2542FOR PUF5- FROM [NEA 92]
PUF5-        200     -1.000      4.0        0.0        0.0        0.0        0.
    27.01       0.0
 29  1.000 20  5.000
2543FOR PUF6-2 FROM [NEA 92]
PUF6-2       200     -2.000      4.0        0.0        0.0        0.0        0.
    29.08       0.0
 29  1.000 20  6.000
2560FOR PUO2+ FROM [RAI 84]
PUO2+        400      1.000      5.000      0.000      0.000      0.000      0.
   -18.600      0.000 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.0
 29  1.000  3  2.000  1 -4.000  2 -1.000
2561FOR PUO2OH(AQ) FROM [BENNE92]
PUO2OH       400      0.000      5.000      0.000      0.000      0.000      0.
   -28.33       0.0
 29  1.000  1 -5.000  2 -1.000  3  3.000
2562FOR PUO2CO3- FROM [BENNE92]
PUO2CO3-     500     -1.000      9.0        0.0        0.0        0.0        0.
   -13.48       0.0
 29  1.000  1 -4.000  2 -1.000  3  2.000 15  1.000
2590FOR PUO2+2 FROM [RAI 84]
PUO2+2       400      2.000      6.000      0.000      0.000      0.000      0.
   -34.760      0.000 0.00000E+00 0.00000E+00 0.00000E+00 0.00000E+00 0.0
 29  1.000  3  2.000  1 -4.000  2 -2.000
2591FOR PUO2OH+ FROM [SHIB98C]
PUO2OH+      400      1.000      6.000      0.000      0.000      0.000      0.
   -40.03       0.0
 29  1.000  1 -5.000  2 -2.000  3  3.000
2592FOR PUO2OH2 FROM [SHIB98C]
PUO2OH2      400      0.000      6.000      0.000      0.000      0.000      0.
   -47.22       0.0
 29  1.000  1 -6.000  2 -2.000  3  4.000
2593FOR PUO2OH3- FROM [SHIB98C]
PUO2OH3-     400     -1.000      6.000      0.000      0.000      0.000      0.
   -59.22       0.0
 29  1.000  1 -7.000  2 -2.000  3  5.000
2594FOR (PUO2)2(OH)2+2 FROM [NEA 92]
PUO22OH2     400      2.000     12.0        0.0        0.0        0.0        0.
   -75.14       0.0
 29  2.000  1-10.000  2 -4.000  3  6.000
2595FOR PUO2CO3 FROM FROM [PASHA97]
PUO2CO3      500      0.000     10.0        0.0        0.0        0.0        0.
   -25.2        0.0
 29  1.000  1 -4.000  2 -2.000  3  2.000 15  1.000
2596FOR PUO2(CO3)2-2 FROM [PASHA97]
PUO2CO32     500     -2.000     14.0        0.0        0.0        0.0        0.
   -19.76       0.0
 29  1.000  1 -4.000  2 -2.000  3  2.000 15  2.000
2597FOR PUO2(CO3)3-4 FROM [PASHA97]
PUO2CO33     500     -4.000     18.0        0.0        0.0        0.0        0.
   -17.23       0.0
 29  1.000  1 -4.000  2 -2.000  3  2.000 15  3.000
2598FOR (PUO2)2(OH)3CO3- FROM [ALLAR83]
PUO22OH3     500     -1.000     16.0        0.0        0.0        0.0        0.
   -70.52       0.0
 29  2.000  1-11.000  2 -4.000  3  7.000 15  1.000
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2599FOR (PUO2)3(OH)3CO3+ FROM [ALLAR83]
PUO23OH3     500      1.000     22.0        0.0        0.0        0.0        0.
  -103.28       0.0
 29  3.000  1-15.000  2 -6.000  3  9.000 15  1.000
2600FOR PUO2SO4(AQ) FROM [SHIB98C]
PUO2SO4A     500      0.000     12.0        0.0        0.0        0.0        0.
   -31.61       0.0
 29  1.000  2 -2.000 16  1.000  3  2.000  1 -4.000
2601FOR PUO2(SO4)2-2 FROM [SHIB98C]
PUO2SO42     500     -2.000     18.0        0.0        0.0        0.0        0.
   -30.62       0.0
 29  1.000  2 -2.000 16  2.000  3  2.000  1 -4.000
2602FOR PUO2HPO4(AQ) FROM [SHIB98C]
PUO2HPO4     500      0.000      6.0        0.0        0.0        0.0        0.
   -15.17       0.0
 29  1.000  1 -3.000 19  1.000  2 -2.000  3  2.000
2603FOR PUO2H2PO4+1 FROM [SHIB98C]
PUO2H2PO     500      1.000      6.0        0.0        0.0        0.0        0.
   -11.94       0.0
 29  1.000  1 -2.000 19  1.000  2 -2.000  3  2.000
2604FOR PUO2NO3+ FROM [SHIB98C][CHOPI99]
PUO2NO3+     500      1.000     11.0        0.0        0.0        0.0        0.
   -34.46       0.0
 29  1.000 17  1.000  2 -2.000  1 -4.000  3  2.000
2605FOR PUO2F+ FROM [FUGER92]
PUO2F+       500      1.000      6.0        0.0        0.0        0.0        0.
   -30.19       0.0
 29  1.000  3  2.000  2 -2.000  1 -4.000 20  1.000
2606FOR PUO2F2(AQ) FROM [FUGER92]
PUO2F2AQ     500      0.000      6.0        0.0        0.0        0.0        0.
   -26.52       0.0
 29  1.000  3  2.000  2 -2.000  1 -4.000 20  2.000
2607FOR PUO2F3- FROM [FUGER92]
PUO2F3-      500     -1.000      6.0        0.0        0.0        0.0        0.
   -24.96       0.0
 29  1.000  3  2.000  2 -2.000  1 -4.000 20  3.000
2608 FOR (PUO2)3(OH)5+ FROM [NEA 92]
PUO23OH5     400      1.000     18.0        0.0        0.0        0.0        0.
  -119.83       0.0
 29  3.000  1-17.000  2 -6.000  3 11.000
2609 FOR PUO2CL+ FROM [FUGER92]
PUO2CL+      500      1.000      6.0        0.0        0.0        0.0        0.
   -34.66       0.0
 29  1.000  3  2.000  2 -2.000  1 -4.000 14  1.000
2700 FOR AMOH+2 FROM [NEA95]
AMOH+2       300      2.000      3.000      0.000      0.000      0.000      0.
