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JAEA-TDB-RN in 2020: Update of JAEA's Thermodynamic Database for Solubility and Speciation of Radionuclides for Performance Assessment of Geological Disposal of High-level and TRU Wastes

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Part of JAEA's Thermodynamic Database (JAEA-TDB) for solubility and speciation of radionuclides (JAEA-TDB-RN) for performance assessment of geological disposal of high-level radioactive and TRU wastes has been updated with subsuming the database for geochemical calculations (JAEA-TDB-GC). This report has focused to update JAEA-TDB-RN after selecting change in standard Gibbs free energy of formation ($\Delta_f G^o_m$), change in standard enthalpy change of formation ($\Delta_f H^o_m$), standard molar entropy (S^o_m) and, heat capacity (C^o_p), change in standard Gibbs free energy of reaction ($\Delta_r G^o_m$), change in standard enthalpy change of reaction ($\Delta_r H^o_m$) and standard entropy change of reaction ($\Delta_r S^o_m$) as well as logarithm of equilibrium constant ($\log_{10} K°$) at standard state. The extent of selection of these thermodynamic data enables to evaluate solubility and speciation of radionuclides at temperatures other than 298.15 K. Furthermore, the latest thermodynamic data for iron which have been critically reviewed, selected and compiled by the Nuclear Energy Agency within Organisation for Economic Co-operation and Development (OECD/NEA) have been accepted. Most of previously selected $\log_{10} K°$ have been refined to confirm internal consistency with JAEA-TDB-GC. Text files of the updated JAEA-TDB have been provided for geochemical calculation programs of PHREEQC and Geochemist's Workbench.

Keywords: Geological Disposal, High-level Radioactive Waste, TRU Waste, Thermodynamic Database, Solubility, Speciation, Radionuclide, Update of JAEA-TDB, Use of Geochemical Calculation Programs

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2020 年版 JAEA 核種 TDB：高レベルおよび TRU 廃棄物地層処分の性能評価に用いる放射性核種の溶解挙動評価のための JAEA 熱力学データベースの更新

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高レベル放射性廃棄物および TRU 廃棄物地層処分の性能評価に用いる JAEA 熱力学データベース（JAEA-TDB）のうち，放射性核種溶解挙動評価部分（JAEA-TDB-RN）について，地球化学計算部分（JAEA-TDB-GC）を包含する形で更新を実施した。今回の更新では，従来の選定値が標準状態における反応の平衡定数（対数値 $\log_{10} K°$）だけであったのに対して，ギブズ標準自由エネルギー変化（$\Delta_f G°_m$），標準モルエンタルピー変化（$\Delta_f H°_m$），標準モルエントロピー（$S°_m$），比熱容量（$C°_{p,m}$），反応の自由エネルギー変化（$\Delta_r G°_m$），反応のエンタルピー変化（$\Delta_r H°_m$）および反応のエントロピー変化（$\Delta_r S°_m$）を追加することで，大幅な選定値の拡充を行うとともに，298.15 K 以外の温度における溶解挙動評価が実施できるよう整備が行われた。また，経済協力開発機構原子力機関（OECD/NEA）がレビュー，選定および集約した鉄についての最新の熱力学データを取り込んだ。さらに，JAEA-TDB-GC と選定値の内部整合性を図るために，多くの反応の $\log_{10} K°$ について再計算を実施した。更新した JAEA-TDB を有効活用するために， PHREEQC および Geochemist’s Workbench といった地球化学計算コード用フォーマットを提供した。

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1. Introduction

Many radionuclides are contained in high-level radioactive waste (HLW) and are part of TRU waste; some of them have long half-lives (more than 10^4 years). It is necessary to predict solubility and speciation of the radionuclides in groundwaters and bentonite porewaters in an engineered barrier system for performance assessment of geological disposal of HLW and TRU waste. Thermodynamic data at standard state (298.15 K, 0.1 MPa and ionic strength of zero) are needed to estimate the solubility and aqueous species in the groundwater and bentonite porewater. These data are also needed to estimate sorption and diffusion behavior of chemical species on/in engineered barriers and host rocks. Therefore, the most reliable thermodynamic data should be compiled to carry out the reliable performance assessment by implementation and regulatory organizations.

The author and his colleagues have developed and updated the JAEA's thermodynamic database (JAEA-TDB) (JAEA is the abbreviation of Japan Atomic Energy Agency) for the performance assessment of geological disposal of radioactive waste [1-5]. Main part of the thermodynamic data in JAEA-TDB were selected and estimated by JAEA, however, some were taken from the data selected in the NEA Thermochemical Data Base Project (NEA-TDB) organized by the Nuclear Energy Agency (NEA) within the Organisation for Economic Co-operation and Development (OECD) [6] and those selected in JNC-TDB [5] (JNC is the abbreviation of Japan Nuclear Cycle Development Institute which is one of the predecessor of JAEA). The thermodynamic data were compiled and converted to be available for use in geochemical calculation programs, e.g., PHREEQC [7] and Geochemist's Workbench (GWB) [8].

Problems of past versions of JAEA-TDB [1-4] were that; 1) prediction of solubility and speciation was able to perform only at 298.15 K due to compilation of only equilibrium constant values at 298.15 K, and 2) no thermodynamic data for geochemical calculations have been updated after publishing JNC-TDB [5]. Although thermodynamic data for geochemical calculations have been replaced to those selected in another JAEA-TDB specialized for geochemical calculations (JAEA-TDB-GC) [9, 10] in the previous update in 2019 [11], the internal consistency in the TDB was far from satisfactory.

In the present update of JAEA-TDB from "the previous update published in 2019" [11], the author has carefully compiled thermodynamic data for solubility and speciation of radionuclides to confirm internal consistency in the TDB through; 1) selection of thermodynamic data on formation and reaction of elements other than the equilibrium constant ($\log_{10} K°$), 2) compilation of thermodynamic data selected in the latest update of JAEA-TDB-GC [9], and 3) refinement of thermodynamic data (especially for $\log_{10} K°$) after revising those for basic elements. The author has updated the part of JAEA-TDB for solubility and speciation of radionuclides (JAEA-TDB-RN) because the author has not developed but just referred JAEA-TDB-GC [9].

The author has also decided to provide text files of updated and expired TDB for use of the geochemical calculation programs of PHREEQC [7] and GWB [8].

2. Guidelines for Selection of Thermodynamic Data

2.1 Basic Information

The objective of developing the JAEA-TDB is to provide an appropriate thermodynamic database for the performance assessment of geological disposal of radioactive waste (especially for HLW and TRU waste). The traceability and transparency of selection of thermodynamic values in the JAEA-TDB should be guaranteed.

The thermodynamic values to be selected in the JAEA-TDB fall in two categories, those that are necessary and those that would be desirable (recommended) to have if adequate data are available. These are further elaborated below:

- Necessary:
  equilibrium constant of reaction (K^{o}) or
  change in standard Gibbs free energy of reaction ($\Delta_r G^{o}_{m} = -RT \ln K^{o}$, where R and T is gas constant and absolute temperature, respectively),
- Recommended:
  change in standard Gibbs free energy of formation ($\Delta_f G^{o}_{m}$),
  change in standard enthalpy change of formation ($\Delta_f H^{o}_{m}$) and that of reaction ($\Delta_r H^{o}_{m}$), standard molar entropy (S^{o}_{m}) and change in standard entropy change of reaction ($\Delta_r S^{o}_{m}$), and heat capacity (C^{o}_{p}).

Twenty-six elements of interest were selected in the safety assessment in JNC's 2nd progress report on research and development of geological disposal of HLW (H12) [12] and that of TRU waste (TRU-2) [13] as follows:

- carbon (C)
- chlorine (Cl)
- cobalt (Co)
- nickel (Ni)
- selenium (Se)
- strontium (Sr)
- zirconium (Zr)
- niobium (Nb)
- molybdenum (Mo)
- technetium (Tc)
- palladium (Pd)
- tin (Sn)
- antimony (Sb)
- iodine (I)
- cesium (Cs)
- samarium (Sm)

- lead (Pb)
- bismuth (Bi)
- polonium (Po)
- radium (Ra)
- actinium (Ac)
- thorium (Th)
- protactinium (Pa)
- uranium (U)
- neptunium (Np)
- plutonium (Pu)
- americium (Am)
- curium (Cm)

Considering the stability and abundance of anions in the geological disposal environment that can form complexes with the radioactive elements of interest, complexes of the following dominant anions will be considered emphasized for selecting thermodynamic data:

- hydroxyl ion (OH^-)
- hydrogen carbonate and carbonate ions (HCO_3^- and CO_3^{2-}, respectively)
- sulfate and hydrosulfide ions (SO_4^{2-} and HS^-, respectively)
- nitrate ion and ammine (NO_3^- and NH_3(aq), respectively)
- dihydrogen, hydrogen phosphate and orthophosphate ions ($H_2PO_4^-$, HPO_4^{2-} and PO_4^{3-}, respectively)
- halide ions (F^-, Cl^-, Br^- and I^-).

Thermodynamic data of several elements with the following organic ligands, which have been published as the NEA-TDB [14], will be incorporated into the JAEA-TDB due to importance for the performance assessment of TRU waste:

- Ethylenediaminetetraacetic acid (EDTA: $(HOOCCH_2)_2NCH_2CH_2N(CH_2COOH)_2$),
- Citric acid (Cit: $HOOCCH_2CCOOHOHCH_2COOH$),
- Oxalic acid (Ox: HOOCCOOH) and
- Isosaccharic acid (ISA: $CH_2OHCHOHCH_2COHCH_2OHCOOH$).

Although it is important to select formation constants with natural organic substances (e.g. humic and fulvic acids) for the JAEA-TDB, it is currently not possible to do so because the humic substances are complex with multiple functional groups, and the proposed models for interpreting complexation behavior of the humic substances are empirical, too simplified, and not able to unambiguously assign values of formation constants for them. Formation constants with organic ligands other than EDTA, Cit, Ox and ISA will be

excluded from the compilation of the JAEA-TDB.

The order of ligands is sorted based on the ranks of elements given in “Standard Order of Arrangement” [15] as shown in Figure 1.

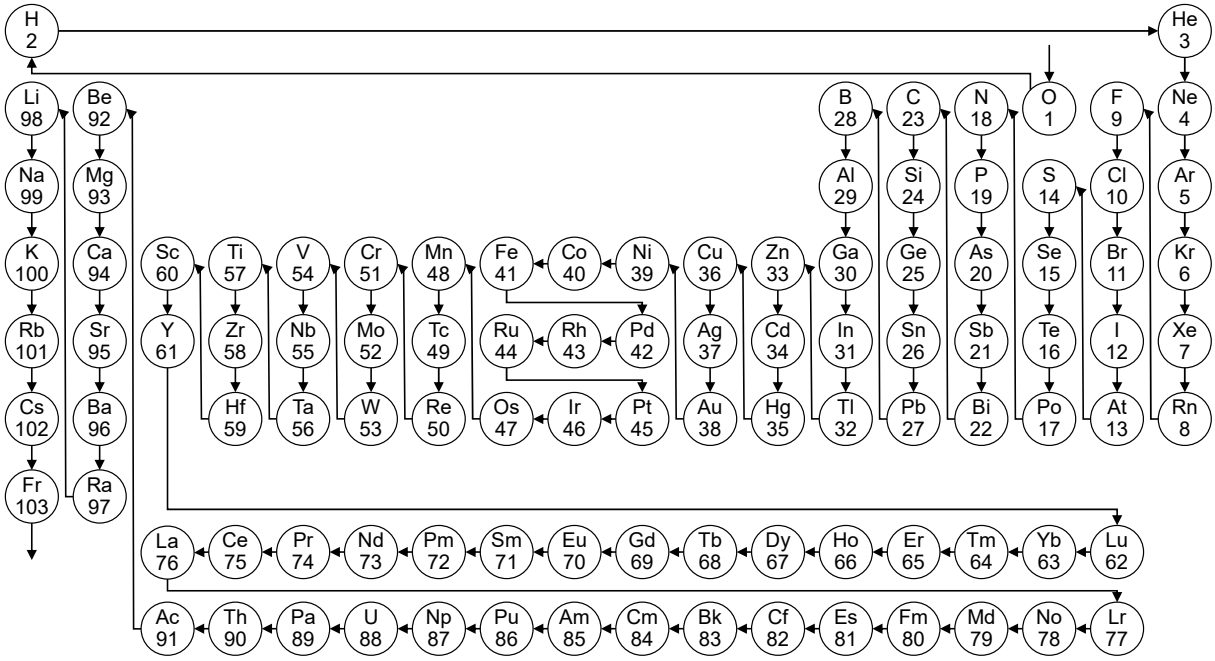

Figure 1 Standard order of arrangement of the elements and compounds based on the periodic classification of the elements (after Wagman et al.[15])

2.2 Relation between Thermodynamic Data on Formation and Reaction

There are some compounds/species for which thermodynamic values on reaction have not been selected and those on formation are available. The thermodynamic values on reaction (e.g., $\log_{10} K^\circ$ and $\Delta_r H^\circ_m$) are required for use in some geochemical calculation programs such as PHREEQC [7]. Therefore, some thermodynamic values on reaction have been determined from those on formation using the following calculation.

Using the Hess’s law, thermodynamic values on formation for some arbitrary reaction, e.g.,

$$a\,\mathrm{A} + b\,\mathrm{B} \rightleftarrows c\,\mathrm{C} + d\,\mathrm{D}\,, \qquad (1)$$

where A, B, C and D are substances involving the reaction, and a, b, c and d are coefficients of the substances A, B, C and D, respectively,

can be obtained using the following equations:

$$\Delta_r G^\circ_m = c\,\Delta_f G^\circ_m(\mathrm{C}) + d\,\Delta_f G^\circ_m(\mathrm{D}) - a\,\Delta_f G^\circ_m(\mathrm{A}) - b\,\Delta_f G^\circ_m(\mathrm{B})\,, \qquad (2)$$

$$\Delta_r H^\circ_m = c\,\Delta_f H^\circ_m(\mathrm{C}) + d\,\Delta_f H^\circ_m(\mathrm{D}) - a\,\Delta_f H^\circ_m(\mathrm{A}) - b\,\Delta_f H^\circ_m(\mathrm{B}) \quad \text{and} \qquad (3)$$

$$\Delta_r S°_m = c\, S°_m(C) + d\, S°_m(D) - a\, S°_m(A) - b\, S°_m(B)\ . \quad (4)$$

Logarithm of equilibrium constant at standard state ($\log_{10} K°$) is derived from $\Delta_r G°_m$ using the following equation:

$$\Delta_r G°_m = -RT \log_e K° \quad (5)$$

where R is the gas constant (8.3145 $J \cdot K^{-1} \cdot mol^{-1}$) and T is absolute temperature (which for 25 °C is 298.15 K) [16]. Therefore, $\log_{10} K°$ equals to $-(\Delta_r G°_m)/(5.708)$ at 298.15 K.
Uncertainty (σ) of the thermodynamic values is obtained from error propagation as follows:

$$\sigma(\Delta_r G°_m) = (c\ \sigma(\Delta_f G°_m(C))^2 + d\ \sigma(\Delta_f G°_m(D))^2 + a\ \sigma(\Delta_f G°_m(A))^2 + b\ \sigma(\Delta_f G°_m(B))^2)^{1/2}, \quad (6)$$

$$\sigma(\Delta_r H°_m) = (c\ \sigma(\Delta_f H°_m(C))^2 + d\ \sigma(\Delta_f H°_m(D))^2 + a\ \sigma(\Delta_f H°_m(A))^2 + b\ \sigma(\Delta_f H°_m(B))^2)^{1/2}, \quad (7)$$

$$\sigma(\Delta_r S°_m) = (c\ \sigma(S°_m(C))^2 + d\ \sigma(S°_m(D))^2 + a\ \sigma(S°_m(A))^2 + b\ \sigma(S°_m(B))^2)^{1/2}, \text{ and} \quad (8)$$

$$\sigma(\log_{10} K°) = \sigma(\Delta_r G°_m)/5.708. \quad (9)$$

The uncertainty in equilibrium constant ($\sigma(\log_{10} K°)$) calculated using equations (6) and (9) is usually larger than that obtained experimentally. The smallest of the uncertainty values have been selected on the basis of either the experimental data or calculations.