    -6.4        0.0
 28  1.000  3  1.000  1 -1.000
2701 FOR AM(OH)2+ FROM [NEA95]
AM(OH)2+     300      1.000      3.000      0.000      0.000      0.000      0.
    -14.1       0.0
 28  1.000  3  2.000  1 -2.000
2702 FOR AM(OH)3  FROM [NEA95]
AM(OH)3      300      0.000      3.000      0.000      0.000      0.000      0.
    -25.7       0.0
 28  1.000  3  3.000  1 -3.000
2703 FOR AMCO3+ FROM [NEA95]
AMCO3+       200      1.000      7.0        0.0        0.0        0.0        0.
     7.80       0.0
 28  1.000 15  1.000
2704 FOR AM(CO3)2- FROM [NEA95]
AMCO32-      200     -1.000     11.0        0.0        0.0        0.0        0.
    12.30       0.0
 28  1.000 15  2.000
2705 FOR AM(CO3)3-3 FROM [NEA95]
AMCO33-3     200     -3.000     15.0        0.0        0.0        0.0        0.
    15.2        0.0
 28  1.000 15  3.000
2706 FOR AMF+2  FROM [NEA95]
AMF+2        200      2.000      3.000      0.000      0.000      0.000      0.
     3.4        0.0
 28  1.000 20  1.000
2707 FOR AMF2+  FROM [NEA95]
AMF2+        200      1.000      3.000      0.000      0.000      0.000      0.
     5.800      0.0
 28  1.000 20  2.000
2708 FOR AMNO3+2 FROM [NEA95]
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AMNO3+2     200     2.000     8.000     0.000     0.000     0.000     0.
    1.330       0.0
 28  1.000 17  1.000
2709FOR AMCL+2  FROM [NEA95]
AMCL+2      200     2.000     3.000     0.000     0.000     0.000     0.
    1.050       0.0
 28  1.000 14  1.000
2710FOR AMSO4+  FROM [NEA95]
AMSO4+      200     1.000     9.000     0.000     0.000     0.000     0.
    3.850       0.0
 28  1.000 16  1.000
2711FOR AM(SO4)2-  FROM [NEA95]
AM(SO4)2    200    -1.000    15.000     0.000     0.000     0.000     0.
    5.400       0.0
 28  1.000 16  2.000
2712FOR AMH2PO4+2  FROM [NEA95]
AMH2PO4+    300     2.000     3.000     0.000     0.000     0.000     0.
   22.562       0.0
 28  1.000 19  1.000  1  2.000
2900 FOR CMOH+2 FROM [YUI99]
CMOH+2      300     2.000     3.000     0.000     0.000     0.000     0.
   -6.4         0.0
 50  1.000  3  1.000  1 -1.000
2901 FOR CM(OH)2+ FROM [YUI99]
CM(OH)2+    300     1.000     3.000     0.000     0.000     0.000     0.
  -14.1         0.0
 50  1.000  3  2.000  1 -2.000
2902 FOR CM(OH)3  FROM [YUI99]
CM(OH)3     300     0.000     3.000     0.000     0.000     0.000     0.
  -25.7         0.0
 50  1.000  3  3.000  1 -3.000
2903 FOR CMCO3+ FROM [YUI99]
CMCO3+      200     1.000     7.0       0.0       0.0       0.0       0.
    7.80        0.0
 50  1.000 15  1.000
2904 FOR CM(CO3)2- FROM [YUI99]
CMCO32-     200    -1.000    11.0       0.0       0.0       0.0       0.
   12.30        0.0
 50  1.000 15  2.000
2905 FOR CM(CO3)3-3 FROM [YUI99]
CMCO33-3    200    -3.000    15.0       0.0       0.0       0.0       0.
   15.2         0.0
 50  1.000 15  3.000
2906 FOR CMF+2  FROM [YUI99]
CMF+2       200     2.000     3.000     0.000     0.000     0.000     0.
    3.4         0.0
 50  1.000 20  1.000
2907 FOR CMF2+  FROM [YUI99]
CMF2+       200     1.000     3.000     0.000     0.000     0.000     0.
    5.800       0.0
 50  1.000 20  2.000
2908 FOR CMNO3+2 FROM [YUI99]
CMNO3+2     200     2.000     8.000     0.000     0.000     0.000     0.
    1.330       0.0
 50  1.000 17  1.000

LOOK MIN
CALCITE     2         4.00     -8.48      0.00      1              0.0000RIGINAL
  15      1.000   4      1.000
-0.17191E+03-0.77993E-01 0.28393E+04 0.71595E+02 0.00000E+00
ARAGONIT    2         4.00     -8.34      0.00      1              0.0000RIGINAL
  15      1.000   4      1.000
-0.17198E+03-0.77993E-01 0.29033E+04 0.71595E+02 0.00000E+00
DOLOMITE    3         8.00    -17.09      0.00      0              0.0000RIGINAL
   4      1.000   5      1.000  15      2.000
SIDERITE    2         6.00    -10.57      0.00      0              0.0000RIGINAL
   8      1.000  15      1.000
STRONTIT    2         4.00     -9.27      0.00      1              0.0000RIGINAL
  12      1.000  15      1.000
 0.15503E+03 0.00000E+00-0.72396E+04-0.56586E+02 0.00000E+00
GYPSUM      3         6.00     -4.60      0.00      1              0.0000RIGINAL
   4      1.000  16      1.000   3      2.000
 0.82090E+02 0.00000E+00-0.38539E+04-0.29812E+02 0.00000E+00
ANHYDRIT    2         6.00     -4.38      0.00      0              0.0000RIGINAL
   4      1.000  16      1.000
CELESTIT    2         6.00     -6.58      0.00      0              0.0000RIGINAL
  12      1.000  16      1.000
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BARITE     2          6.00      -9.98       0.00      0                0.0000RIGINAL
  11     1.000  16       1.000
HYDROXAP   4          0.00     -40.47       0.00      0                0.0000RIGINAL
   3     1.000  19       3.000   4           5.000  1      -1.000
VIVIANIT   3          6.00     -36.00       0.00      0                0.0000RIGINAL
   8     3.000  19       2.000   3           8.000
FLUORITE   2          0.00     -10.96       0.00      0                0.0000RIGINAL
   4     1.000  20       2.000
FEOH3A     3          3.00       4.89       0.00      0                0.0000RIGINAL
  69     1.000   3       3.000   1          -3.000
GIBBSITE   3          0.00       8.77       0.00      0                0.0000RIGINAL
  10     1.000   3       3.000   1          -3.000
KAOLINIT   4          0.00     -36.92       0.00      0                0.0000RIGINAL
   3    -7.000   1       2.000  13           2.000  84       2.000
FES PPT    5          0.00     -37.603      0.00      0                0.0000RIGINAL
   8     1.000  16       1.000   3          -4.000  1        8.000  2       8.000
BIRNESIT   4          4.00      18.09       0.00      0                0.000[NEA85]
  78     1.000   3       2.000   2          -1.000  1       -4.000
MANGANIT   3          3.00      -0.24       0.00      0                0.000[NEA85]
  78     1.000   3       2.000   1          -3.000
SIL GEL    2          0.00      -2.70       0.00      0                0.000[NEA85]
  13     1.000   3      -2.000
SIL GLAS   2          0.00      -3.02       0.00      0                0.000[NEA85]
  13     1.000   3      -1.000
SEP PPT    4          0.00     -37.21       0.00      0                0.000[NEA85]
   5     2.000  13       3.000  62           4.000  3       -4.500
MACKINIT   5          0.00     -38.323      0.00      0                0.000[NEA85]
   8     1.000  16       1.000   1          8.000  3       -4.000  2       8.000
MUSCOVIT   4          0.00      14.60       0.00      0                0.000[NEA85]
  10     3.000  13       3.000   7          1.000  1      -10.000
CLINOZOI   5          0.00      43.61       0.00      0                0.000[NEA85]
  10     3.000  13       3.000   4          2.000  3        1.000  1      -13.
EPIDOTE,   7          3.00      45.43       0.00      0                0.000[NEA85]
  10     2.000  13       3.000   4          2.000  8        1.000  3        1.
   1   -13.000   2      -1.000
TREMOLIT   5          0.00      57.70       0.00      0                0.000[NEA85]
   5     5.000  13       8.000   4          2.000  3       -8.000  1      -14.
ANDRADIT   5          6.00      55.10       0.00      0                0.000[NEA85]
  13     3.000   4       3.000   8          2.000  1      -12.000  2       -2.
MONTMOCA   5          0.00      41.88       0.00      0                0.000[NEA85]
  10    14.000  13      22.000   4          1.000  3      -16.000  1      -44.
ANORTHHE   4          0.00      26.70       0.00      0                0.000[NEA85]
  10     2.000  13       2.000   4          1.000  1       -8.000
ANORTHTR   4          0.00      26.37       0.00      0                0.000[NEA85]
  10     2.000  13       2.000   4          1.000  1       -8.000
LIME, QU   3          0.00      32.70       0.00      0                0.000[NEA85]
   4     1.000   3       1.000   1          -2.000
ILLITEK3   6          0.00      67.15       0.00      0                0.000[NEA85]
   5     1.000  10       9.000  13          14.000  7        3.000  3       -8.
   1   -32.000
PHLOGOPI   5          0.00      36.33       0.00      0                0.000[NEA85]
   5     3.000  10       1.000  13          3.000  7        1.000  1      -10.
CLINOC26   6         16.00     447.61       0.00      0                0.000[NEA85]
   5    26.000  10      20.000  13          24.000  8        8.000  3       48.
   1  -128.000
MG2SI206   4          0.00      23.26       0.00      0                0.000[NEA85]
   5     2.000  13       2.000   3          -2.000  1       -4.000
TALC       4          0.00      20.60       0.00      0                0.000[NEA85]
   5     3.000  13       4.000   3          -4.000  1       -6.000
CLINOC40   5          0.00     546.83       0.00      0                0.000[NEA85]
   5    40.000  10      16.000  13          24.000  3       48.000  1     -128.
SEPIOLIT   4          0.00      32.83       0.00      0                0.000[NEA85]
   5     4.000  13       6.000   3          -1.000  1       -8.000
CLINOCH8   7         53.00     178.37       0.00      0                0.000[NEA85]
   5     8.000  10      25.000  13          20.000  8       26.000  3       64.
   1  -144.000   2      -1.000
MONTMOMG   5          0.00      57.04       0.00      0                0.000[NEA85]
   5     1.000  10      14.000  13          22.000  3      -16.000  1      -44.
MAGNESIO   5          6.00      42.82       0.00      0                0.000[NEA85]
   5     1.000   8       2.000   3          4.000  1       -8.000  2       -2.
PERICLAS   3          0.00      21.58       0.00      0                0.000[NEA85]
   5     1.000   3       1.000   1          -2.000
MONTMONA   5          0.00      58.54       0.00      0                0.000[NEA85]
   6     2.000  10      14.000  13          22.000  3      -16.000  1      -44.
PARAGONI   4          0.00      18.87       0.00      0                0.000[NEA85]
   6     1.000  10       3.000  13          3.000  1      -10.000
ALBITE     5          0.00       3.54       0.00      0                0.000[NEA85]
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   6      1.000  10       1.000  13       3.000   3      -4.000   1       -4.
ILLITEK2   5          0.00       28.54       0.00   0                       0.000[NEA85]
  10     10.000  13      14.000   7       2.000   3      -8.000   1       -32.
MONTMOK    5          0.00       57.51       0.00   0                       0.000[NEA85]
  10     14.000  13      22.000   7       2.000   3     -16.000   1       -44.
ALUNITE    5         12.00        1.61       0.00   0                       0.000[NEA85]
  10      3.000  16       2.000   7       1.000   3       6.000   1        -6.
MICROCLI   5          0.00        1.78       0.00   0                       0.000[NEA85]
  10      1.000  13       3.000   7       1.000   3      -4.000   1        -4.
ORTHOCLA   5          0.00        0.86       0.00   0                       0.000[NEA85]
  10      1.000  13       3.000   7       1.000   3      -4.000   1        -4.
ANNITE     5          6.00       22.33       0.00   0                       0.000[NEA85]
  10      1.000  13       3.000   7       1.000   8       3.000   1       -10.
HEMATITE   4          6.00       22.40       0.00   0                       0.000[NEA85]
   8      2.000   3       3.000   1      -6.000   2      -2.000
FE2SI206   4          4.00       10.60       0.00   0                       0.000[NEA85]
  13      2.000   8       2.000   3      -2.000   1      -4.000
ALMANDIN   4          6.00       33.41       0.00   0                       0.000[NEA85]
  10      2.000  13       3.000   8       3.000   1     -12.000
MAGNETIT   4          8.00       30.65       0.00   0                       0.000[NEA85]
   8      3.000   3       4.000   1      -8.000   2      -2.000
PYRRHOTI   5          0.00     -321.28       0.00   0                       0.000[NEA85]
  16      8.000   8       7.000   3     -32.000   1      64.000   2        62.