There is another equation to obtain $\Delta_r S°_m$ as follows:

$$\Delta_r S°_m = (\Delta_r H°_m - \Delta_r G°_m) / T\ . \quad (10)$$

This equation is useful to check internal consistency of the selected values. The uncertainty of $\Delta_r S°_m$ ($\sigma(\Delta_r S°_m)$) using the equation (10) is, however, usually much larger than that using the equation (7). Therefore, $\Delta_r S°_m$ and $\sigma(\Delta_r S°_m)$ should be selected using the equations (4) and (8), respectively.

For use with geochemical calculation programs, dissociation reactions are defined for all compounds and gaseous species, i.e., the objective compounds and species are put on the left-hand side and aqueous master species of the objective elements are put on right-hand side in their reactions.

2.3 General Procedure for the Selection of Thermodynamic Data

2.3.1 Elements of Interest and Two Individual Parts of JAEA-TDB

Development of JAEA-TDB has been performed in the following two parts individually in recent years: 1) the database for geochemical reactions between rocks / minerals and groundwaters (JAEA-TDB-GC), and 2) those for solubility and speciation of radionuclides (JAEA-TDB-RN). Elements of interest in the both parts are shown on a periodic table in Figure 2, comparing of those in the NEA Thermochemical Data Base Project (NEA-TDB). The present report provides the selected thermodynamic data for JAEA-TDB-RN compiled with the selected data in JAEA-TDB-GC of which the development has been shown in elsewhere [17].

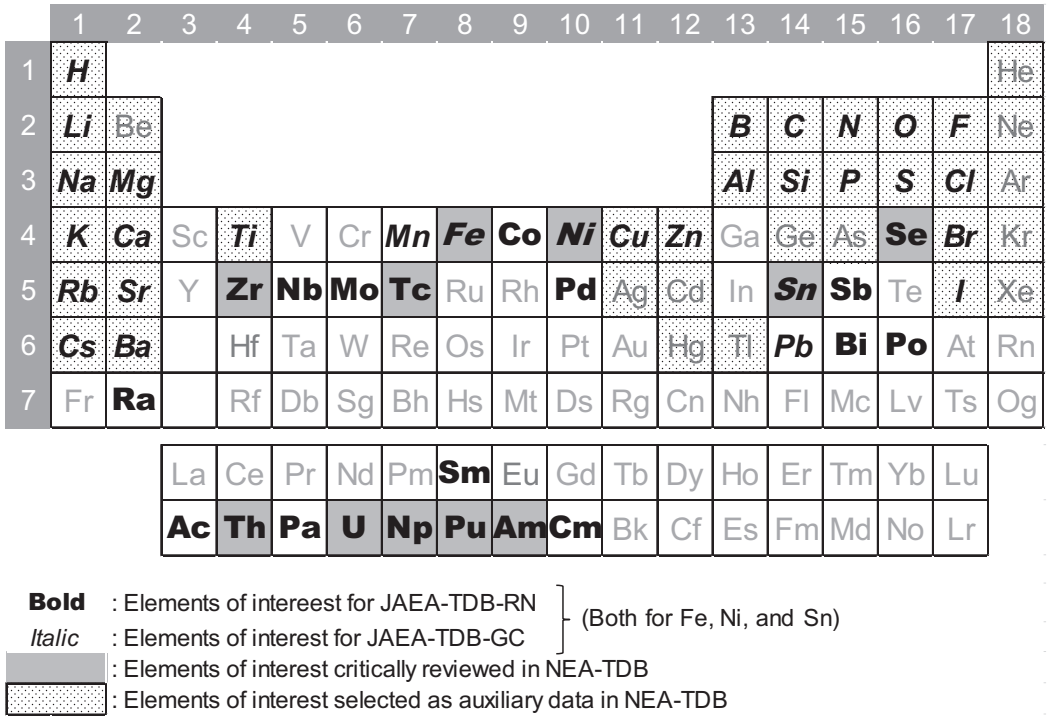

Figure 2 Elements of interest in JAEA-TDB comparing with those in the NEA Thermochemical Data Base Project (NEA-TDB)

2.3.2 Collecting Thermodynamic Values

Thermodynamic values for iron [18, 19], nickel [20], selenium [21], zirconium [22], technetium [23], tin [24], thorium [25], uranium [23], neptunium [23], plutonium [23], americium [23] and those with selected organic ligands [14] which have been critically reviewed by the NEA should be collected. Other thermodynamic values for these elements, which were not reviewed by the NEA, may have to be collected as necessary. Selected or referred thermodynamic values in the JNC-TDB [5] and the PSI/Nagra-TDB [26] of which thermodynamic data have been reviewed and compiled on the basis of the NEA's guidelines [6] should also be collected. Thermodynamic values for elements excluded in the above TDBs should be collected through literature survey. Thermodynamic values for some elements with poor or no experimental values should be estimated using chemical analogues and/or models.

2.3.3 Procedure for Review and Selection of Thermodynamic Values

Review and selection of thermodynamic values obtained from experimental data should be based on the NEA's "TDB-1" guideline [27], which describes how to review and select thermodynamic data based on the number of data source available. Even though the "TDB-1" [27] mentions that only original experimental data are evaluated, not estimates, values from compilations or secondary citations, thermodynamic values or databases selected by the NEA can be transferred to the JAEA-TDB after checking the consistency of these

values with the existing database. Based on the same (unique) policy, thermodynamic values contained in TDBs developed on the basis of the "TDB-1" guideline [27], which are the PSI/Nagra-TDB [26] and part of the JNC-TDB (Lothenbach *et al.* [28]), can be treated as already reviewed values. If the latest thermodynamic values and/or non-selected values in the above TDBs are considered to be reliable, the review and selection of thermodynamic values should be performed for all candidate values, and the consistency of the database should be reevaluated in a manner similar to the reevaluation of the NEA-TDB.

Thermodynamic values on formation ($\Delta_f G^o_m$, $\Delta_f H^o_m$, S^o_m and C^o_p) compiled in JAEA-TDB-GC [17] have been adopted without any modifications, except for those for iron [18, 19], nickel [20] and tin [24] which have also been reviewed and selected in NEA-TDB. It is found that most of thermodynamic data on formations and reactions of fundamental elements in JAEA-TDB-GC [17] are similar to those selected in NEA-TDB (the auxiliary data).

Refinement of the selected thermodynamic data has been performed in order to make sure internal consistency in the TDB as follows:

1. Select thermodynamic values on reaction ($\log_{10} K^o$, $\Delta_r G^o_m$, $\Delta_r H^o_m$ and $\Delta_r S^o_m$) when reliable,
2. Calculate thermodynamic values on formation ($\Delta_f G^o_m$, $\Delta_f H^o_m$, S^o_m) from those on reaction selected above,
3. Select thermodynamic values on formation ($\Delta_f G^o_m$, $\Delta_f H^o_m$, S^o_m and C^o_p) when the related thermodynamic values on reaction ($\log_{10} K^o$, $\Delta_r G^o_m$, $\Delta_r H^o_m$ and $\Delta_r S^o_m$) have not been selected,
4. Calculate thermodynamic values on reaction ($\log_{10} K^o$, $\Delta_r G^o_m$, $\Delta_r H^o_m$ and $\Delta_r S^o_m$) using the selected values on formation ($\Delta_f G^o_m$, $\Delta_f H^o_m$ and S^o_m), and
5. Check internal consistency through calculation of $\Delta_r S^o_m$ using the equations (4) and (10).

For the calculation of $\Delta_f G^o_m$ of aqueous species and compounds of interest, some $\Delta_f G^o_m$ values for basic species (can be nominated as "solution master species" in PHREEQC program [7]) have been taken from Fuger and Oetting [29] and Wagman et al. [15].

Selection of thermodynamic values for iron, nickel and tin of which both JAEA-TDB-GC [17] and NEA-TDB [18-20, 24] have been selected will be discussed later.

2.3.4 Correction of Ionic Strength

All thermodynamic values should be standardized at zero ionic strength. Correction of ionic strength to determine the equilibrium constant values at zero ionic strength should be performed on the basis of the NEA's "TDB-2" guideline [30], which recommends the Brønsted-Guggenheim-Scatchard Model (usually called the "specific ion interaction theory (SIT)"). In the model, the activity coefficient γ_j of an ion j of charge z_j in the electrolyte solution of molarity m_k (mol kg^{-1}) and ionic strength I_m (mol kg^{-1}) is assumed as follows:

$$\log \gamma_j = -z_j{}^2 D + \sum_k \varepsilon_{(j,k,I_m)} m_k \ , \quad (11)$$

where D denotes the Debye-Hückel term as defined as a function of I_m as shown in the following equation; $\varepsilon_{(j,k,I_m)}$ denotes the ion interaction coefficient of ion j against the counterion(s) k at a certain I_m:

$$D = \frac{0.509\sqrt{I_m}}{1+1.5\sqrt{I_m}} \ . \quad (12)$$

The ionic strength I_m equals the molarity m_k in case of 1:1 electrolyte (e.g. NaCl, $NaClO_4$). The ion interaction coefficients $\varepsilon_{(j,k,I_m)}$ are assumed to be zero for ions of the same charge sign (e.g. between Na^+ and UO_2^{2+}) and for uncharged species (e.g. $UO_2(OH)_2(aq)$).

2.3.5 Temperature Correction

All thermodynamic values should be selected at 298.15 K. If thermodynamic values are available only at other temperatures, those should be converted to 298.15 K on the basis of the "TDB-4" guideline by the NEA [31].

2.3.6 Assignment of Uncertainties

Uncertainties of experimental and thermodynamic values should be assigned on the basis of the NEA's "TDB-3" guideline [16] Assignment of uncertainties for values obtained from chemical analogues and/or models, however, should be discussed because no guidelines are available. Assignment of uncertainties by an expert judgment (or "educated guess" in the TDB-1 [27]) would not be avoidable for some thermodynamic values. Propagation of uncertainties should be carefully treated so as not to overestimate uncertainties.

2.3.7 Use of Chemical Analogues and Models for Estimation of Thermodynamic Data

Some thermodynamic values which are important for the performance assessment of geological disposal of radioactive wastes should be selected even if the reliability of the values is questionable. In this case, the value may be selected as a tentative value, specifying low reliability of the value and the need for the value to be more reliably determined.

Application of chemical analogues should be considered to estimate thermodynamic values on some species which have not been published values based on experimental data. At the moment, application of a chemical analogue among actinoides with the same oxidation state should be considered. Some chemical analogues may be combined with chemical models that have been proposed to estimate thermodynamic values where no values based on experimental data are available. Some of the models are able to estimate thermodynamic values by semi-empirical and/or qualitative interactions between central atom and coordinated species [32-34] .

The selection of tentative values should be carried out with special care, and we should explain the procedure of the selection logically.

3. Selection and Refinement of Thermodynamic Data in JAEA-TDB-RN

This chapter describes selection and refinement of thermodynamic data in JAEA-TDB-RN with categorizing the following groups:

- Lanthanoides and actinoides: Sm, Ac, Th, Pa, U, Np, Pu, Am and Cm,
- Transient metals: Fe, Co, Ni, Zr, Nb, Mo, Tc and Pd
- Other elements: Se, Sn, Sb, Bi, Po and Ra, and
- Various elements with selected organic ligands (oxalate, citrate, ethylenediaminetetraacetate (EDTA) and isosaccharnate (ISA)).

All the selected data have been tabulated in Appendix A with order of atomic numbers and subsequent tables for various elements with selected organic ligands.

3.1 Discussion of Elements of Interest in Both JAEA-TDB-GC and JAEA-TDB-RN

Before starting the selection and refinement of thermodynamic data, selected thermodynamic data for Fe, Ni and Sn should be discussed, because the most of selected vales in JAEA-TDB-GC [17] are different from those in JAEA-TDB-RN and/or NEA-TDB.

3.1.1 Iron (Fe)

Although Fe is out of interest in JAEA-TDB-RN, selected thermodynamic data should be discussed because the NEA has published the selected data [18, 19]. The selected thermodynamic data for typical Fe species and compounds in JAEA-TDB-GC [17] and NEA-TDB [18, 19] are listed in Table 1. It is found that all the selected data are consistent within uncertainties. The author has accepted the selected values in JAEA-TDB-GC [17] due to comprehensiveness of the data and avoiding change of $\log_{10} K°$ values for iron-containing minerals. The author has also accepted the selected values in NEA-TDB that has not compiled in JAEA-TDB-GC [17]. Refinement of thermodynamic data has been performed based on the guideline in section 2.

3.1.2 Nickel (Ni)

Thermodynamic data for Ni have been selected in both JAEA-TDB-GC [17] and NEA-TDB [20]. The selected thermodynamic data for typical iron species and compounds in JAEA-TDB-GC and NEA-TDB are listed in Table 2. The author has accepted the selected data in NEA-TDB [20] because the selected data are more comprehensive than those in JAEA-TDB-GC [17] and have been critically reviewed. Refinment of thermodynamic data has been performed based on the guideline in section 2.

Table 1 Comparison of selected thermodynamic data for typical iron (Fe) species and compounds between JAEA-TDB-GC (GC) [17] and NEA-TDB (NEA) [18, 19]

Species / compound	$\Delta_f G°_m$ (kJ.mol^{-1})		$\Delta_f H°_m$ (kJ.mol^{-1})		$S°_m$ (J.K^{-1}.mol^{-1})		$C°_{p,m}$ (J.K^{-1}.mol^{-1})	
	GC	NEA	GC	NEA	GC	NEA	GC	NEA
α-Fe	0.000	0.000	0.000	0.000	27.280	27.085	24.978	25.084
					± 0.126	± 0.160	± 0.418	± 0.500
Fe^{2+}	-91.504	-90.719	-92.257	-90.295	-105.855	-102.171	-32.313	-23.000
	± 0.837	± 0.641	± 2.092	± 0.522	± 5.858	± 2.778		± 10.000
Fe^{3+}	-17.238	-16.226	-49.580	-50.056	-277.399	-282.404	-77.822	-108.000
	± 6.694	± 0.650	± 6.694	± 0.973	± 21.757	± 3.927		± 20.000
Fe_2O_3(hematite)	-745.505	-744.448	-827.260	-826.290	87.613	87.400	104.767	103.930
α-Fe_2O_3(cr)	± 1.255	± 2.632	± 1.255	± 2.630	± 1.255	± 0.160	± 1.674	± 0.170
Fe_3O_4(magnetite)	-1014.913	-1012.719	-1118.174	-1115.780	145.729	145.890	151.670	150.780
α-Fe_3O_4(cr)	± 3.347	± 1.609	± 3.347	± 1.600	± 0.418	± 0.300	± 1.255	± 1.250
$FeOH^+$	-275.600	-275.916	-326.812		-41.840		62.760	
	± 7.113	± 2.372	± 9.623		± 20.920			
$FeOH^{2+}$	-241.835	-241.094	-292.880	-299.886	-106.274	-132.871	-34.309	
	± 6.694	± 0.764		± 3.154		± 10.886		
FeS_2(pyrite)	-160.247	-162.219	-171.544	-173.630	52.928	52.920	62.099	62.270
	± 8.368	± 2.361	± 8.368	± 2.360	± 0.126	± 0.140	± 0.628	± 0.200

Table 2 Comparison of selected thermodynamic data for typical nickel (Ni) species and compounds between JAEA-TDB-GC (GC) [17] and NEA-TDB (NEA) [20]

Species / compound	$\Delta_f G°_m$ (kJ.mol^{-1})		$\Delta_f H°_m$ (kJ.mol^{-1})		$S°_m$ (J.K^{-1}.mol^{-1})		$C°_{p,m}$ (J.K^{-1}.mol^{-1})	
	GC	NEA	GC	NEA	GC	NEA	GC	NEA
Ni(cr)	0.000	0.000	0.000	0.000	29.874	29.870	25.773	26.070
					± 0.837	± 0.200	± 0.837	± 0.100
Ni^{2+}	-45.606	-45.773	-53.974	-55.012	-128.867	-131.800	-48.953	-46.100
	± 8.368	± 0.771	± 8.368	± 0.878	± 8.368	± 1.400		± 7.500
$NiOH^+$	-221.124	-228.458	-283.089	-287.042	-75.312		129.704	
		± 1.111		± 1.914				
β-$Ni(OH)_2$	-457.102	-457.100	-542.288	-542.300	79.998	80.000	82.015	82.010
	± 1.255	± 1.400	± 1.674	± 1.500	± 0.837	± 0.800	± 0.293	± 0.300
$Ni(OH)_3^-$	-580.187	-590.519	-782.730		-80.701		276.194	
		± 9.735						
$Ni(OH)_4^{2-}$	-742.978		-997.817		-22.912		77.504	
$NiCO_3$(aq)		-597.646						
		± 2.441						
$NiCO_3$(cr)		-636.416		-713.320		85.400		90.300
		± 1.292		± 1.424		± 2.000		± 4.100

3.1.3 Tin (Sn)

Thermodynamic data for Sn have been selected in both JAEA-TDB-GC [17] and NEA-TDB [24]. The selected thermodynamic data for typical Sn species and compounds in JAEA-TDB-GC [17] and NEA-TDB [24] are listed in Table 3. It is found that the selected $\Delta_f G°_m$ value of Sn^{4+} in NEA-TDB [24] are completely different from the conventional value selected in JAEA-TDB-GC [17] as hatched in Table 3, while other selected values are quite similar to each other. Although the author has mainly accepted the selected data in NEA-TDB [24] and those by Rai et al.[35] for Sn(IV)-OH^- system, the author has decided to accept thermodynamic data of aqueous species and compounds of tin selected in JAEA-TDB-GC [17] from the comprehensive point of view,

except for Sn^{4+} in NEA-TDB [24] due to reliability of potentiometric measurements conducted by Gajda et al. [36] Refinement of thermodynamic data has been performed based on the guideline in section 2.

Table 3 Comparison of selected thermodynamic data for typical tin (Sn) species and compounds between JAEA-TDB-GC (GC) [17] and NEA-TDB (NEA) [24]

Species / compound	$\Delta_f G°_m$ (kJ.mol^{-1})		$\Delta_f H°_m$ (kJ.mol^{-1})		$S°_m$ (J.K^{-1}.mol^{-1})		$C°_{p,m}$ (J.K^{-1}.mol^{-1})	
	GC	NEA	GC	NEA	GC	NEA	GC	NEA
β-Sn	0.000	0.000	0.000	0.000	51.170	51.180		27.110
					± 0.084	± 0.080		± 0.080
Sn^{2+}	-27.489	-27.390	-8.786	-9.617	-16.736	-19.889	-64.852	
	± 1.506	± 0.300	± 0.837	± 1.236	± 4.184	± 4.266		
Sn^{4+}	**2.469**	**46.711**	-28.451		-313.800		-96.650	
	± 1.757	**± 3.871**	± 62.760		± 209.200		± 20.920	
SnO_2(cassiterite)	-519.950	-516.640	-580.781	-577.630	52.300	51.770	54.572	55.260
	± 0.544	± 0.206	± 0.418	± 0.200	± 1.255	± 0.140	± 0.879	± 0.090
$SnOH^+$	-245.182	-244.381	-267.065		80.333		-53.974	
	± 2.929	± 2.303						
$Sn(OH)_3^-$	-644.294	-644.992	-796.621		109.253		-114.591	
	± 1.674	± 3.440						
$Sn(OH)_5^-$	-1137.630	-1132.965	-1379.607		144.030		40.769	
	± 4.184	± 2.379						
$Sn(OH)_6^{2-}$	-1316.663	-1312.625	-1689.838		-62.609		-62.337	
	± 2.092	± 1.839						

3.2 Lanthanoides and Actinoides

3.2.1 Thorium (Th)

Most of thermodynamic data for Th have been taken from NEA-TDB [25] and some literature values [37, 38]. Refinement of thermodynamic data has been performed based on the guideline in section 2.

3.2.2 Uranium (U), Neptunium (Np), Plutonium (Pu) and Americium (Am)

Most of thermodynamic data for U, Np, Pu and Am have been taken from NEA-TDB [23]. Some $\log_{10} K°$ values for hydrolysis species and carbonatehydroxo complexes of tetravalent actinoides (U, Np and Pu) have been taken from Fujiwara et al. [39].

Thermodynamic data for Pu(III) have been taken from those for Am(III) on the basis of chemical analogues [40] in the previous JAEA-TDB [11] because those for Am(III) have been more comprehensive than those for Pu(III). Refinement of thermodynamic data for Pu(III) has been performed in the present TDB as follows:

1. Accept thermodynamic data for Pu(III) in NEA-TDB [23],
2. Take from $\log_{10} K°$ values for the same chemical species and compounds of Am(III) [23] when those for Pu(III) are not available,
3. Calculate thermodynamic values on formation ($\Delta_f G°_m$, $\Delta_f H°_m$, $S°_m$) from those on reaction selected above, and

4. Calculate thermodynamic values on reaction ($\log_{10} K^{\circ}$, $\Delta_r G^{\circ}_m$, $\Delta_r H^{\circ}_m$ and $\Delta_r S^{\circ}_m$) using the selected values on formation ($\Delta_f G^{\circ}_m$, $\Delta_f H^{\circ}_m$ and S°_m).

The species and compounds of Pu(III) and Am(III) selected in NEA-TDB are listed in Table 4. Based on Table 4, $\log_{10} K°$ values for some hydrolysis species, hydroxides, halide complexes, nitrate complexes, phosphate complexes, carbonate complexes and silicate complexes have been taken from those for Am(III).

The latest $\log_{10} K°$ values for ISA complexes of U(IV/VI) ($U(OH)_4(isa)^-$, $U(OH)_4(isa)_2^{2-}$ and $UO_2(OH)_3(isa)_2^{3-}$) published by Kobayashi et al. [41] have been accepted in the present report.

Refinement of thermodynamic data has been performed based on the guideline in section 2.

Table 4 Species and compounds of Pu(III) and Am(III) of which thermodynamic data have been selected in NEA-TDB [23]

Pu(III)	Am(III)	Pu(III)	Am(III)
Pu^{3+}	Am^{3+}	PuOI(cr)	PuI_3(g)
Pu_2O_3(cr)			AmS(cr)
$PuOH^{2+}$	$AmOH^{+2}$	$PuSO_4^+$	$AmSO_4^+$
	$Am(OH)_2^+$	$Pu(SO_4)_2^-$	$Am(SO_4)_2^-$
$Pu(OH)_3$(cr)	$Am(OH)_3$(cr)		AmN_3^{2+}
	$Am(OH)_3$(am)		$AmNO_2^{2+}$
	$Am(OH)_3$(aq)		$AmNO_3^{2+}$
	AmF^{+2}	$PuPO_4$(s, hyd)	$AmPO_4$(am,hyd)
	AmF_2^+		$AmH_2PO_4^{2+}$
PuF_3(cr)	AmF_3(cr)		$AmCO_3^+$
PuF_3(g)	AmF_3(g)		$Am(CO_3)_2^-$
PuOF(cr)			$Am(CO_3)_3^{3-}$
$PuCl^{2+}$	$AmCl^{2+}$		$Am_2(CO_3)_3$(am)
	$AmCl_2^+$		$AmHCO_3^{2+}$
$PuCl_3$(cr)	$AmCl_3$(cr)		$AmCO_3OH·0.5H_2O$(cr)
$PuCl_3$(g)			$AmCO_3OH$(am,hyd)
PuOCl(cr)	AmOCl(cr)		$AmSiO(OH)_3^{2+}$
$PuCl_3·6H_2O$(cr)		$PuSCN^{2+}$	$AmSCN^{2+}$
$PuBr_3$(cr)	$AmBr_3$(cr)		$NaAm(CO_3)_2·5H_2O$(cr)
$PuBr_3$(g)		Cs_3PuCl_6(cr)	
PuOBr(cr)	AmOBr(cr)	$CsPu_2Cl_7$(cr)	
PuI^{2+}		$Cs_2NaPuCl_6$(cr)	$Cs_2NaAmCl_6$(cr)
PuI_3(cr)	AmI_3(cr)		

3.2.3 Samarium (Sm), Actinium (Ac) and Curium (Cm)

Since thermodynamic data for Sm, Ac and Cm have not been selected in NEA-TDB, $\log_{10} K°$ values for these elements have been taken from those for Am(III) on the basis of chemical analogues [40] in the previous JAEA-TDB [11]. The author has accepted the selected $\log_{10} K°$ values and calculated $\Delta_r G^{\circ}_m$ values for Sm using $\Delta_r G^{\circ}_m$ of Sm^{3+} selected by Wagman et al. [15]. Refinement of thermodynamic data has been performed based on the guideline in section 2.

3.2.4 Protactinium (Pa)

Since thermodynamic data for Pa have not been selected in NEA-TDB, $\log_{10} K°$ values for these elements have been taken from the previous JAEA-TDB [11] without any refinements.

3.3 Other Elements

3.3.1 Selenium (Se), Zirconium (Zr) and Technetium (Tc)

Most of thermodynamic data for Se, Zr and Tc have been taken from NEA-TDB [21-23]. Some $\log_{10} K°$ values for some species and compounds of these elements have been taken from elsewhere [42-44]. Refinement of thermodynamic data has been performed based on the guideline in section 2.

3.3.2 Cobalt (Co), Niobium (Nb), Molybdenum (Mo) and Palladium (Pd)

Since thermodynamic data for Co, Nb, Mo and Pd have not been selected in NEA-TDB, $\log_{10} K°$ values for these elements have been taken from the previous JAEA-TDB [11] without any refinements. Values of the change in Gibbs free energy of formation ($\Delta_r G°_m$) for species and compounds of Co, Mo and Pd have been calculated using the selected $\log_{10} K°$ values and $\Delta_r G°_m$ vales of Co(cr), Mo(cr) and Pd(cr), respectively, selected by Wagman et al. [15]

3.3.3 Antimony (Sb), Bismuth (Bi), Polonium (Po)

Since thermodynamic data for Sb, Bi and Po have not been selected in NEA-TDB, $\log_{10} K°$ values for these elements have been taken from the previous JAEA-TDB [11] without any refinements. Values of the change in Gibbs free energy of formation ($\Delta_r G°_m$) for species and compounds of Sb and Bi have been calculated using the selected $\log_{10} K°$ values and $\Delta_r G°_m$ vales of Sb(cr) and Bi(cr), respectively, selected by Wagman et al. [15]

3.3.4 Radium (Ra)

Thermodynamic data for Ra have been extended and refined using a model on correlation of those with ionic radius among alkaline earth metal ions [45]. Prediction of $\Delta_f G°_m$ and $S°_m$ has been performed through extrapolation of thermodynamic data for strontium and barium selected in JAEA-TDB-GC [17]. Other thermodynamic data have been calculated from the predicted $\Delta_f G°_m$ and $S°_m$ values.

Evaluation of thermodynamic data for $SrSO_4$(aq) and $BaSO_4$(aq) have been performed in the prediction [45] as shown in Figure 3. The predicted values are listed in Table 5. These evaluated data will be compiled into the next update of JAEA-TDB-GC [17].

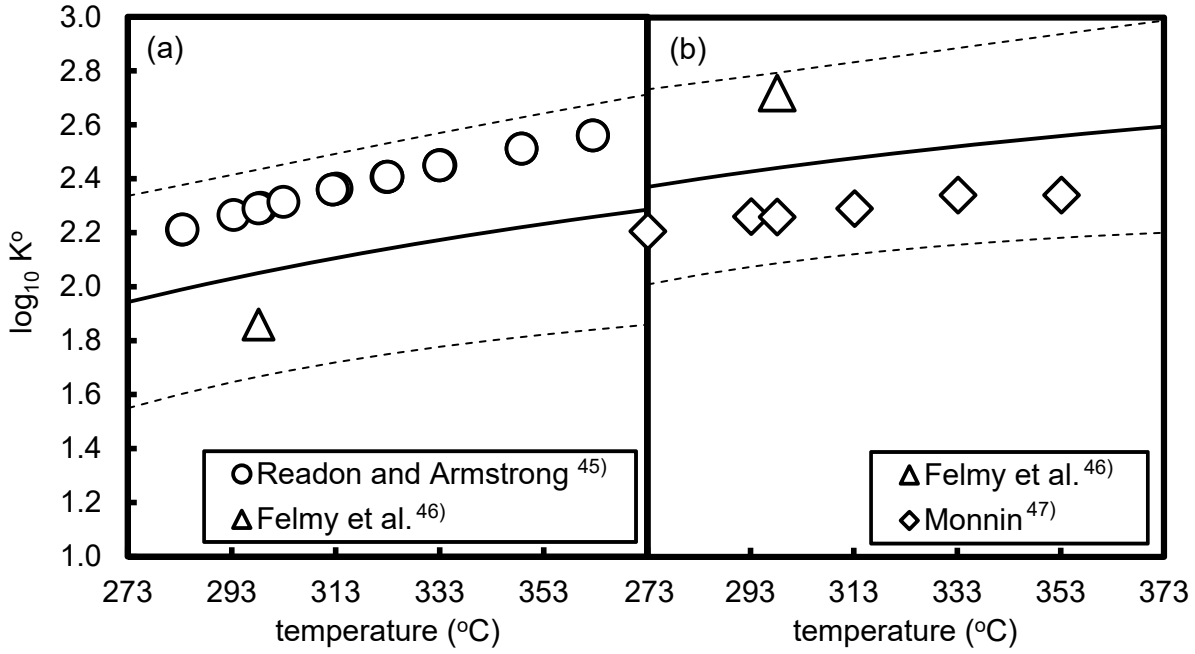

Figure 3 Evaluation of formation constant of (a) $SrSO_4$(aq) and (b) $BaSO_4$(aq) at the standard state

Table 5 Thermodynamic data of $SrSO_4$(aq) and $BaSO_4$(aq) used for prediction of thermodynamic data for radium [45)]

Species	$\Delta_f G^0_m$ (kJ.mol^{-1})	$\Delta_f H^0_m$ (kJ.mol^{-1})	S^0_m (J.K^{-1}.mol^{-1})	Reaction	$\log_{10} K°$	$\Delta_r G^0_m$ (kJ.mol^{-1})	$\Delta_r H^0_m$ (kJ.mol^{-1})	$\Delta_r S^0_m$ (J.K^{-1}.mol^{-1})
$SrSO_4$(aq)	-1320.000 ± 2.000	-1453.887 ± 5.173	49.000 ± 16.000	$Sr^{2+} + SO_4^{2-}$ ⇄ $SrSO_4$(aq)	2.051 ± 0.386	-11.705 ± 2.201	6.622 ± 5.214	61.678 ± 16.133
$BaSO_4$(aq)	-1316.000 ± 1.000	-1439.988 ± 4.589	89.000 ± 15.000	$Ba^{2+} + SO_4^{2-}$ ⇄ $BaSO_4$(aq)	2.442 ± 0.351	-13.939 ± 2.003	4.245 ± 4.902	61.386 ± 15.014

All the selected data have been re-calculated by the author due to give thermodynamic data to three decimal places.