LAWRENCI   2          2.00        6.82       0.00   0                       0.000[NEA85]
  14      2.000   8       1.000
MOLYSITE   3          3.00       24.56       0.00   0                       0.000[NEA85]
  14      3.000   8       1.000   2      -1.000
GOETHITE   4          3.00       11.29       0.00   0                       0.000[NEA85]
   8      1.000   3       2.000   1      -3.000   2      -1.000
PYRRHOTI   5          0.00      -39.78       0.00   0                       0.000[NEA85]
  16      1.000   8       1.000   3      -4.000   1       8.000   2         8.
PYRITE     5          0.00      -85.95       0.00   0                       0.000[NEA85]
  16      2.000   8       1.000   3      -8.000   1      16.000   2        14.
RHODOCHR   2          6.00      -10.54       0.00   0                       0.000[NEA85]
  15      1.000   9       1.000
PYROLUSI   4          4.00       41.55       0.00   0                       0.000[NEA85]
   9      1.000   3       2.000   1      -4.000   2      -2.000
ALABANDI   5          0.00      -34.11       0.00   0                       0.000[NEA85]
  16      1.000   9       1.000   3      -4.000   1       8.000   2         8.
TOPAZ, O   4          0.00       12.81       0.00   0                       0.000[NEA85]
  10      2.000  13       1.000   3       2.000   1      -6.000
CHALCEDO   2          0.00       -3.49       0.00   0                       0.000[NEA85]
  13      1.000   3      -2.000
QUARTZ     2          0.00       -3.78       0.00   0                       0.000[NEA85]
  13      1.000   3      -2.000
SILICA H   4         -1.00       -2.47       0.00   0                       0.000[NEA85]
  13      1.000   3      -2.000   1       1.000   2       1.000
COBALTOU   2          2.00        8.79       0.00   0                       0.000[NEA85]
  14      2.000  27       1.000
COBALTOU   3          2.00       13.44       0.00   0                       0.000[NEA85]
  27      1.000   3       1.000   1      -2.000
H2 GAS     1         -2.00       -3.15       0.00   0                       0.0000RIGINAL
  61      1.000
CH4 GAS    4         -4.00      -43.931      0.00   0                       0.000
  15      1.000   1      10.00    2       8.000   3      -3.000
FERROSIL   4          2.00        7.42       0.000  0                       0.000
   8      1.000  13       1.000   3      -1.000   1      -2.000
GREENALI   4          6.00       22.59       0.000  0                       0.000
   8      3.000  13       2.000   3       1.000   1      -6.000
FAYALITE   3          4.00       19.05       0.000  0                       0.000
   8      2.000  13       1.000   1      -4.000
SR3P042    2          0.00       -27.8       0.000  0                       0.000[CROSS87]
  12      3.000  19       2.000
SRHP04     3          0.00      -19.31       0.000  0                       0.000[CROSS87]
  12      1.000  19       1.000   1       1.000
SRN032     2         10.00        0.59       0.000  0                       0.000[CROSS87]
  12      1.000  17       2.000
SROH2      3          0.00       24.98       0.000  0                       0.000[CROSS87]
  12      1.000   3       2.000   1      -2.000
SRS04      2          6.00       -6.42       0.000  0                       0.000[CROSS87]
  12      1.000  16       1.000
SRC03      2          4.00       -9.25       0.000  0                       0.000[CROSS87]
  12      1.000  15       1.000
I2         2          0.00       18.18       0.000  0                       0.000[CROSS87]
  23      2.000   2      -2.000
K-FELDSP   5          0.00      0.0832       0.00   0                          [LLNL83]
  13      3.000   3      -4.000   1      -4.000   7       1.000  10        1.0
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SILI(AM)   2        0.00     -2.71      0.00     0              0.000[LLNL83]
  13     1.000   3     -2.000
H(G)       2       -1.00     35.61      0.00     0              0.000[NEA95]
   1     1.000   2      1.000
H2(G)      2       -2.00      0.00      0.00     0              0.000[NEA95]
   1     2.000   2      2.000
O(G)       3        2.00     82.15      0.00     0              0.000[NEA95]
   3     1.000   1     -2.000   2     -2.000
O2(G)      3        4.00     83.09      0.00     0              0.000[NEA95]
   3     2.000   1     -4.000   2     -4.000
H2O(G)     1        0.00      1.50      0.00     0              0.000[NEA95]
   3     1.000
CA(CR)     2       -2.00     96.85      0.00     0              0.000[NEA95]
   4     1.000   2      2.000
CA(G)      2       -2.00    122.08      0.00     0              0.000[NEA95]
   4     1.000   2      2.000
CAO(CR)    3        0.00     32.70      0.00     0              0.000[NEA95]
   4     1.000   3      1.000   1     -2.000
NA(CR)     2       -1.00     45.89      0.00     0              0.000[NEA95]
   6     1.000   2      1.000
NA(G)      2       -1.00     59.38      0.00     0              0.000[NEA95]
   6     1.000   2      1.000
K(CR)      2       -1.00     49.49      0.00     0              0.000[NEA95]
   7     1.000   2      1.000
K(G)       2       -1.00     60.09      0.00     0              0.000[NEA95]
   7     1.000   2      1.000
BA(CR)     2       -2.00     97.70      0.00     0              0.000[NEA95]
  11     1.000   2      2.000
BAO(CR)    3        0.00     48.07      0.00     0              0.000[NEA95]
  11     1.000   3      1.000   1     -2.000
SR(CR)     2       -2.00     98.79      0.00     0              0.000[NEA95]
  12     1.000   2      2.000
SRO(CR)    3        0.00     42.23      0.00     0              0.000[NEA95]
  12     1.000   3      1.000   1     -2.000
SI(CR)     4       -4.00     62.93      0.00     0              0.000[NEA95]
  13     1.000   3     -4.000   1      4.000   2      4.000
SI(G)      4       -4.00    133.97      0.00     0              0.000[NEA95]
  13     1.000   3     -4.000   1      4.000   2      4.000
SIO2(QUA   2        0.00     -4.00      0.00     0              0.000[NEA95]
  13     1.000   3     -2.000
CL(G)      2        1.00     41.44      0.00     0              0.000[NEA95]
  14     1.000   2     -1.000
CL2(G)     2        2.00     45.98      0.00     0              0.000[NEA95]
  14     2.000   2     -2.000
HCL(G)     2        0.00      6.29      0.00     0              0.000[NEA95]
  14     1.000   1      1.000
SRCL2(CR   2        0.00      7.24      0.00     0              0.000[NEA95]
  12     1.000  14      2.000
BACL2(CR   2        0.00      2.30      0.00     0              0.000[NEA95]
  11     1.000  14      2.000
C(CR)      4        0.00    -32.15      0.00     0              0.000[NEA95]