3.4 Various Elements with Selected Organics

As mentioned above, the author decided to select four organic ligands (oxalate, citrate, EDTA and ISA) for elements of interest. Most of thermodynamic data for Ni, Se, Zr, Tc, U, Np, Pu and Am with the selected organic ligands have been taken from NEA-TDB [14)]. Equilibrium constant ($\log_{10} K°$) values for other elements have been estimated using a linear-free energy relationship (LFER) [49)]. Many $\log_{10} K°$ value for metal ions with ISA have been updated in the previous JAEA-TDB [11)] mainly based on the latest review [50, 51)]. Refinement of thermodynamic data has been performed based on the guideline in section 2.

4. Preparation of Text Files for Geochemical Calculation Programs

Text files of JAEA-TDB-RN in 2020 for PHREEQC [7] and Geochemist's Workbench [8] have been provided as shown in Table 6. Integration between JAEA-TDB-RN and JAEA-TDB-GC [17] has been performed in these files; therefore calculation of solubility and speciation of radionuclides as well as that of geochemical reactions is available. These files are enclosed in CD-ROM and also available via the Internet with our Website (https://migrationdb.jaea.go.jp/).

Tiny revision of the files may be carried out after publication of the present report for some reasons. The number just before the extension (i.e., *n* in 210329x*n*.tdb; x: c, s or g) will be increased when revised. The revised text files will be uploaded to our Website (https://migrationdb.jaea.go.jp/) when necessary.

Table 6 Correspondence among file name, TDB type and geochemical calculation program of text files of JAEA-TDB-RN in 2020

File name	TDB type	Corresponding geochemical calculation program
201203c0.tdb	JAEA-TDB-RN in 2020	PHREEQC without using SIT
201203s0.tdb	JAEA-TDB-RN in 2020	PHREEQC using SIT
201203g0.tdb	JAEA-TDB-RN in 2020	Geochemist's Workbench

5. Conclusions

JAEA's Thermodynamic Database for solubility and speciation of radionuclides (JAEA-TDB-RN) has been updated. Additional selection of thermodynamic data at standard state on formation and reaction as well as logarithm of equilibrium constant ($\log_{10} K°$) has been performed. Furthermore, refinement of many thermodynamic data has also been carefully and successfully carried out to make internal consistency with JAEA-TDB for geochemical reactions (JAEA-TDB-GC). The extent of selection of these thermodynamic data enables to evaluate solubility and speciation of radionuclides at temperatures other than 298.15 K. Text files of the updated JAEA-TDB after ingegrating JAEA-TDB-GC and JAEA-TDB-RN have been provided for geochemical calculation programs of PHREEQC and Geochemist's Workbench.

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Appendix 1 Updated Thermodynamic Data Compiled for JAEA-TDB

Selected thermodynamic data for aqueous species, solid phases and gaseous species in the present update of JAEA-TDB-RN are shown in Tables A1 – A23 with order of atomic number of elements of interest and Tables A24 and A25 for various elements with selected organic ligands (oxalate, citrate, EDTA and ISA).

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Table A1 Selected thermodynamic data for iron (Fe) in JAEA-TDB-RN in 2020 (1/10)

Values indicated by **boldface** are calculated and selected in the present report.

Species / compound	$\Delta_f G^0_m$ (kJ.mol^{-1})	$\Delta_f H^0_m$ (kJ.mol^{-1})	S^0_m (J.K^{-1}.mol^{-1})	$C^0_{p,m}$ (J.K^{-1}.mol^{-1})	Reaction	$\log_{10} K°$	$\Delta_r G^0_m$ (kJ.mol^{-1})	$\Delta_r H^0_m$ (kJ.mol^{-1})	$\Delta_r S^0_m$ (J.K^{-1}.mol^{-1})
α-Fe	0.000	0.000	27.280	24.978					
			± 0.126	± 0.418					
	[2020JAE]	[2020JAE]	[2020JAE]	[2020JAE]					
Fe^{2+}	-91.504	-92.257	-105.855	-32.313	α-Fe + 2 H^+ ⇄ Fe^{2+} + H_2(g)	**16.031**	**-91.504**	**-92.257**	**-2.456**
	± 0.837	± 2.092	± 5.858			**± 0.147**	**± 0.837**	**± 2.092**	**± 5.859**
	[2020JAE]	[2020JAE]	[2020JAE]	[2020JAE]					
Fe^{3+}	-17.238	-49.580	-277.399	-77.822	Fe^{2+} + H^+ ⇄ Fe^{3+} + 0.5 H_2(g)	**-13.011**	**74.266**	**42.677**	**-106.205**
	± 6.694	± 6.694	± 21.757			**± 1.182**	**± 6.746**	**± 7.014**	**± 22.532**
	[2020JAE]	[2020JAE]	[2020JAE]	[2020JAE]					
$Fe_{0.932}O$(cr)	-244.593	-265.800	56.69	48.970	0.932 Fe^{2+} + H_2O(l) ⇄ $Fe_{0.932}O$(cr) + 2 H^+ + 0.136 e^-	**-13.642**	**77.871**	**106.022**	**94.310**
	± 1.906	± 1.900	± 0.490	± 0.290		**± 0.361**	**± 2.062**	**± 2.724**	**± 5.482**
	[2013LEM/BER]	[2013LEM/BER]	[2013LEM/BER]	[2013LEM/BER]					
FeO(s)	-251.458	-272.044	60.752	49.919	Fe^{2+} + H_2O(l) ⇄ FeO(s) + 2 H^+	**-13.530**	**77.228**	**106.052**	**96.684**
	± 2.510	± 2.092	± 1.674	± 0.544		**± 0.464**	**± 2.648**	**± 2.960**	**± 6.093**
	[2020JAE]	[2020JAE]	[2020JAE]	[2020JAE]					
Fe_2O_3(hematite)	-745.505	-827.260	87.613	104.767	2 Fe^{3+} + 3 H_2O(l) ⇄ Fe_2O_3(hematite) + 6 H^+	**-0.091**	**0.519**	**129.415**	**432.642**
	± 1.255	± 1.255	± 1.255	± 1.674		**± 2.356**	**± 13.451**	**± 13.451**	**± 43.532**
	[2020JAE]	[2020JAE]	[2020JAE]	[2020JAE]					
Fe_2O_3(maghemite)	-728.853	-808.976	93.052	104.977	2 Fe^{3+} + 3 H_2O(l) ⇄ Fe_2O_3(maghemite) + 6 H^+	**-3.008**	**17.171**	**147.699**	**438.082**
	± 8.368	± 8.368	± 0.418	± 1.674		**± 2.767**	**± 15.792**	**± 15.792**	**± 43.516**
	[2020JAE]	[2020JAE]	[2020JAE]	[2020JAE]					
Fe_3O_4(magnetite)	-1014.913	-1118.174	145.729	151.670	Fe^{2+} + 2 Fe^{3+} + 4 H_2O(l) ⇄ Fe_3O_4(magnetite) + 8 H^+	**-10.476**	**59.798**	**216.597**	**526.690**
	± 3.347	± 3.347	± 0.418	± 1.255		**± 2.423**	**± 13.832**	**± 13.965**	**± 43.909**
	[2020JAE]	[2020JAE]	[2020JAE]	[2020JAE]					
FeOOH(goethite)	-490.114	-560.991	59.831	78.032	Fe^{3+} + 2 H_2O(l) ⇄ FeOOH(goethite) + 3 H^+	**-0.261**	**1.490**	**60.266**	**197.384**
	± 2.092	± 2.092	± 2.092	± 0.837		**± 1.229**	**± 7.017**	**± 7.017**	**± 21.858**
	[2020JAE]	[2020JAE]	[2020JAE]	[2020JAE]					
FeOOH(lepidocrocite)	-479.905	-549.192	65.078	69.061	Fe^{3+} + 2 H_2O(l) ⇄ FeOOH(lepidocrocite) + 3 H^+	**-2.049**	**11.698**	**72.065**	**202.631**
	± 2.092	± 2.092	± 0.293	± 0.544		**± 1.229**	**± 7.017**	**± 7.017**	**± 21.759**
	[2020JAE]	[2020JAE]	[2020JAE]	[2020JAE]					
β-FeOOH·0.652H_2O·0.0096HCl(cr)			81.800	91.100					
			± 2.000	± 2.000					
			[2020LEM/PAL]	[2020LEM/PAL]					
$FeOH^+$	-275.600	-326.812	-41.840	62.760	Fe^{2+} + H_2O(l) ⇄ $FeOH^+$ + H^+	**-9.300**	**53.087**	**51.283**	**-5.908**
	± 7.113	± 9.623	± 20.920			**± 1.255**	**± 7.163**	**± 9.849**	**± 21.725**
	[2020JAE]	[2020JAE]	[2020JAE]	[2020JAE]					
$FeOH^{2+}$	-241.835	-292.880	-106.274	-34.309	Fe^{3+} + H_2O(l) ⇄ $FeOH^{2+}$ + H^+	**-2.205**	**12.585**	**42.539**	**101.203**
	± 6.694					**± 1.659**	**± 9.468**		
	[2020JAE]	[2020JAE]	[2020JAE]	[2020JAE]					

Table A1 Selected thermodynamic data for iron (Fe) in JAEA-TDB-RN in 2020 (2/10)

Species / compound	$\Delta_f G^0_m$ (kJ.mol^{-1})	$\Delta_f H^0_m$ (kJ.mol^{-1})	S^0_m (J.K^{-1}.mol^{-1})	$C^0_{p,m}$ (J.K^{-1}.mol^{-1})	Reaction	$\log_{10} K°$	$\Delta_r G^0_m$ (kJ.mol^{-1})	$\Delta_r H^0_m$ (kJ.mol^{-1})	$\Delta_r S^0_m$ (J.K^{-1}.mol^{-1})
$Fe(OH)_2$(am)	-485.386	-567.350	87.864	91.257	$Fe^{2+} + 2\ H_2O(l) \rightleftarrows Fe(OH)_2(am) + 2\ H^+$	**-14.100**	**80.483**	**96.583**	**53.873**
	± 4.184	± 12.552	± 41.840			**± 0.748**	**± 4.272**	**± 12.727**	**± 42.248**
	[2020JAE]	[2020JAE]	[2020JAE]	[2020JAE]					
$Fe(OH)_2$(mic)	-493.377	-575.300	88.282	91.257	$Fe^{2+} + 2\ H_2O(l) \rightleftarrows Fe(OH)_2(mic) + 2\ H^+$	**-12.700**	**72.492**	**88.634**	**54.292**
	± 5.021	± 12.134	± 46.024			**± 0.892**	**± 5.094**	**± 12.314**	**± 46.396**
	[2020JAE]	[2020JAE]	[2020JAE]	[2020JAE]					
$Fe(OH)_2$(aq)	-449.403	-549.276	29.288	75.362	$Fe^{2+} + 2\ H_2O(l) \rightleftarrows Fe(OH)_2(aq) + 2\ H^+$	**-20.404**	**116.466**	**114.658**	**-4.703**
	± 8.786	± 12.134	± 25.104			**± 1.547**	**± 8.828**	**± 12.314**	**± 25.779**
	[2020JAE]	[2020JAE]	[2020JAE]	[2020JAE]					
$Fe(OH)_2^+$	-459.361	-541.087	23.481	-125.888	$Fe^{3+} + 2\ H_2O(l) \rightleftarrows Fe(OH)_2^+ + 2\ H^+$	-4.800	27.399		
	± 6.694					± 0.400	27.399		
	[2020JAE]	[2020JAE]	[2020JAE]	[2020JAE]		[2013LEM/BER]	[2013LEM/BER]		
$Fe_2(OH)_2^{4+}$	**-492.744**	**-626.837**	**-321.364**		$2\ Fe^{3+} + 2\ H_2O(l) \rightleftarrows Fe_2(OH)_2^{4+} + 2\ H^+$	-2.820	16.097	44.000	93.588
	± 13.405	**± 13.722**	**± 44.712**			± 0.110	± 0.628	± 3.000	± 10.280
						[2013LEM/BER]	[2013LEM/BER]	[2013LEM/BER]	[2013LEM/BER]
$Fe(OH)_3$(am)	-706.301	-825.712	129.997	111.357	$Fe^{3+} + 3\ H_2O(l) \rightleftarrows Fe(OH)_3(am) + 3\ H^+$	**-3.939**	**22.485**	**81.383**	**197.627**
	± 3.766	± 2.092	± 10.042			**± 1.347**	**± 7.687**	**± 7.021**	**± 23.964**
	[2020JAE]	[2020JAE]	[2020JAE]	[2020JAE]					
$Fe(OH)_3$(mic)	-710.527	-829.938	129.997	109.997	$Fe^{3+} + 3\ H_2O(l) \rightleftarrows Fe(OH)_3(mic) + 3\ H^+$	**-3.199**	**18.259**	**77.157**	**197.627**
	± 3.766	± 2.092	± 10.042			**± 1.347**	**± 7.687**	**± 7.021**	**± 23.964**
	[2020JAE]	[2020JAE]	[2020JAE]	[2020JAE]					
$Fe(OH)_3$(aq)	-647.181	-831.779	-88.282	149.419	$Fe^{3+} + 3\ H_2O(l) \rightleftarrows Fe(OH)_3(aq) + 3\ H^+$	**-14.296**	**81.605**	**75.316**	**-20.652**
	± 7.113	± 20.920	± 75.312			**± 1.712**	**± 9.772**	**± 21.967**	**± 78.392**
	[2020JAE]	[2020JAE]	[2020JAE]	[2020JAE]					
$Fe(OH)_3^-$	-636.345	-812.031	7.113	167.410	$Fe^{2+} + 3\ H_2O(l) \rightleftarrows Fe(OH)_3^- + 3\ H^+$	**-29.206**	**166.707**	**137.741**	**-96.801**
	± 8.368	± 15.062	± 29.288			**± 1.474**	**± 8.415**	**± 15.210**	**± 29.869**
	[2020JAE]	[2020JAE]	[2020JAE]	[2020JAE]					
$Fe(OH)_4^-$	-840.482	-1018.804	165.268	221.752	$Fe^{3+} + 4\ H_2O(l) \rightleftarrows Fe(OH)_4^- + 4\ H^+$	**-21.984**	**125.487**	**174.130**	**162.975**
	± 6.694	± 12.552	± 33.472	± 41.840		**± 1.660**	**± 9.476**	**± 14.232**	**± 39.923**
	[2020JAE]	[2020JAE]	[2020JAE]	[2020JAE]					
FeF^+	-381.413	-424.467	-87.446	87.186	$Fe^{2+} + F^- \rightleftarrows FeF^+$	**1.429**	**-8.159**	**3.138**	**31.589**
	[2020JAE]	[2020JAE]	[2020JAE]	[2020JAE]					
FeF^{2+}	-333.256	-364.594	-107.529	31.957	$Fe^{3+} + F^- \rightleftarrows FeF^{2+}$	**6.003**	**-34.267**	**20.334**	**183.050**
	[2020JAE]	[2020JAE]	[2020JAE]	[2020JAE]					
FeF_2(cr)	-669.499	-712.100	86.990	68.090	$Fe^{2+} + 2\ F^- \rightleftarrows FeF_2(cr)$	**2.539**	**-14.494**	**50.852**	**219.204**
	± 8.500	± 8.500	± 0.200	± 0.500		**± 1.515**	**± 8.645**	**± 8.855**	**± 5.961**
	[2013LEM/BER]	[2013LEM/BER]	[2013LEM/BER]	[2013LEM/BER]					
FeF_3(cr)		-991.700		91.300	$Fe^{3+} + 3\ F^- \rightleftarrows FeF_3(cr)$			**63.923**	
		± 10.000		± 2.000				**± 12.200**	
		[2013LEM/BER]		[2013LEM/BER]					

Table A1 Selected thermodynamic data for iron (Fe) in JAEA-TDB-RN in 2020 (3/10)

Species / compound	$\Delta_f G^0_m$ (kJ.mol^{-1})	$\Delta_f H^0_m$ (kJ.mol^{-1})	S^0_m (J.K^{-1}.mol^{-1})	$C^0_{p,m}$ (J.K^{-1}.mol^{-1})	Reaction	$\log_{10} K°$	$\Delta_r G^0_m$ (kJ.mol^{-1})	$\Delta_r H^0_m$ (kJ.mol^{-1})	$\Delta_r S^0_m$ (J.K^{-1}.mol^{-1})
$FeCl^+$	-221.878 [2020JAE]	-256.312 [2020JAE]	-42.258 [2020JAE]	86.190 [2020JAE]	$Fe^{2+} + Cl^- \rightleftarrows FeCl^+$	**-0.161**	**0.916**	**3.025**	**6.862**
$FeCl^{2+}$	-156.984 [2020JAE]	-212.631 [2020JAE]	-178.657 [2020JAE]	14.096 [2020JAE]	$Fe^{3+} + Cl^- \rightleftarrows FeCl^{2+}$	**1.481**	**-8.456**	**4.029**	**42.007**
$FeCl_2$(aq)	-307.440 [2020JAE]	-328.402 [2020JAE]	179.912 [2020JAE]	122.173 [2020JAE]	$Fe^{2+} + 2\ Cl^- \rightleftarrows FeCl_2$(aq)	**-8.171**	**46.643**	**98.014**	**172.297**
$FeCl_2^+$	**-292.269** [2020JAE]				$Fe^{3+} + 2\ Cl^- \rightleftarrows FeCl_2^+$	0.700 ± 0.200 [2013LEM/BER]	-3.996 ± 1.142 [2013LEM/BER]		
$FeCl_2$(s)	-302.189 ± 0.544 [2020JAE]	-341.532 ± 0.502 [2020JAE]	118.198 ± 0.418 [2020JAE]	76.776 ± 0.837 [2020JAE]	$Fe^{2+} + 2\ Cl^- \rightleftarrows FeCl_2$(s)	**-9.091 ± 0.178**	**51.894 ± 1.018**	**84.885 ± 2.159**	**110.583 ± 5.882**
$FeCl_2 \cdot H_2O$(cr)	**-514.373 ± 2.071**				H_2O(l) + $FeCl_2$(cr) ⇄ $FeCl_2 \cdot H_2O$(cr)	-4.380 ± 0.350 [2013LEM/BER]	25.000 ± 2.000 [2013LEM/BER]		
$FeCl_2 \cdot 2H_2O$(cr)	**-804.870**				$FeCl_2 \cdot 4H_2O$(cr) ⇄ $FeCl_2 \cdot 2H_2O$(cr) + 2 H_2O(g)	-4.131 ± 0.263 [2013LEM/BER]	23.580 ± 1.500 [2013LEM/BER]		
$FeCl_2 \cdot 4H_2O$(cr)	**-1284.715 ± 1.205**	**-1547.687 ± 3.266**	**300.615 ± 11.269**		4 H_2O(l) + $FeCl_2$(cr) ⇄ $FeCl_2 \cdot 4H_2O$(cr)	5.921 ± 0.176 [2013LEM/BER]	-33.795 ± 1.007 [2013LEM/BER]	-62.800 ± 3.200 [2013LEM/BER]	-97.283 ± 11.252 [2013LEM/BER]
$FeCl_3$(aq)	**-416.709 ± 1.146**				$FeCl_2^+ + Cl^- \rightleftarrows FeCl_3$(aq)	-1.200 ± 0.200 [2013LEM/BER]	6.850 ± 1.142 [2013LEM/BER]		
$FeCl_3$(s)	-331.515 ± 0.251 [2020JAE]	-395.982 ± 0.084 [2020JAE]	145.478 ± 0.837 [2020JAE]	96.609 ± 0.837 [2020JAE]	$Fe^{3+} + 3\ Cl^- \rightleftarrows FeCl_3$(s)	**-13.944 ± 1.175**	**79.592 ± 6.706**	**154.837 ± 6.700**	**252.672 ± 21.779**
$FeCl_3 \cdot 2H_2O$(cr)		-1011.446 ± 1.503 [2013LEM/BER]			$Fe^{3+} + 3\ Cl^- + 2\ H_2O$(l) ⇄ $FeCl_3 \cdot 2H_2O$(cr)			**111.050 ± 6.869**	
$FeCl_3 \cdot 2.5H_2O$(cr)		-1162.386 ± 1.503 [2013LEM/BER]			$Fe^{3+} + 3\ Cl^- + 2.5\ H_2O$(l) ⇄ $FeCl_3 \cdot 2.5H_2O$(cr)			**103.029 ± 6.871**	
$FeCl_3 \cdot 3.5H_2O$(cr)		-1473.416 ± 1.503 [2013LEM/BER]			$Fe^{3+} + 3\ Cl^- + 3.5\ H_2O$(l) ⇄ $FeCl_3 \cdot 3.5H_2O$(cr)			**77.838 ± 6.876**	
$FeCl_3 \cdot 6H_2O$(cr)		-2221.926 ± 1.503 [2013LEM/BER]		342.000 ± 4.000 [2013LEM/BER]	$Fe^{3+} + 3\ Cl^- + 6\ H_2O$(l) ⇄ $FeCl_3 \cdot 6H_2O$(cr)			**43.923 ± 6.895**	

Table A1 Selected thermodynamic data for iron (Fe) in JAEA-TDB-RN in 2020 (4/10)

Species / compound	$\Delta_f G^0_m$ (kJ.mol^{-1})	$\Delta_f H^0_m$ (kJ.mol^{-1})	S^0_m (J.K^{-1}.mol^{-1})	$C^0_{p,m}$ (J.K^{-1}.mol^{-1})	Reaction	$\log_{10} K°$	$\Delta_r G^0_m$ (kJ.mol^{-1})	$\Delta_r H^0_m$ (kJ.mol^{-1})	$\Delta_r S^0_m$ (J.K^{-1}.mol^{-1})
$FeCl_4^-$	**-536.583**				$FeCl_3(aq) + Cl^- \rightleftarrows FeCl_4^-$	-2.000	11.416		
	± 4.158					± 0.700	± 3.996		
						[2013LEM/BER]	[2013LEM/BER]		
FeOCl(cr)	-358.618	-405.875	82.700	70.490	$Fe^{3+} + Cl^- + H_2O(l) \rightleftarrows FeOCl(cr) + 2\ H^+$	**-4.746**	**27.092**	**96.623**	**233.441**
	± 3.002	± 3.001	± 0.200	± 0.200		**± 1.286**	**± 7.338**	**± 7.338**	**± 21.759**
	[2013LEM/BER]	[2013LEM/BER]	[2013LEM/BER]	[2013LEM/BER]					
β-$Fe_2Cl(OH)_3$(s)	**-927.668**				$2\ Fe^{2+} + Cl^- + 3\ H_2O(l) \rightleftarrows \beta\text{-}Fe_2Cl(OH)_3(s) + 3\ H^+$	-17.200	98.178		
	± 2.051					± 0.200	± 1.142		
						[2020LEM/PAL]	[2020LEM/PAL]		
$FeBr_2$(cr)	-235.779	-247.495	140.000	80.230	$Fe^{2+} + 2\ Br^- \rightleftarrows FeBr_2(cr)$	**-11.179**	**63.812**	**87.769**	**80.169**
	± 1.337	± 0.989	± 3.000	± 1.200		**± 0.282**	**± 1.612**	**± 2.334**	**± 6.594**
	[2013LEM/BER]	[2013LEM/BER]	[2013LEM/BER]	[2013LEM/BER]					
$FeBr_3$(cr)	-240.767	-262.592	182.200		$Fe^{3+} + 3\ Br^- \rightleftarrows FeBr_3(cr)$	**-15.522**	**88.602**	**151.498**	**211.070**
	± 2.471	± 0.628	± 8.000			**± 1.253**	**± 7.154**	**± 6.739**	**± 23.189**
	[2013LEM/BER]	[2013LEM/BER]	[2013LEM/BER]						
FeI_2(cr)	-127.076	-117.900	174.000	83.690	$Fe^{2+} + 2\ I^- \rightleftarrows FeI_2(cr)$	**-11.961**	**68.275**	**88.162**	**66.471**
	± 7.783	± 5.000	± 20.000	± 5.000		**± 1.402**	**± 8.005**	**± 5.673**	**± 20.844**
	[2013LEM/BER]	[2013LEM/BER]	[2013LEM/BER]	[2013LEM/BER]					
FeS(pyrrhotite)	-100.751	-100.416	60.312	54.647	$Fe^{2+} + HS^- \rightleftarrows FeS(pyrrhotite) + H^+$	**3.716**	**-21.213**	**7.950**	**97.968**
	± 0.418	± 0.418	± 0.042			**± 0.180**	**± 1.025**		
	[2020JAE]	[2020JAE]	[2020JAE]	[2020JAE]					
FeS(s, mackinawaite)	**-97.720**				$Fe^{2+} + H_2S(aq) \rightleftarrows FeS(s, mackinawaite) + 2\ H^+$	-3.800	21.691		
						± 0.400	± 2.283		
						[2013LEM/BER]	[2013LEM/BER]		
$Fe_{1.000}S$(cr, troilite)	-101.259	-100.910	60.310	50.610	$Fe^{2+} + HS^- \rightleftarrows Fe_{1.000}S(cr, troilite) + H^+$	**3.805**	**-21.721**	**7.456**	**97.966**
	± 2.002	± 2.000	± 0.220	± 0.170		**± 0.387**	**± 2.210**		
	[2020LEM/PAL]	[2020LEM/PAL]	[2020LEM/PAL]	[2020LEM/PAL]					
$Fe_{11/12}S$(cr, 6*C* pyrrhotite)		-97.480			$0.917\ Fe^{2+} + HS^- \rightleftarrows Fe_{11/12}S(cr, 6C\ pyrrhotite) + H^+$			**3.198**	
		± 3.930							
		[2020LEM/PAL]							
$Fe_{9/10}S$(cr, 5*C* pyrrhotite)	-97.893	-95.890	63.150	51.140	$0.9\ Fe^{2+} + HS^-$	**4.819**	**-27.506**	**3.250**	**103.288**
	± 2.232	± 2.230	± 0.250	± 0.300	$\rightleftarrows Fe_{9/10}S(cr, 5C\ pyrrhotite) + H^+ + 0.2\ e^-$	**± 0.419**	**± 2.393**		
	[2020LEM/PAL]	[2020LEM/PAL]	[2020LEM/PAL]	[2020LEM/PAL]					
$Fe_{0.875}S$(cr, 4*C* pyrrhotite)	-97.005	-95.530	60.700	49.880	$0.875\ Fe^{2+} + HS^-$	**5.064**	**-28.905**	**1.303**	**101.459**
	± 2.003	± 2.000	± 0.340	± 0.350	$\rightleftarrows Fe_{0.875}S(cr, 4C\ pyrrhotite) + H^+ + 0.25\ e^-$	**± 0.381**	**± 2.173**		
	[2020LEM/PAL]	[2020LEM/PAL]	[2020LEM/PAL]	[2020LEM/PAL]					
FeS_2(cr, pyrite)	-160.247	-171.544	52.928	62.099	$Fe^{2+} + 2\ HS^- \rightleftarrows FeS_2(cr, pyrite) + 2\ H^+ + 2\ e^-$	**16.236**	**-92.676**	**-47.070**	**153.063**
	± 8.368	± 8.368	± 0.126	± 0.628		**± 1.481**	**± 8.451**		
	[2020JAE]	[2020JAE]	[2020JAE]	[2020JAE]					
FeS_2(cr, marcasite)	-158.317	-169.430	53.920	62.660	$Fe^{2+} + 2\ HS^- \rightleftarrows FeS_2(cr, marcasite) + 2\ H^+ + 2\ e^-$	**15.898**	**-90.745**	**-44.956**	**154.056**
	± 2.442	± 2.438	± 0.410	± 0.400		**± 0.475**	**± 2.714**		
	[2020LEM/PAL]	[2020LEM/PAL]	[2020LEM/PAL]	[2020LEM/PAL]					

Table A1 Selected thermodynamic data for iron (Fe) in JAEA-TDB-RN in 2020 (5/10)

Species / compound	$\Delta_f G^0_m$ (kJ.mol^{-1})	$\Delta_f H^0_m$ (kJ.mol^{-1})	S^0_m (J.K^{-1}.mol^{-1})	$C^0_{p,m}$ (J.K^{-1}.mol^{-1})	Reaction	$\log_{10} K°$	$\Delta_r G^0_m$ (kJ.mol^{-1})	$\Delta_r H^0_m$ (kJ.mol^{-1})	$\Delta_r S^0_m$ (J.K^{-1}.mol^{-1})
Fe_3S_4(cr, greigite)	-309.000 ± 10.000 [2020LEM/PAL]				3 Fe^{2+} + 4 HS^- ⇄ Fe_3S_4(cr, greigite) + 4 H^+ + 2 e^-	**14.427 ± 1.830**	**-82.353 ± 10.445**		
$FeSO_4^+$	**-785.956 ± 6.734**				Fe^{3+} + SO_4^{2-} ⇄ $FeSO_4^+$	4.250 ± 0.100 [2013LEM/BER]	-24.259 ± 0.571 [2013LEM/BER]		
$FeSO_4$(s)	-825.085 ± 8.368 [2020JAE]	-928.848 ± 8.368 [2020JAE]	120.959 ± 1.255 [2020JAE]	98.667 [2020JAE]	Fe^{2+} + SO_4^{2-} ⇄ $FeSO_4$(s)	**-1.906 ± 1.476**	**10.878 ± 8.422**	**73.011 ± 8.636**	**207.987 ± 6.012**
$FeSO_4$(aq)	-849.908 ± 0.795 [2020JAE]	-993.700 ± 8.368 [2020JAE]	-12.134 ± 20.920 [2020JAE]	-104.600 ± 121.336 [2020JAE]	Fe^{2+} + SO_4^{2-} ⇄ $FeSO_4$(aq)	**2.443 ± 0.218**	**-13.945 ± 1.243**	**8.159 ± 8.636**	**74.894 ± 21.730**
$FeSO_4·H_2O$(szomolnokite)	-1080.221 [2020JAE]	-1243.987 ± 1.674 [2020JAE]	153.411 [2020JAE]	108.730 [2020JAE]	Fe^{2+} + SO_4^{2-} + H_2O(l) ⇄ $FeSO_4·H_2O$(szomolnokite)	**1.240**	**-7.075**	**43.710 ± 2.714**	**170.515**
$FeSO_4·4H_2O$(rozenite)	-1792.718 ± 0.837 [2020JAE]	-2128.484 ± 1.674 [2020JAE]	276.144 ± 4.184 [2020JAE]	274.834 [2020JAE]	Fe^{2+} + SO_4^{2-} + 4 H_2O(l) ⇄ $FeSO_4·4H_2O$(rozenite)	**1.406 ± 0.233**	**-8.025 ± 1.332**	**16.728 ± 2.744**	**83.479 ± 7.224**
$FeSO_4·7H_2O$(melanterite)	-2507.718 ± 0.628 [2020JAE]	-3012.509 ± 0.586 [2020JAE]	409.112 ± 0.837 [2020JAE]	394.928 ± 2.929 [2020JAE]	Fe^{2+} + SO_4^{2-} + 7 H_2O(l) ⇄ $FeSO_4·7H_2O$(melanterite)	**2.011 ± 0.235**	**-11.477 ± 1.342**	**-9.782 ± 2.330**	**6.678 ± 5.967**
$Fe_2(SO_4)_3·7.53H_2O$(cr)		-4852.290 ± 5.710 [2020LEM/PAL]			2 Fe^{3+} + 3 SO_4^{2-} + 7.53 H_2O(l) ⇄ $Fe_2(SO_4)_3·7.53H_2O$(cr)			**78.458 ± 8.923**	
$Fe_2(SO_4)_3·9H_2O$(cr)		-5294.520 ± 5.760 [2020LEM/PAL]			2 Fe^{3+} + 3 SO_4^{2-} + 9 H_2O(l) ⇄ $Fe_2(SO_4)_3·9H_2O$(cr)			**56.410 ± 8.970**	
$Fe_2(SO_4)_3$(cr)	-2263.397 ± 3.906 [2013LEM/BER]	-2584.100 ± 3.900 [2013LEM/BER]	305.600 ± 0.600 [2013LEM/BER]	272.930 ± 1.000 [2013LEM/BER]	2 Fe^{3+} + 3 SO_4^{2-} ⇄ $Fe_2(SO_4)_3$(cr)	**-0.781 ± 2.455**	**4.457 ± 14.015**	**243.866 ± 14.002**	**803.914 ± 43.544**
$Fe_2(SO_4)_3·5H_2O$(cr)		-4106.500 ± 5.900 [2013LEM/BER]			2 Fe^{3+} + 3 SO_4^{2-} + 5 H_2O(l) ⇄ $Fe_2(SO_4)_3·5H_2O$(cr)			**101.077 ± 9.026**	
$Fe_2(SO_4)_2^-$	**-1541.660 ± 6.791**				$FeSO_4^+$ + SO_4^{2-} ⇄ $Fe(SO_4)_2^-$	1.970 ± 0.130 [2013LEM/BER]	-11.245 ± 0.742 [2013LEM/BER]		
$Fe_{4.78}(SO_4)_6(OH)_{2.34}$ $(H_2O)_{20.71}$(cr)		-12046.200 ± 12.600 [2013LEM/BER]			4.78 Fe^{3+} + 6 SO_4^{2-} + 23.05 H_2O(l) ⇄ $Fe_{4.78}(SO_4)_6(OH)_{2.34}(H_2O)_{20.71}$(cr) + 2.34 H^+			**236.977 ± 34.566**	
$(H_3O)_{0.91}Fe_{2.91}(SO_4)_2$ $(OH)_{5.64}(H_2O)_{0.18}$(cr)	-3163.853 ± 6.925 [2013LEM/BER]	-3693.900 ± 6.500 [2013LEM/BER]	446.500 ± 8.000 [2013LEM/BER]		2.91 Fe^{3+} + 2 SO_4^{2-} + 6.73 H_2O(l) ⇄ $(H_3O)_{0.91}Fe_{2.91}(SO_4)_2(OH)_{5.64}(H_2O)_{0.18}$(cr) + 4.73 H^+	**4.999 ± 3.628**	**-28.533 ± 20.706**	**193.274 ± 20.566**	**745.494 ± 63.826**