  15     1.000   3     -3.000   1      6.000   2      4.000
C(G)       4        0.00     85.45      0.00     0              0.000[NEA95]
  15     1.000   3     -3.000   1      6.000   2      4.000
CO(G)      4        2.00    -14.64      0.00     0              0.000[NEA95]
  15     1.000   3     -2.000   1      4.000   2      2.000
CO2(G)     3        4.00    -18.15      0.00     0              0.000[NEA95]
  15     1.000   3     -1.000   1      2.000
S(CR)      4        0.00    -35.84      0.00     0              0.000[NEA95]
  16     1.000   3     -4.000   1      8.000   2      6.000
S(G)       4        0.00      5.63      0.00     0              0.000[NEA95]
  16     1.000   3     -4.000   1      8.000   2      6.000
S2(G)      4        0.00    -57.71      0.00     0              0.000[NEA95]
  16     2.000   3     -8.000   1     16.000   2     12.000
SO2(G)     4        4.00   -478.35      0.00     0              0.000[NEA95]
  16     1.000   3     -2.000   1      4.000   2      2.000
H2S(G)     4       -2.00    -41.70      0.00     0              0.000[NEA95]
  16     1.000   3     -4.000   1     10.000   2      8.000
N(G)       4        0.00    -25.42      0.00     0              0.000[NEA95]
  17     1.000   3     -3.000   1      6.000   2      5.000
N2(G)      4        0.00   -210.46      0.00     0              0.000[NEA95]
  17     2.000   3     -6.000   1     12.000   2     10.000
NH3(G)     4       -3.00   -108.10      0.00     0              0.000[NEA95]
  17     1.000   3     -3.000   1      9.000   2      8.000
SR(NO3)2   2       10.00      0.40      0.00     0              0.000[NEA95]
  12     1.000  17      2.000
B(CR)      4       -3.00     45.17      0.00     0              0.000[NEA95]
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  18      1.000   3      -3.000    1       3.000    2       3.000
B(G)       4          -3.00     136.45      0.00      0                0.000[NEA95]
  18      1.000   3      -3.000    1       3.000    2       3.000
B2O3(CR)   2           0.00       5.75      0.00      0                0.000[NEA95]
  18      2.000   3      -3.000
B(OH)3(C   1           0.00      -0.07      0.00      0                0.000[NEA95]
  18      1.000
P(AM)      4          -5.00      13.48      0.00      0                0.000[NEA95]
  19      1.000   3      -4.000    1       8.000    2       5.000
P(CR)      4          -5.00      13.48      0.00      0                0.000[NEA95]
  19      1.000   3      -4.000    1       8.000    2       5.000
P(G)       4          -5.00      62.55      0.00      0                0.000[NEA95]
  19      1.000   3      -4.000    1       8.000    2       5.000
P2(G)      4         -10.00      45.08      0.00      0                0.000[NEA95]
  19      2.000   3      -8.000    1      16.000    2      10.000
P4(G)      4         -20.00      58.19      0.00      0                0.000[NEA95]
  19      4.000   3     -16.000    1      32.000    2      20.000
F(G)       2           1.00      60.23      0.00      0                0.000[NEA95]
  20      1.000   2      -1.000
F2(G)      2           2.00      98.64      0.00      0                0.000[NEA95]
  20      2.000   2      -2.000
HF(G)      2           0.00       1.07      0.000     0                0.000[NEA95]
  20      1.000   1       1.000
SIF4(G)    4           0.00     -15.33      0.00      0                0.000[NEA95]
  13      1.000  20       4.000   3      -4.000    1       4.000
BF3(G)     4           0.00      -2.98      0.00      0                0.000[NEA95]
  18      1.000  20       3.000   3      -3.000    1       3.000
BR(G)      2           1.00      32.63      0.00      0                0.000[NEA95]
  22      1.000   2      -1.000
BR2(G)     2           2.00      36.93      0.00      0                0.000[NEA95]
  22      2.000   2      -2.000
HBR(G)     2           0.00       8.85      0.00      0                0.000[NEA95]
  22      1.000   1       1.000
I(G)       2           0.00      21.36      0.00      0                0.000[NEA95]
  23      1.000   2      -1.000
I2(CR)     2           0.00      18.12      0.00      0                0.000[NEA95]
  23      2.000   2      -2.000
I2(G)      2           0.00      21.51      0.000     0                0.000[NEA95]
  23      2.000   2      -2.000
HI(G)      2          -1.00       9.36      0.000     0                0.000[NEA95]
  23      1.000   1       1.000
NI(OH)2    3           0.00      12.73      0.000     0                0.000[BAEYE89]
  31      1.000   3       2.000   1      -2.000
NICO3(s)   2           4.00      -6.97      0.000     0                0.000[BAEYE89]
  31      1.000  15       1.000
NIO(cr)    3           0.00      12.44      0.000     0                0.000[BAEYE89]
  31      1.000   3       1.000   1      -2.000
NIS        5          -2.00     -42.83      0.000     0                0.000[BAEYE89]
  31      1.000   3      -4.000    1       8.000   16       1.000   2       8.000
NI3(PO4)2  2           0.00     -29.59      0.000     0                0.000[BAEYE89]
  31      3.000  19       2.000
NI2P2O7    4           0.00     -33.57      0.000     0                0.000[BAEYE89]
  31      2.000  19       2.000   1       2.000    3      -1.000
OLIVINE    3           0.00      18.84      0.000     0                0.000[BAEYE89]
  31      2.000  13       1.000   1      -4.000
SPINEL     3           0.00      20.24      0.000     0                0.000[BAEYE89]
  31      2.000  13       1.000   1      -4.000
NISIO3     4           0.00      -2.28      0.000     0                0.000[BAEYE89]
  31      1.000  13       1.000   1      -2.000    3      -1.000
NI3S2      5          -6.00     -82.00      0.530     0                0.000[BAEYE89]
  31      3.000  16       2.000   3      -8.000    1      16.000   2      18.000
SE         4           0.00     -88.92      0.000     0                0.000[CROSS87]
  32      1.000   3      -4.000   2       6.000    1       8.000
SEO2       4           4.00     -35.82      0.000     0                0.000[CROSS87]
  32      1.000   3      -2.000   2       2.000    1       4.000
SE2O5      4          10.00     -19.6       0.000     0                0.000[CROSS87]
  32      2.000   3      -3.000   2       2.000    1       6.000
SEO3       3           6.00      19.2       0.000     0                0.000[CROSS87]
  32      1.000   3      -1.000   1       2.000
FESE2      5           0.00    -181.10      0.00      0                0.000[CROSS87]
  32      2.000   8       1.000   3      -8.000    1      16.000   2      14.