Table A1 Selected thermodynamic data for iron (Fe) in JAEA-TDB-RN in 2020 (6/10)

Species / compound	$\Delta_f G^0_m$ (kJ.mol^{-1})	$\Delta_f H^0_m$ (kJ.mol^{-1})	S^0_m (J.K^{-1}.mol^{-1})	$C^0_{p,m}$ (J.K^{-1}.mol^{-1})	Reaction	$\log_{10} K°$	$\Delta_r G^0_m$ (kJ.mol^{-1})	$\Delta_r H^0_m$ (kJ.mol^{-1})	$\Delta_r S^0_m$ (J.K^{-1}.mol^{-1})
$(H_3O)_{1.34}Fe(SO_4)_{2.17}$ $(H_2O)_{3.06}$(cr)		-3201.220 ± 3.560 [2013LEM/BER]			Fe^{3+} + 2.17 SO_4^{2-} + 4.4 H_2O(l) + 1.34 H^+ ⇄ $(H_3O)_{1.34}Fe(SO_4)_{2.17}(H_2O)_{3.06}$(cr)			**79.885 ± 7.650**	
$(H_3O)Fe_3(SO_4)_2(OH)_6$(cr)			448.200 ± 0.700 [2013LEM/BER]	437.500 ± 2.000 [2013LEM/BER]					
$FeO(SO_4)_{0.157}(OH)_{0.686}$ $(H_2O)_{0.972}$(cr)		-884.100 ± 2.000 [2013LEM/BER]			Fe^{3+} + 0.157 SO_4^{2-} + 2.658 H_2O(l) ⇄ $FeO(SO_4)_{0.157}(OH)_{0.686}(H_2O)_{0.972}$(cr) + 2.686 H^+			**68.046 ± 6.993**	
$FeO(SO_4)_{0.168}(OH)_{0.664}$ $(H_2O)_{1.226}$(cr)		-960.600 ± 2.000 [2013LEM/BER]			Fe^{3+} + 0.168 SO_4^{2-} + 2.89 H_2O(l) ⇄ $FeO(SO_4)_{0.168}(OH)_{0.664}(H_2O)_{1.226}$(cr) + 2.664 H^+			**67.866 ± 6.994**	
$FeSe_{1.95}$			81.400 ± 2.000 [2020LEM/PAL]	69.300 ± 2.000 [2020LEM/PAL]					
$Fe_{1.042}Se$(cr)	-75.233 ± 4.009 [2020LEM/PAL]	-74.700 ± 4.000 [2020LEM/PAL]	72.100 ± 0.800 [2020LEM/PAL]	57.100 ± 0.700 [2020LEM/PAL]	1.042 Fe^{2+} + SeO_3^{2-} + 6 H^+ + 6.084 e^- ⇄ $Fe_{1.042}Se$(cr) + 3 H_2O(l)	**57.645 ± 0.784**	**-329.042 ± 4.473**	**-328.923 ± 4.704**	**-0.300 ± 9.334**
Fe_7Se_8(cr,α)	-547.084 ± 39.038 [2020LEM/PAL]	-521.000 ± 39.000 [2020LEM/PAL]	613.800 ± 5.000 [2020LEM/PAL]	442.100 ± 4.000 [2020LEM/PAL]	7 Fe^{2+} + 8 SeO_3^{2-} + 48 H^+ + 46 e^- ⇄ Fe_7Se_8(cr,α) + 24 H_2O(l)	**472.982 ± 7.353**	**-2699.802 ± 41.969**	**-2678.039 ± 42.702**	**67.765 ± 69.690**
Fe_3Se_4(cr,γ)	-257.000 ± 20.024 [2020LEM/PAL]	-248.000 ± 20.000 [2020LEM/PAL]	279.800 ± 3.000 [2020LEM/PAL]	220.100 ± 2.000 [2020LEM/PAL]	3 Fe^{2+} + 4 SeO_3^{2-} + 24 H^+ + 22 e^- ⇄ Fe_3Se_4(cr,γ) + 12 H_2O(l)	**241.608 ± 3.749**	**-1379.111 ± 21.402**	**-1372.648 ± 21.480**	**19.194 ± 33.248**
$FeSe_2$(cr)	-111.722 ± 9.022 [2020LEM/PAL]	-120.000 ± 9.000 [2020LEM/PAL]	83.500 ± 2.000 [2020LEM/PAL]	70.600 ± 2.000 [2020LEM/PAL]	Fe^{2+} + 2 SeO_3^{2-} + 12 H^+ + 10 e^- ⇄ $FeSe_2$(cr) + 6 H_2O(l)	**125.880 ± 1.706**	**-718.529 ± 9.736**	**-728.453 ± 9.533**	**-34.391 ± 15.336**
$FeSeO_3^+$	**-447.556 ± 7.327**				Fe^{3+} + H_2SeO_3(aq) ⇄ $FeSeO_3^+$ + 2 H^+	0.900 ± 0.500 [2020LEM/PAL]	-5.137 ± 2.854 [2020LEM/PAL]		
$Fe_2(SeO_3)_3 \cdot 3H_2O$(cr)	**-2086.068 ± 14.056**				2 Fe^{3+} + 3 H_2SeO_3(aq) + 3 H_2O(l) ⇄ $Fe_2(SeO_3)_3 \cdot 3H_2O$(cr) + 6 H^+	11.300 ± 0.600 [2020LEM/PAL]	-64.501 ± 3.425 [2020LEM/PAL]		
$Fe_{1.111}Te$(cr,β)	-29.014 ± 1.811 [2020LEM/PAL]	-26.060 ± 1.810 [2020LEM/PAL]	89.220 ± 0.150 [2020LEM/PAL]	55.030 ± 0.090 [2020LEM/PAL]					
$FeTe_2$(cr,ε)			100.220 ± 0.200 [2020LEM/PAL]	73.640 ± 0.100 [2020LEM/PAL]					
Fe_2TeO_6(cr)				180.700 ± 4.000 [2020LEM/PAL]					

Table A1 Selected thermodynamic data for iron (Fe) in JAEA-TDB-RN in 2020 (7/10)

Species / compound	$\Delta_f G^0_m$ (kJ.mol^{-1})	$\Delta_f H^0_m$ (kJ.mol^{-1})	S^0_m (J.K^{-1}.mol^{-1})	$C^0_{p,m}$ (J.K^{-1}.mol^{-1})	Reaction	$\log_{10} K°$	$\Delta_r G^0_m$ (kJ.mol^{-1})	$\Delta_r H^0_m$ (kJ.mol^{-1})	$\Delta_r S^0_m$ (J.K^{-1}.mol^{-1})
$FeHPO_4$(aq)	-1201.185	-1376.996	-45.606	-79.496	$Fe^{2+} + H^+ + PO_4^{3-} \rightleftarrows FeHPO_4$(aq)	**15.921**	**-90.876**	**-7.364**	**282.002**
	± 2.092	± 8.786	± 29.288	± 112.968		**± 1.518**	**± 8.666**	**± 12.313**	**± 88.851**
	[2020JAE]	[2020JAE]	[2020JAE]	[2020JAE]					
$FeH_2PO_4^+$	-1196.038	-1358.628	-1.255	242.672	$Fe^{2+} + 2\ H^+ + PO_4^{3-} \rightleftarrows FeH_2PO_4^+$	**15.019**	**-85.730**	**11.004**	**326.352**
	± 1.674	± 10.460	± 33.472	± 83.680		**± 1.502**	**± 8.575**	**± 13.558**	**± 90.316**
	[2020JAE]	[2020JAE]	[2020JAE]	[2020JAE]					
$Fe_3(PO_4)_2 \cdot 8H_2O$(vivianite)	-4410.564	-5130.421	435.136	569.614	$3\ Fe^{2+} + 2\ PO_4^{3-} + 8\ H_2O$(l)	**35.210**	**-200.983**	**-12.192**	**636.822**
	± 4.184	± 12.552	± 41.840		$\rightleftarrows Fe_3(PO_4)_2 \cdot 8H_2O$(vivianite)	**± 3.057**	**± 17.451**	**± 21.857**	**± 173.405**
	[2020JAE]	[2020JAE]	[2020JAE]	[2020JAE]					
$Fe_2P_2O_7$(cr)			220.500	196.380					
			± 2.430	± 2.160					
			[2020LEM/PAL]	[2020LEM/PAL]					
$Fe(PO_3)_3$			210.000	203.200					
(cr, monoclinic)			± 3.000	± 3.000					
			[2020LEM/PAL]	[2020LEM/PAL]					
$Fe(PO_3)_3 \cdot 0.128H_2O$			215.400	208.480					
(cr, monoclinic)			± 2.370	± 2.290					
			[2020LEM/PAL]	[2020LEM/PAL]					
$FePO_4$(cr, trigonal)	-1161.338	-1267.560	122.210	101.960	$Fe^{3+} + PO_4^{3-} \rightleftarrows FePO_4$(cr, trigonal)	**21.951**	**-125.296**	**59.396**	**621.361**
	± 1.411	± 1.350	± 1.340	± 1.120		**± 1.894**	**± 10.809**	**± 10.801**	**± 86.473**
	[2020LEM/PAL]	[2020LEM/PAL]	[2020LEM/PAL]	[2020LEM/PAL]					
$FePO_4 \cdot 2H_2O$			174.000	180.500					
(cr, orthorhombic)			± 7.000	± 0.200					
			[2020LEM/PAL]	[2020LEM/PAL]					
Fe_3PO_7(cr)			219.730	211.440					
			± 2.420	± 2.330					
			[2020LEM/PAL]	[2020LEM/PAL]					
$Fe_4(P_2O_7)_3$(cr)			561.030	503.440					
			± 6.170	± 5.540					
			[2020LEM/PAL]	[2020LEM/PAL]					
$Fe_3(P_2O_7)_2$(cr)			384.120	346.000					
			± 4.230	± 3.460					
			[2020LEM/PAL]	[2020LEM/PAL]					
$FeAsO_4$(cr)		-897.250			$Fe^{3+} + AsO_4^{3-} \rightleftarrows FeAsO_4$(cr)			**40.470**	
		± 4.700						**± 9.105**	
		[2020LEM/PAL]							
$FeAsO_4 \cdot 2H_2O$(cr, scorodite)	-1283.269	-1507.180	188.000	185.400	$Fe^{3+} + AsO_4^{3-} + 2\ H_2O$(l)	**25.106**	**-143.306**	**2.217**	**488.353**
	± 4.725	± 4.680	± 2.100	± 1.900	$\rightleftarrows FeAsO_4 \cdot 2H_2O$(cr, scorodite)	**± 1.598**	**± 9.124**	**± 9.097**	**± 21.867**
	[2020LEM/PAL]	[2020LEM/PAL]	[2020LEM/PAL]	[2020LEM/PAL]					
$FeAsO_4 \cdot 3.5H_2O$(cr, kaňkite)	-1628.340	-1938.590	248.300	244.900	$Fe^{3+} + AsO_4^{3-} + 3.5\ H_2O$(l)	**23.231**	**-132.603**	**-0.435**	**443.769**
	± 4.738	± 4.660	± 2.800	± 2.400	$\rightleftarrows FeAsO_4 \cdot 3.5H_2O$(cr, kaňkite)	**± 1.600**	**± 9.135**	**± 9.092**	**± 21.946**
	[2020LEM/PAL]	[2020LEM/PAL]	[2020LEM/PAL]	[2020LEM/PAL]					

Table A1 Selected thermodynamic data for iron (Fe) in JAEA-TDB-RN in 2020 (8/10)

Species / compound	$\Delta_f G^0_m$ (kJ.mol^{-1})	$\Delta_f H^0_m$ (kJ.mol^{-1})	S^0_m (J.K^{-1}.mol^{-1})	$C^0_{p,m}$ (J.K^{-1}.mol^{-1})	Reaction	$\log_{10} K°$	$\Delta_r G^0_m$ (kJ.mol^{-1})	$\Delta_r H^0_m$ (kJ.mol^{-1})	$\Delta_r S^0_m$ (J.K^{-1}.mol^{-1})
$FeAsO_4 \cdot 2H_2O$ (cr, parascorodite)		-1504.940 ± 4.670 [2020LEM/PAL]			$Fe^{3+} + AsO_4^{3-} + 2\ H_2O(l) \rightleftarrows FeAsO_4 \cdot 2H_2O$(cr, parascorodite)			**4.457 ± 9.092**	
$Fe_4(AsO_4)_4 \cdot 3H_2O$(cr)	**-3975.633 ± 32.348**	-4559.684 ± 18.357 [2020LEM/PAL]	616.800 ± 2.000 [2020LEM/PAL]	558.000 ± 5.600 [2020LEM/PAL]	$4\ Fe^{3+} + 4\ H_3AsO_4(aq) + 3\ H_2O(l) \rightleftarrows Fe_4(AsO_4)_4 \cdot 3H_2O(cr) + 12\ H^+$	22.890 ± 1.480 [2020LEM/PAL]	-130.657 ± 8.448 [2020LEM/PAL]		
$FeCO_3$(aq)	-648.708 ± 2.971 [2020JAE]	-766.509 ± 8.368 [2020JAE]	-54.392 ± 41.840 [2020JAE]	-125.520 ± 125.520 [2020JAE]	$Fe^{2+} + HCO_3^- \rightleftarrows FeCO_3(aq) + H^+$	**-5.209 ± 0.541**	**29.736 ± 3.089**	**15.682 ± 8.628**	**-46.986 ± 42.251**
$FeCO_3$(siderite)	-679.590 ± 0.920 [2020JAE]	-752.610 ± 0.920 [2020JAE]	95.479 ± 2.092 [2020JAE]	82.216 ± 2.092 [2020JAE]	$Fe^{2+} + HCO_3^- \rightleftarrows FeCO_3(cr) + H^+$	**0.195 ± 0.219**	**-1.113 ± 1.248**	**29.581 ± 2.285**	**102.943 ± 5.914**
$Fe(CO_3)_2^{2-}$	**-1186.698 ± 1.292**				$FeCO_3(cr) + H_2O(l) + CO_2(g) \rightleftarrows Fe(CO_3)_2^{2-} + 2\ H^+$	-21.794 ± 0.158 [2013LEM/BER]	124.400 ± 0.900 [2013LEM/BER]		
$Fe(CO_3)_3^{3-}$	**-1738.181 ± 13.263**				$Fe^{3+} + 3\ CO_3^{2-} \rightleftarrows Fe(CO_3)_3^{3-}$	24.000 ± 2.000	-136.993 ± 11.416		
$Fe(OH)CO_3$(aq)	**-843.480 ± 13.238**				$Fe^{3+} + H_2O(l) + CO_3^{2-} \rightleftarrows Fe(OH)CO_3(aq) + H^+$	10.700 ± 2.000 [2013LEM/BER]	-61.076 ± 11.416 [2013LEM/BER]		
$Fe(CN)_6^{4-}$	680.226 ± 21.260 [2020LEM/PAL]	**452.627 ± 50.253**	**134.345 ± 183.013**		$Fe^{2+} + 6\ CN^- \rightleftarrows Fe(CN)_6^{4-}$	**45.997 ± 9.553**	**-262.555 ± 54.530**	-358.860 ± 0.330 [2020LEM/PAL]	**-324.639 ± 189.865**
$Fe(CN)_6^{3-}$	714.921 **± 21.284** [2020LEM/PAL]	**564.867 ± 50.257**	**329.093 ± 183.058**		$Fe(CN)_6^{4-} + H^+ \rightleftarrows Fe(CN)_6^{3-} + 0.5\ H_2(g)$	-6.078 ± 0.178 [2020LEM/PAL]	34.695 ± 1.017 [2020LEM/PAL]	112.240 ± 0.656 [2020LEM/PAL]	260.087 ± 4.059 [2020LEM/PAL]
$HFe(CN)_6^{3-}$	655.796 **± 21.268** [2020LEM/PAL]	**454.727 ± 50.342**	**223.327 ± 183.299**		$Fe(CN)_6^{4-} + H^+ \rightleftarrows HFe(CN)_6^{3-}$	4.280 ± 0.100 [2020LEM/PAL]	-24.430 ± 0.571 [2020LEM/PAL]	2.100 ± 3.000 [2020LEM/PAL]	88.982 ± 10.243 [2020LEM/PAL]
$H_2Fe(CN)_6^{2-}$	642.097 **± 21.336** [2020LEM/PAL]				$HFe(CN)_6^{3-} + H^+ \rightleftarrows H_2Fe(CN)_6^{2-}$	2.400 ± 0.300 [2020LEM/PAL]	-13.699 ± 1.712 [2020LEM/PAL]		
$FeSCN^{2+}$	**58.180 ± 10.720**				$Fe^{3+} + SCN^- \rightleftarrows FeSCN^{2+}$	3.060 ± 0.050 [2020LEM/PAL]	-17.467 ± 0.285 [2020LEM/PAL]		
$Fe(SCN)_2^+$	**139.348 ± 12.194**				$FeSCN^{2+} + SCN^- \rightleftarrows Fe(SCN)_2^+$	2.230 ± 0.500 [2020LEM/PAL]	-12.729 ± 2.854 [2020LEM/PAL]		
$FeSiO_3$(clino)				90.600 ± 5.000 [2013LEM/BER]					

Table A1 Selected thermodynamic data for iron (Fe) in JAEA-TDB-RN in 2020 (9/10)

Species / compound	$\Delta_f G^0_m$ (kJ.mol^{-1})	$\Delta_f H^0_m$ (kJ.mol^{-1})	S^0_m (J.K^{-1}.mol^{-1})	$C^0_{p,m}$ (J.K^{-1}.mol^{-1})	Reaction	$\log_{10} K°$	$\Delta_r G^0_m$ (kJ.mol^{-1})	$\Delta_r H^0_m$ (kJ.mol^{-1})	$\Delta_r S^0_m$ (J.K^{-1}.mol^{-1})
$FeSiO_3$(ortho)			94.600 ± 3.000 [2013LEM/BER]						
$FeSiO_3$(ferrosilite)	-1119.597 ± 4.184 [2020JAE]	-1195.193 [2020JAE]	90.500 [2020JAE]	91.035 [2020JAE]	Fe^{2+} + $Si(OH)_4$(aq) ⇄ $FeSiO_3$(ferrosilite) + H_2O(l) + 2 H^+	**-7.445 ± 0.813**	**42.497 ± 4.640**	**68.150**	**76.481**
Fe_2SiO_4(fayalite)	-1381.682 ± 4.184 [2020JAE]	-1481.554 ± 4.184 [2020JAE]	148.323 ± 1.674 [2020JAE]	132.901 [2020JAE]	2 Fe^{2+} + $Si(OH)_4$(aq) ⇄ Fe_2SiO_4(fayalite) + 4 H^+	**-19.113 ± 0.851**	**109.098 ± 4.860**	**159.884 ± 6.845**	**170.236 ± 15.653**
γ-Fe_2SiO_4				128.000 ± 0.300 [2013LEM/BER]					
$FeB(OH)_4^+$	-1265.786 ± 2.092 [2020JAE]	-1453.522 ± 12.552 [2020JAE]	9.205 ± 37.656 [2020JAE]	276.144 ± 83.680 [2020JAE]	Fe^{2+} + $B(OH)_3$(aq) + H_2O(l) ⇄ $FeB(OH)_4^+$ + H^+	**-5.547 ± 0.433**	**31.665 ± 2.469**	**-0.891 ± 12.765**	**-117.160 ± 38.938**
$((Fe^{2+})_{4.87}(Fe^{3+})_{2.76}Mn_{1.07}Mg_{0.15}Ti_{0.15}O_3)(Si_{5.94}Al_{0.03}Ti_{0.03}O_{17})$(cr)				786.100 ± 0.800 [2013LEM/BER]					
$((Fe^{2+})_{5.38}(Fe^{3+})_{0.66}Mn_{0.08}Mg_{0.8}Ca_{0.05})(Si_8O_{22})\{(OH)_{1.37}Cl_{0.03}O_{0.6}\}$(cr)				684.900 ± 2.600 [2013LEM/BER]					
$((Fe^{2+})_{5.2766}(Fe^{3+})_{0.12}Mn_{0.0825}Mg_{1.5209})(Si_{7.9163}Al_{0.0837}O_{22.0363})(OH)_{1.9637}$(cr)				684.900 ± 3.000 [2013LEM/BER]					
$FeCr_2O_4$(cr)			152.200 ± 3.000 [2020LEM/PAL]	133.900 ± 4.000 [2020LEM/PAL]					
$NiFe_2O_4$(cr)	-962.271 ± 3.044 [2020LEM/PAL]	-1070.900 ± 2.800 [2020LEM/PAL]	130.000 ± 4.000 [2020LEM/PAL]	144.800 ± 2.000 [2020LEM/PAL]	2 Fe^{2+} + Ni^{2+} + 4 H_2O(l) ⇄ $NiFe_2O_4$(cr) + 8 H^+ + 2 e^-	**-37.708 ± 0.627**	**215.241 ± 3.581**	**311.980 ± 5.128**	**324.497 ± 12.463**
$MgFe(OH)_4^+$	-1306.412 ± 7.531 [2020JAE]	-1489.755 ± 8.368 [2020JAE]	50.919 ± 31.798 [2020JAE]	676.134 ± 171.544 [2020JAE]	Fe^{3+} + Mg^{2+} + 4 H_2O(l) ⇄ $MgFe(OH)_4^+$ + 4 H^+	**-19.891 ± 1.777**	**113.541 ± 10.143**	**169.138 ± 10.779**	**186.698 ± 39.342**
$NaFe(OH)_4$(aq)	-1100.643 ± 7.113 [2020JAE]	-1257.710 ± 12.552 [2020JAE]	222.170 ± 37.656 [2020JAE]	472.792 ± 96.232 [2020JAE]	Fe^{3+} + Na^+ + 4 H_2O(l) ⇄ $NaFe(OH)_4$(aq) + 4 H^+	**-22.285 ± 1.713**	**127.206 ± 9.777**	**175.519 ± 14.232**	**161.469 ± 43.491**
$KFe(OH)_4$(aq)	-1118.048 ± 7.113 [2020JAE]	-1273.317 ± 15.899 [2020JAE]	293.717 ± 30.962 [2020JAE]	471.537 ± 96.232 [2020JAE]	Fe^{3+} + K^+ + 4 H_2O(l) ⇄ $KFe(OH)_4$(aq) + 4 H^+	**-22.842 ± 1.713**	**130.382 ± 9.777**	**171.787 ± 17.256**	**190.380 ± 37.844**
$KFe(CN)_6^{3-}$	**384.350 ± 21.262**	**204.057 ± 50.263**	**292.454 ± 183.046**		$Fe(CN)_6^{4-}$ + K^+ ⇄ $KFe(CN)_6^{3-}$	2.350 ± 0.050 [2020LEM/PAL]	-13.414 ± 0.285 [2020LEM/PAL]	3.600 ± 1.000 [2020LEM/PAL]	57.065 ± 3.488 [2020LEM/PAL]

Table A1 Selected thermodynamic data for iron (Fe) in JAEA-TDB-RN in 2020 (10/10)

Species / compound	$\Delta_f G^0_m$ (kJ.mol^{-1})	$\Delta_f H^0_m$ (kJ.mol^{-1})	S^0_m (J.K^{-1}.mol^{-1})	$C^0_{p,m}$ (J.K^{-1}.mol^{-1})	Reaction	$\log_{10} K°$	$\Delta_r G^0_m$ (kJ.mol^{-1})	$\Delta_r H^0_m$ (kJ.mol^{-1})	$\Delta_r S^0_m$ (J.K^{-1}.mol^{-1})
$KFe(CN)_6^{2-}$	**424.125**	**297.115**	**405.823**		$Fe(CN)_6^{3-} + K^+ \rightleftarrows KFe(CN)_6^{2-}$	1.460	-8.334	2.100	34.996
	± 21.287	**± 21.305**	**± 8.777**			± 0.050 [2020LEM/PAL]	± 0.285 [2020LEM/PAL]	± 1.300 [2020LEM/PAL]	± 4.464 [2020LEM/PAL]
$K_4Fe(CN)_6·3H_2O$ (cr, monoclinic)	**-1187.543**	**-1468.741**	**651.693**	481.400	$Fe(CN)_6^{4-} + 4\ K^+ + 3\ H_2O(l)$	4.620	-26.374	-55.174	-96.596
	± 21.290	**± 50.257**	**± 183.051**	± 3.700 [2020LEM/PAL]	$\rightleftarrows K_4Fe(CN)_6·3H_2O$(cr, monoclinic)	± 0.170 [2020LEM/PAL]	± 0.972 [2020LEM/PAL]	± 0.460 [2020LEM/PAL]	± 3.607 [2020LEM/PAL]
$K_4Fe(CN)_6$(cr)	**-471.863**	**-613.785**	**419.477**	332.900	$K_4Fe(CN)_6·3H_2O$(cr, monoclinic)	-0.724	4.132	15.123	36.864
	± 21.304	**± 21.274**	**± 7.970**	± 1.800 [2020LEM/PAL]	$\rightleftarrows K_4Fe(CN)_6$(cr) + 3 H_2O(l)	± 0.125 [2020LEM/PAL]	± 0.713 [2020LEM/PAL]	± 0.524 [2020LEM/PAL]	± 2.968 [2020LEM/PAL]
$K_3Fe(CN)_6$(cr)	**-143.050**	**-263.705**	**426.021**	316.700	$Fe(CN)_6^{3-} + 3\ K^+ \rightleftarrows K_3Fe(CN)_6$(cr)	1.854	-10.585	-54.381	-146.893
	± 21.318	**± 21.290**	**± 9.119**	± 1.300 [2020LEM/PAL]		± 0.198 [2020LEM/PAL]	± 1.133 [2020LEM/PAL]	± 0.994 [2020LEM/PAL]	± 5.055 [2020LEM/PAL]

[2020JAE] Japan Atomic Energy Agency [A1)].
[2013LEM/BER] Lemire et al. [A2)]
[2020LEM/PAL] Lemire et al. [A3)]

Table A2 Selected thermodynamic data for cobalt (Co) in JAEA-TDB-RN in 2020 (1/4)

Values indicated by **boldface** are calculated and selected in the present report.

Species / compound	$\Delta_f G^0_m$ (kJ.mol^{-1})	$\Delta_f H^0_m$ (kJ.mol^{-1})	S^0_m (J.K^{-1}.mol^{-1})	$C^0_{p,m}$ (J.K^{-1}.mol^{-1})	Reaction	$\log_{10} K°$	$\Delta_r G^0_m$ (kJ.mol^{-1})	$\Delta_r H^0_m$ (kJ.mol^{-1})	$\Delta_r S^0_m$ (J.K^{-1}.mol^{-1})
α-Co(hexagonal)	0.000 [1982WAG/EVA]	0.000 [1982WAG/EVA]	30.040 [1982WAG/EVA]	24.810 [1982WAG/EVA]					
Co^{2+}	**-54.398 ± 0.999**				α-Co(hexagonal) ⇄ Co^{2+} + 2 e^-	9.530 ± 0.175 [2009KIT/KIR]	**-54.398 ± 0.999**		
$CoOH^+$	**-237.525 ± 1.010**				Co^{2+} + H_2O(l) ⇄ H^+ + $CoOH^+$	-9.470 ± 0.020 [2009KIT/KIR]	**54.055 ± 0.114**		
$Co(OH)_2$(aq)	**-426.018 ± 6.361**				Co^{2+} + 2 H_2O(l) ⇄ 2 H^+ + $Co(OH)_2$(aq)	-18.000 ± 1.100 [2009KIT/KIR]	**102.745 ± 6.279**		
$Co(OH)_3^-$	**-586.142 ± 3.039**				Co^{2+} + 3 H_2O(l) ⇄ 3 H^+ + $Co(OH)_3^-$	-31.500 ± 0.500 [2009KIT/KIR]	**179.803 ± 2.854**		
Co_2OH^{3+}	**-285.769 ± 5.306**				2 Co^{2+} + H_2O(l) ⇄ H^+ + Co_2OH^{3+}	-10.548 ± 0.861 [2009KIT/KIR]	**60.208 ± 4.915**		
$Co_4(OH)_4^{4+}$	**-1010.086 ± 4.192**				4 Co^{2+} + 4 H_2O(l) ⇄ 4 H^+ + $Co_4(OH)_4^{4+}$	-27.371 ± 0.211 [2009KIT/KIR]	**156.235 ± 1.204**		
CoF^+	**-344.539 ± 1.224**				Co^{2+} + F^- ⇄ CoF^+	1.470 ± 0.040 [2009KIT/KIR]	**-8.391 ± 0.228**		
$CoCl^+$	**-190.311 ± 1.081**				Co^{2+} + Cl^- ⇄ $CoCl^+$	0.810 ± 0.070 [2009KIT/KIR]	**-4.624 ± 0.400**		
CoS(aq)	**-45.856 ± 11.820**				Co^{2+} + HS^- ⇄ CoS(aq) + H^+	0.600 ± 2.062 [2009KIT/KIR]	**-3.425 ± 11.770**		
$CoHS^+$	**-71.776 ± 1.916**				Co^{2+} + HS^- ⇄ $CoHS^+$	5.141 ± 0.277 [2009KIT/KIR]	**-29.345 ± 1.581**		
$CoSO_4$(aq)	**-811.414 ± 1.136**				Co^{2+} + SO_4^{2-} ⇄ $CoSO_4$(aq)	2.200 ± 0.050 [2009KIT/KIR]	**-12.558 ± 0.285**		
$Co(SO_4)_2^{2-}$	**-1559.698 ± 1.388**				Co^{2+} + 2 SO_4^{2-} ⇄ $Co(SO_4)_2^{2-}$	2.870 ± 0.050 [2009KIT/KIR]	**-16.382 ± 0.285**		
$CoNO_3^+$	**-159.493 ± 2.723**				Co^{2+} + NO_3^- ⇄ $CoNO_3^+$	-1.020 ± 0.060 [2009KIT/KIR]	**5.822 ± 0.342**		