FESE       5           0.00     -84.78      0.00      0                0.000[YUI99]
  32      1.000   8       1.000   3      -4.000    1       8.000   2       8.
ZRO2(am)   2           0.00      -8.00      0.000     0                0.000[YUI99]
  33      1.000   3      -2.000
NB2O5      2           0.00     -16.00      0.00      0                      [LOTHE99]
  41      2.000   3      -5.000
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TC(CR)     4          0.00     -23.94       0.00     0                0.000[PHIL88]
  24     1.000   3       -1.000   1       2.000    2       4.000
TC(OH)2    3          2.00     -21.63       0.00     0                0.000[PHIL88]
  24     1.000   3        1.000   2       2.000
TC(OH)3(   4          3.00     -14.63       0.00     0                0.000[NEA89]
  24     1.000   3        2.000   1      -1.000    2       1.000
TCO2.2H2   3          4.00      -4.23       0.00     0                0.000[NEA89]
  24     1.000   3        3.000   1      -2.000
TCO2(C)    3          4.00     -19.76       0.00     0                0.000[PHIL88]
  24     1.000   3        1.000   1      -2.000
TCO3(C)    4          6.00      19.96       0.00     0                0.000[NEA89]
  24     1.000   3        2.000   1      -4.000    2      -2.000
NATCO4(C   5          7.00      35.54       0.00     0                0.000[NEA89]
   6     1.000  24        1.000   3       3.000    1      -6.000    2      -3.
TC2O7(C)   4         14.00      13.11       0.00     0                0.000[NEA89]
  24     2.000   3        5.000   1     -10.000    2      -6.00
PERTECHN   4          7.00      38.97       0.00     0                0.000[NEA89]
  24     1.000   3        3.000   1      -5.000    2      -3.000
TC3O4(S)   4          8.00     -56.89       0.00     0                0.000[NEA89]
  24     3.000   3        1.000   1      -2.000    2       4.000
TC4O7(S)   4         14.00     -36.79       0.00     0                0.000[NEA89]
  24     4.000   3        3.000   1      -6.000    2       2.000
PD(CR)     2          0.00     -32.90       0.00     0                0.000[LOTHE99]
  42     1.000   2        2.000
SN(CR)     4         -4.00      -0.77       0.000    0                0.000[LOTHE99]
  34     1.000   1        4.000   3      -4.000    2       4.000
SNOH2(S)   4         -2.00      -2.58       0.000    0                0.000[LOTHE99]
  34     1.000   1        2.000   3      -2.000    2       2.000
SNO(CR)    4         -2.00      -2.99       0.000    0                0.000[LOTHE99]
  34     1.000   1        2.000   3      -3.000    2       2.000
SNOHCL(S   5         -2.00      -7.82       0.000    0                0.000[LOTHE99]
  34     1.000   1        3.000   3      -3.000   14       1.000    2       2.000
SNO2(AM)   2          0.00      -7.46       0.000    0                0.000[LOTHE99]
  34     1.000   3       -2.000
SNO2(CAS   2          0.00      -8          0.000    0                0.000[LOTHE99]
  34     1.000   3       -2.000
SM(OH)3A   3          0.00      17.006      0.000    0                0.000[YUI99]
  35     1.000   3        3.000   1      -3.000
SM(OH)3C   3          0.00      15.206      0.000    0                0.000[YUI99]
  35     1.000   3        3.000   1      -3.000
SMOHCO3    4          4.00      -7.200      0.000    0                0.000[YUI99]
  35     1.000   3        1.000   1      -1.000   15       1.000
SMPO4(A)   2          0.00     -24.79       0.000    0                0.000[YUI99]
  35     1.000  19        1.000
SM2(CO3)   2         12.00     -33.40       0.000    0                0.000[YUI99]
  35     2.000  15        3.000
SB(CR      4          0.00     -11.99       0.00     0                     [LOTHE99]
  46     1.000   3       -3.000   1       3.000    2       3.000
VALENTIN   2          6.00      -8.72       0.00     0                     [LOTHE99]
  46     2.000   3       -3.000
STIBNITE   5          0.00    -156.219      0.00     0                     [LOTHE99]
  46     2.000  16        3.000   3     -18.000    1      30.000    2      24.000
SB2O5      4          2.00      36.28                                     [LOTHE99]
  46     2.000   3       -1.000   1       4.000    2       4.000
CS(CR)     2         -1.00      51.06       0.00     0                0.000[NEA95]
  30     1.000   2        1.000
CS(G)      2         -1.00      59.74       0.00     0                0.000[NEA95]
  30     1.000   2        1.000
CSNO3      2          5.00      -0.41       0.000    0                0.000[CROSS87]
  30     1.000  17        1.000
CS2O       3          0.00      89.89       0.00     0                     [PHIL88]
  30     2.000   3        1.000   1      -2.000
CSOH       3          0.00      27.42       0.00     0                     [PHIL88]
  30     1.000   3        1.000   1      -1.000
CS2SO4     2          6.00       0.87       0.00     0                     [PHIL88]
  30     2.000  16        1.000
CS2CO3     2          4.00      10.07       0.00     0                     [PHIL88]
  30     2.000  15        1.000
CS2UO4(C   5          6.00      44.84       0.00     0                0.000[NEA95]
  25     1.000  30        2.000   3       4.000    1      -8.000    2      -2.000
CS2U2O7(   5         12.00      49.01       0.00     0                0.000[NEA95]
  25     2.000  30        2.000   3       7.000    1     -14.000    2      -4.000
CS2U4O12   5         22.00      52.03       0.00     0                0.000[NEA95]
  25     4.000  30        2.000   3      12.000    1     -24.000    2      -6.000
PB(CR)     2          0.00       4.25       0.000    0                0.000[LOTHE99]
  36     1.000   2        2.000
PBO(RED)   3          2.00      12.68       0.000    0                0.000[LOTHE99]
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  36      1.000   3       1.000   1      -2.000
PBO(YELL   3          2.00      12.96      0.000      0                0.000[LOTHE99]
  36      1.000   3       1.000   1      -2.000
PB(OH)2    3          2.00      13.05      0.000      0                0.000[LOTHE99]
  36      1.000   3       2.000   1      -2.000
PBSO4(S)   2          8.00      -7.81      0.000      0                0.000[LOTHE99]
  36      1.000  16       1.000
PBCL2(S)   2          2.00      -4.81      0.000      0                0.000[LOTHE99]
  36      1.000  14       2.000
PBOHCL(S   4          2.00       0.62      0.000      0                0.000[LOTHE99]
  36      1.000  14       1.000   3      1.000   1      -1.000
PBF2(S)    2          2.00      -7.52      0.000      0                0.000[LOTHE99]
  36      1.000  20       2.000
PBFCL(S)   3          2.00      -8.82      0.000      0                0.000[LOTHE99]
  36      1.000  20       1.000  14      1.000
PBCO3(S    2          6.00     -13.23      0.000      0                0.000[LOTHE99]
  36      1.000  15       1.000
PB3(CO3    4         14.00     -17.64      0.000      0                0.000[LOTHE99]
  36      3.000  15       2.000   3      2.000   1      -2.000
PB10(CO    4         44.00     -41.21      0.000      0                0.000[LOTHE99]
  36     10.000  15       6.000   3      7.000   1      -8.000
PBOHNO3    4          7.00       2.94      0.000      0                0.000[LOTHE99]
  36      1.000  17       1.000   3      1.000   1      -1.000
PBHPO4(S   3          2.00     -23.78      0.000      0                0.000[LOTHE99]
  36      1.000  19       1.000   1      1.000
PB(H2PO4   3          2.00     -48.94      0.000      0                0.000[LOTHE99]
  36      1.000  19       2.000   1      4.000
PB3PO42    2          6.00     -44.40      0.000      0                0.000[LOTHE99]
  36      3.000  19       2.000
PB4PO42O   4          8.00     -37.09      0.000      0                0.000[LOTHE99]
  36      4.000  19       2.000   1     -2.000   3       1.000
PB5PO43O   4         10.00     -62.80      0.000      0                0.000[LOTHE99]
  36      5.000  19       3.000   1     -1.000   3       1.000
PB5PO43C   3         10.00     -84.40      0.000      0                0.000[LOTHE99]
  36      5.000  19       3.000  14      1.000
PB5PO43F   3         10.00     -71.60      0.000      0                0.000[LOTHE99]
  36      5.000  19       3.000  20      1.000
PBS(S)     5          0.00     -45.863     0.000      0                0.000[LOTHE99]
  36      1.000  16       1.000   1      8.000   2       8.000   3      -4.
PBO2(S)    4          4.00      48.98      0.000      0                0.000[LOTHE99]
  36      1.000   3       2.000   1     -4.000   2      -2.000
PB3O4(S)   4          8.00      70.98      0.000      0                0.000[LOTHE99]
  36      3.000   3       4.000   1     -8.000   2      -2.000
BI(CR      2         -3.00     -16.74       0.00      0                     [LOTHE99]
  47      1.000   2       3.000
BI2O3      3          0.00       0.76       0.00      0                     [LOTHE99]
  47      2.000   3       3.000   1     -6.000
BIOCL(S)   4          0.00      -8.47       0.00      0                     [LOTHE99]
  47      1.000   3       1.000   1     -2.000  14       1.000
(BIO)2CO   4          4.00     -14.27       0.00      0                     [LOTHE99]
  47      2.000   3       2.000   1     -4.000  15       1.000
(BIO)4OH   4          4.00      -8.68       0.00      0                     [LOTHE99]
  47      4.000   3       6.000   1    -10.000  15       1.000
BIONO3(S   4          5.00      -2.75       0.00      0                     [LOTHE99]
  47      1.000   3       1.000   1     -2.000  17       1.000
PO(OH)4    3          4.00      19.52       0.00      0                     [NBS82]
  48      1.000   3       4.000   1     -4.000
RASO4      2          6.00     -10.40      0.000      0                0.000[CROSS87]
  37      1.000  16       1.000
RACO3      2          4.00      -7.00      0.000      0                0.000[CROSS87]
  37      1.000  15       1.000
AC(OH)3A   3          0.00     17.006      0.000      0                0.000[YUI99]
  49      1.000   3       3.000   1     -3.000
AC(OH)3C   3          0.00     15.206      0.000      0                0.000[YUI99]
  49      1.000   3       3.000   1     -3.000
ACOHCO3    4          4.00     -7.200      0.000      0                0.000[YUI99]
  49      1.000   3       1.000   1     -1.000  15       1.000
ACPO4(A)   2          0.00     -24.79      0.000      0                0.000[YUI99]
  49      1.000  19       1.000
AC2(CO3)   2         12.00     -33.40      0.000      0                0.000[YUI99]
  49      2.000  15       3.000
THO2(AM)   3          0.00     10.500      0.000      0                0.000[FELM91]
  38      1.000   3       2.000   1     -4.000
THO2(CR)   3          0.00      1.800      0.000      0                0.000[RAI 87]
  38      1.000   3       2.000   1     -4.000
THF4NAFH   4          0.00     -34.13      0.000      0                0.000[FELM93]
  38      1.000   3       1.000   6      1.000  20       5.000
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THF4.H2O    3          0.00     -29.01      0.000     0                0.000[FELM93]
  38    1.000    3        1.000   20        4.000
THF4NH4F    3         -3.00     -33.990     0.000     0                0.000[FELM93]
  38    1.000  148        1.000   20        5.000
PAO2        3          4.00       0.60      0.000     0                0.000[BAES 76]
  39    1.000    3        2.000    1       -4.000
PACL4       2          4.00      24.01      0.000     0                0.000[SHIB98A]
  39    1.000   14        4.000
PA2O5       4         10.00      -8.72      0.000     0                0.000[SHIB98A]
  39    2.000    3        5.000    2       -2.000     1      -10.000
PACL5       3          5.00      32.85      0.000     0                0.000[SHIB98A]
  39    1.000   14        5.000    2       -1.000
UO2(AM)     3          4.00       2.56      0.00      0                0.000[RAI 97]
   1   -4.000    3        2.000   25        1.000
UO3(ALPH    4          6.00      17.67      0.00      0                0.000[NEA92]
  25    1.000    3        3.000    1       -6.000     2       -2.000
UO3(BETA    4          6.00      17.34      0.00      0                0.000[NEA92]
  25    1.000    3        3.000    1       -6.000     2       -2.000
UO3(GAMM    4          6.00      16.74      0.00      0                0.000[NEA92]
  25    1.000    3        3.000    1       -6.000     2       -2.000
UO3.0.9H    4          6.00      14.04      0.00      0                0.000[NEA92]
  25    1.000    3        3.900    1       -6.000     2       -2.000
UO3.2H2O    4          6.00      13.85      0.00      0                0.000[NEA92]
  25    1.000    3        5.000    1       -6.000     2       -2.000
UF6(CR)     3          6.00      26.24      0.00      0                0.000[NEA92]
  20    6.000   25        1.000    2       -2.000
UO2(IO3)    5         16.00     224.29      0.00      0                0.000[NEA92]
  23    2.000   25        1.000    3        8.000     1      -16.000     2      -14.000
UO2SO4.2    5         12.00       7.449     0.00      0                0.000[NEA92]
  16    1.000   25        1.000    3        4.500     1       -4.000     2       -2.000
UO2SO4.3    5         12.00       7.453     0.0       0                0.000[NEA92]
  16    1.000   25        1.000    3        5.500     1       -4.000     2       -2.000
NA4UO2(C    6         18.00     -17.90      0.00      0                0.000[NEA92]
   6    4.000   15        3.000   25        1.000     3        2.000     1       -4.000
   2   -2.000
UO2(OH)2    4          6.00      13.97      0.00      0                0.000[NEA92]
  25    1.000    3        4.000    1       -6.000     2       -2.000
UO2CO3(C    5         10.00      -5.43   -148.44      0                0.000[92GRE/FU
  15    1.000   25        1.000    3        2.000     1       -4.000     2       -2.000
NP(OH)3     4          3.00      15.93      0.000     0                0.000[CROSS87]
  40    1.000    3        3.000    1       -3.000     2        1.000
NPO2(AM)    3          4.00       1.51      0.000     0                0.000[RAI 87]
  40    1.000    1       -4.000    3        2.000
NPO2OH(A    4          5.00      16.13      0.000     0                0.000[SHIB98B]
  40    1.000    3        3.000    1       -5.000     2       -1.000
NANPO2C     6          9.00      -0.11      0.000     0                0.000[SHIB98B]
  40    1.000    3        2.000    1       -4.000     2       -1.000    15        1.000
   6    1.000
NA3NPO2     6         13.00      -3.41      0.000     0                0.000[SHIB98B]
  40    1.000    3        2.000    1       -4.000     2       -1.000    15        2.000
   6    3.000
PU(OH)3A    4          3.00      -0.004     0.000     0                0.000[YUI99]
  29    1.000    3        3.000    1       -3.000     2        1.000
PUOHCO3     5          7.00     -24.21      0.000     0                0.000[YUI99]
  29    1.000    3        1.000    1       -1.000    15        1.000     2        1.000
PU(OH)3C    4          3.00      -1.804     0.000     0                0.000[YUI99]
  29    1.000    3        3.000    1       -3.000     2        1.000
PU2(CO3)    3         18.00     -67.42      0.000     0                0.000[YUI99]
  29    2.000   15        3.000    2        2.000
PUPO4(A)    3          3.00     -41.80      0.000     0                0.000[YUI99]
  29    1.000   19        1.000    2        1.000
PUO2(AM)    3          4.00      -0.85      0.00      0                0.000[RAI 84]
  29    1.000    3        2.000    1       -4.000
PUO2OH      4          5.00      23.43      0.00      0                0.000[SHIB98C]
  29    1.000    3        3.000    2       -1.000     1       -5.000
PUO2OH2     4          6.00      39.16      0.00      0                0.000[LIERS86]
  29    1.000    3        4.000    2       -2.000     1       -6.000
PUO2CO3     5         10.00      19.91      0.00      0                0.000[PASHA97]
  29    1.000    3        2.000   15        1.000     1       -4.000     2       -2.000
AM(OH)3A    3          3.00      17.00      0.000     0                0.000[NEA95]
  28    1.000    3        3.000    1       -3.000
AM(OH)3C    3          3.00      15.206     0.000     0                0.000[NEA95]
  28    1.000    3        3.000    1       -3.000
AM2(CO3)    2         18.00     -33.40      0.000     0                0.000[NEA95]
  28    2.000   15        3.000
AMOHCO3     4          7.00      -7.20      0.000     0                0.000[NEA95]
  28    1.000    3        1.000    1       -1.000    15        1.000
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AMPO4(A)   2          3.00    -24.79     0.000     0              0.000[NEA95]
  28      1.000  19       1.000
CM(OH)3A   3          3.00     17.006     0.000     0              0.000[YUI99]
  50      1.000   3       3.000   1      -3.000
CM(OH)3C   3          3.00     15.206     0.000     0              0.000[YUI99]
  50      1.000   3       3.000   1      -3.000
CMOHCO3    4          7.00     -7.200     0.000     0              0.000[YUI99]
  50      1.000   3       1.000   1      -1.000  15       1.000
CMPO4(A)   2          3.00    -24.79     0.000     0              0.000[YUI99]
  50      1.000  19       1.000
CM2(CO3)   2         18.00    -33.40     0.000     0              0.000[YUI99]
  50      2.000  15       3.000

END                                                                          !

 1: Ni --->  300
 2: Se --->  400
 3: Zr --->  500
 4: Nb --->  600
 5: Tc --->  700
 6: Pd --->  800
 7: Sn --->  900 (Sn(II)--->900, SN(IV)--->950)
 8: Sb ---> 1000 (Sb(III)--->1000, Sb(V)--->1050)
 9: Cs ---> 1100
10: Nd ---> 1200
11: Sm ---> 1300
12: Pb ---> 1400
13: Bi ---> 1500
14: Po ---> 1600
15: Ra ---> 1700
16: Ac ---> 1800
17: Th ---> 1900
18: Pa ---> 2000                                                             !
19: U  ---> 2100 (U(III)--->2100, U(IV)--->2130, U(V)--->2160, U(VI)--->2190
                , U(?)--->2240)
20: Np ---> 2300 (NP(III)--->2300, NP(IV)--->2330, NP(V)--->2360, NP(VI)--->2390)
21: Pu ---> 2500 (Pu(III)--->2500, Pu(IV)--->2530, Pu(V)--->2560, Pu(VI)--->2590)
22: Am ---> 2700 (Am(III)--->2700, Am(IV)--->2730, Am(V)--->2760, Am(VI)--->2790)
23: Cm ---> 2900

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