Table A2 Selected thermodynamic data for cobalt (Co) in JAEA-TDB-RN in 2020 (2/4)

Species / compound	$\Delta_f G^0_m$ (kJ.mol^{-1})	$\Delta_f H^0_m$ (kJ.mol^{-1})	S^0_m (J.K^{-1}.mol^{-1})	$C^0_{p,m}$ (J.K^{-1}.mol^{-1})	Reaction	$\log_{10} K°$	$\Delta_r G^0_m$ (kJ.mol^{-1})	$\Delta_r H^0_m$ (kJ.mol^{-1})	$\Delta_r S^0_m$ (J.K^{-1}.mol^{-1})
$CoNH_3^{2+}$	**-93.684 ± 1.204**				$Co^{2+} + NH_4^+ \rightleftarrows CoNH_3^{2+} + H^+$	-7.037 ± 0.102 [2009KIT/KIR]	**40.167 ± 0.582**		
$Co(NH_3)_2^{2+}$	**-130.117 ± 1.678**				$Co^{2+} + 2\ NH_4^+ \rightleftarrows Co(NH_3)_2^{2+} + 2\ H^+$	-14.574 ± 0.205 [2009KIT/KIR]	**83.189 ± 1.170**		
$Co(NH_3)_3^{2+}$	**-165.408 ± 2.711**				$Co^{2+} + 3\ NH_4^+ \rightleftarrows Co(NH_3)_3^{2+} + 3\ H^+$	-22.311 ± 0.405 [2009KIT/KIR]	**127.352 ± 2.312**		
$Co(NH_3)_4^{2+}$	**-197.845 ± 2.875**				$Co^{2+} + 4\ NH_4^+ \rightleftarrows Co(NH_3)_4^{2+} + 4\ H^+$	-30.548 ± 0.410 [2009KIT/KIR]	**174.369 ± 2.340**		
$Co(NH_3)_5^{2+}$	**-226.286 ± 3.068**				$Co^{2+} + 5\ NH_4^+ \rightleftarrows Co(NH_3)_5^{2+} + 5\ H^+$	-39.485 ± 0.415 [2009KIT/KIR]	**225.382 ± 2.369**		
$Co(NH_3)_6^{2+}$	**-248.449 ± 3.287**				$Co^{2+} + 6\ NH_4^+ \rightleftarrows Co(NH_3)_6^{2+} + 6\ H^+$	-49.522 ± 0.421 [2009KIT/KIR]	**282.674 ± 2.403**		
$CoHPO_4$(aq)	**-1160.535 ± 8.467**				$Co^{2+} + H^+ + PO_4^{3-} \rightleftarrows CoHPO_4$(aq)	15.300 ± 0.143 [2009KIT/KIR]	**-87.333 ± 0.816**		
$CoP_2O_7^{2-}$	**-2025.979 ± 17.650**				$Co^{2+} + 2\ H^+ + 2\ PO_4^{3-} \rightleftarrows CoP_2O_7^{2-} + H_2O$(l)	29.985 ± 0.966 [2009KIT/KIR]	**-171.156 ± 5.514**		
$HCoP_2O_7^-$	**-2059.257 ± 17.286**				$Co^{2+} + 3\ H^+ + 2\ PO_4^{3-} \rightleftarrows HCoP_2O_7^- + H_2O$(l)	35.815 ± 0.737 [2009KIT/KIR]	**-204.434 ± 4.207**		
$CoHAsO_4$(aq)	**-785.393 ± 7.288**				$Co^{2+} + H^+ + AsO_4^{3-} \rightleftarrows CoHAsO_4$(aq)	14.477 ± 1.052 [2009KIT/KIR]	**-82.635 ± 6.005**		
$CoCO_3$(aq)	**-607.495 ± 1.163**				$Co^{2+} + CO_3^{2-} \rightleftarrows CoCO_3$(aq)	-5.929 ± 0.102 [2009KIT/KIR]	**33.843 ± 0.582**		
$CoHCO_3^+$	**-649.329 ± 1.531**				$Co^{2+} + H^+ + CO_3^{2-} \rightleftarrows CoHCO_3^+$	1.400 ± 0.202 [2009KIT/KIR]	**-7.991 ± 1.153**		
$Co(CN)_4^{2-}$	**463.787 ± 33.625**				$Co^{2+} + 4\ CN^- \rightleftarrows Co(CN)_4^{2-}$	30.017 ± 0.533 [2009KIT/KIR]	**-171.338 ± 3.042**		
$Co(CN)_5^{3-}$	**645.815 ± 42.158**				$Co^{2+} + 5\ CN^- \rightleftarrows Co(CN)_5^{3-}$	28.327 ± 0.888 [2009KIT/KIR]	**-161.692 ± 5.069**		

Table A2 Selected thermodynamic data for cobalt (Co) in JAEA-TDB-RN in 2020 (3/4)

Species / compound	$\Delta_f G^0_m$ (kJ.mol^{-1})	$\Delta_f H^0_m$ (kJ.mol^{-1})	S^0_m (J.K^{-1}.mol^{-1})	$C^0_{p,m}$ (J.K^{-1}.mol^{-1})	Reaction	$\log_{10} K°$	$\Delta_r G^0_m$ (kJ.mol^{-1})	$\Delta_r H^0_m$ (kJ.mol^{-1})	$\Delta_r S^0_m$ (J.K^{-1}.mol^{-1})
$CoSCN^+$	**28.270**				$Co^{2+} + SCN^- \rightleftarrows CoSCN^+$	1.790	**-10.217**		
	± 8.438					± 0.073	**± 0.417**		
						[2009KIT/KIR]			
$Co(SCN)_2$(aq)	**116.160**				$Co^{2+} + 2\ SCN^- \rightleftarrows Co(SCN)_2$(aq)	2.665	**-15.212**		
	± 16.779					± 0.115	**± 0.656**		
						[2009KIT/KIR]			
$Co(SCN)_3^-$	**207.173**				$Co^{2+} + 3\ SCN^- \rightleftarrows Co(SCN)_3^-$	2.993	**-17.084**		
	± 25.158					± 0.229	**± 1.307**		
						[2009KIT/KIR]			
CoO(cr)	**-220.806**				$CoO(cr) + 2\ H^+ \rightleftarrows Co^{2+} + H_2O(l)$	12.399	**-70.774**		
	± 2.114					± 0.326	**± 1.861**		
						[2009KIT/KIR]			
β-$Co(OH)_2$	**-457.812**				β-$Co(OH)_2 + 2\ H^+ \rightleftarrows Co^{2+} + 2\ H_2O(l)$	12.430	**-70.951**		
	± 1.407					± 0.170	**± 0.970**		
						[2009KIT/KIR]			
$CoCl_2 \cdot 6H_2O$(cr)	**-1722.737**				$CoCl_2 \cdot 6H_2O(cr) \rightleftarrows Co^{2+} + 2\ Cl^- + 6\ H_2O(l)$	3.037	**-17.335**		
	± 1.188					± 0.018	**± 0.103**		
						[2009KIT/KIR]			
β-$Co(IO_3)_2$	**-335.545**				β-$Co(IO_3)_2 \rightleftarrows Co^{2+} + 2\ IO_3^-$	-4.395	**25.087**		
	± 16.773					± 0.088	**± 0.502**		
						[2009KIT/KIR]			
$Co(IO_3)_2 \cdot 2H_2O$(cr)	**-813.940**				$Co(IO_3)_2 \cdot 2H_2O(cr) \rightleftarrows Co^{2+} + 2\ IO_3^- + 2\ H_2O(l)$	-5.101	**29.117**		
	± 16.797					± 0.177	**± 1.010**		
						[2009KIT/KIR]			
α-CoS	**-84.899**				$\alpha\text{-CoS} + H^+ \rightleftarrows Co^{2+} + HS^-$	-7.440	**42.468**		
	± 1.281					± 0.120	**± 0.685**		
						[2009KIT/KIR]			
β-CoS	**-105.791**				$\beta\text{-CoS} + H^+ \rightleftarrows Co^{2+} + HS^-$	-11.100	**63.359**		
	± 9.764					± 1.700	**± 9.704**		
						[2009KIT/KIR]			
α-$CoSO_4 \cdot 6H_2O$	**-2234.676**				$\alpha\text{-}CoSO_4 \cdot 6H_2O \rightleftarrows Co^{2+} + 6\ H_2O(l) + SO_4^{2-}$	-2.229	**12.723**		
	± 2.027					± 0.279	**± 1.593**		
						[2009KIT/KIR]			
β-$CoSO_4 \cdot 6H_2O$	**-2234.076**				$\beta\text{-}CoSO_4 \cdot 6H_2O \rightleftarrows Co^{2+} + 6\ H_2O(l) + SO_4^{2-}$	-2.124	**12.124**		
	± 2.946					± 0.467	**± 2.666**		
						[2009KIT/KIR]			
$CoSO_4 \cdot 7H_2O$(cr)	**-2471.949**				$CoSO_4 \cdot 7H_2O(cr) \rightleftarrows Co^{2+} + 7\ H_2O(l) + SO_4^{2-}$	-2.245	**12.815**		
	± 1.347					± 0.058	**± 0.331**		
						[2009KIT/KIR]			
$Co_3(AsO_3)_2$(cr,hyd)	**-1280.311**				$Co_3(AsO_3)_2(cr,hyd) + 2\ H_2O(l) + 4\ e^- \rightleftarrows 3\ Co^{2+} + 4\ H^+ + 2\ AsO_4^{3-}$	-51.640	**294.763**		
	± 14.324					± 2.012	**± 11.485**		
						[2009KIT/KIR]			

Table A2 Selected thermodynamic data for cobalt (Co) in JAEA-TDB-RN in 2020 (4/4)

Species / compound	$\Delta_f G^0_m$ (kJ.mol^{-1})	$\Delta_f H^0_m$ (kJ.mol^{-1})	S^0_m (J.K^{-1}.mol^{-1})	$C^0_{p,m}$ (J.K^{-1}.mol^{-1})	Reaction	$\log_{10} K°$	$\Delta_r G^0_m$ (kJ.mol^{-1})	$\Delta_r H^0_m$ (kJ.mol^{-1})	$\Delta_r S^0_m$ (J.K^{-1}.mol^{-1})
$Co_3(AsO_4)_2 \cdot 8H_2O$(cr)	**-2868.434**				$Co_3(AsO_4)_2 \cdot 8H_2O$(cr) ⇄ 3 Co^{2+} + 2 AsO_4^{3-} + 8 H_2O(l)	-27.929	**159.420**		
	± 7.148					± 0.883	**± 5.040**		
						[2009KIT/KIR]			
$CoCO_3$(cr)	**-645.322**				$CoCO_3$(cr) + H^+ ⇄ Co^{2+} + HCO_3^-	-0.698	**3.984**		
	± 1.157					± 0.100	**± 0.571**		
						[2009KIT/KIR]			
$CoCO_3 \cdot 5.5H_2O$(cr)	**-1930.133**				$CoCO_3 \cdot 5.5H_2O$(cr) + H^+ ⇄ Co^{2+} + HCO_3^- + 5.5 H_2O(l)	2.752	**-15.709**		
	± 1.187					± 0.053	**± 0.303**		
						[2009KIT/KIR]			

[2009KIT/KIR] Kitamura et al. [A4)]
[1982WAG/EVA] Wagman et al.[A5)]

Table A3 Selected thermodynamic data for nickel (Ni) in JAEA-TDB-RN in 2020 (1/5)

Values indicated by **boldface** are calculated and selected in the present report.

Species / compound	$\Delta_f G^0_m$ (kJ.mol^{-1})	$\Delta_f H^0_m$ (kJ.mol^{-1})	S^0_m (J.K^{-1}.mol^{-1})	$C^0_{p,m}$ (J.K^{-1}.mol^{-1})	Reaction	$\log_{10} K°$	$\Delta_r G^0_m$ (kJ.mol^{-1})	$\Delta_r H^0_m$ (kJ.mol^{-1})	$\Delta_r S^0_m$ (J.K^{-1}.mol^{-1})
Ni(cr)	0.000	0.000	29.870	26.070					
			± 0.200	± 0.100					
	[2005GAM/BUG]	[2005GAM/BUG]	[2005GAM/BUG]	[2005GAM/BUG]					
Ni(g)	384.686	430.100	182.190	23.360	$Ni^{2+} + 2\ e^- \rightleftarrows Ni(g)$	**-75.413**	**430.459**	**485.112**	**183.311**
	± 8.400	± 8.400	± 0.080	± 0.100		**± 1.478**	**± 8.435**	**± 8.446**	**± 1.403**
	[2005GAM/BUG]	[2005GAM/BUG]	[2005GAM/BUG]	[2005GAM/BUG]					
Ni(l)	14.035	17.500	41.490						
	± 0.272	± 0.250	± 0.300						
	[2005GAM/BUG]	[2005GAM/BUG]	[2005GAM/BUG]						
Ni^{2+}	-45.773	-55.012	-131.800	-46.100	$Ni(cr) \rightleftarrows Ni^{2+} + 2\ e^-$	8.019	-45.773	**-55.012**	**-30.991**
	± 0.771	± 0.878	± 1.400	± 7.500		± 0.135	± 0.771	**± 0.878**	**± 1.415**
	[2005GAM/BUG]	[2005GAM/BUG]	[2005GAM/BUG]	[2005GAM/BUG]		[2005GAM/BUG]	[2005GAM/BUG]		
NiO(cr)	-211.660	-239.700	38.400	44.400	$Ni^{2+} + H_2O(l) \rightleftarrows NiO(cr) + 2\ H^+$	**-12.490**	**71.296**	**101.150**	**100.277**
	± 0.422	± 0.400	± 0.400	± 0.100		**± 0.155**	**± 0.885**	**± 0.970**	**± 1.458**
	[2005GAM/BUG]	[2005GAM/BUG]	[2005GAM/BUG]	[2005GAM/BUG]					
$NiOH^+$	**-228.501**	**-287.050**	**-64.073**		$Ni^{2+} + H_2O(l) \rightleftarrows NiOH^+ + H^+$	-9.540	54.455	53.800	-2.196
	± 1.115	**± 1.916**	**± 6.454**			± 0.140	± 0.799	± 1.700	± 6.300
						[2005GAM/BUG]	[2005GAM/BUG]	[2005GAM/BUG]	[2005GAM/BUG]
$Ni(OH)_2$(aq)	-399.195	-501.076	25.104	-92.048	$Ni^{2+} + 2\ H_2O(l) \rightleftarrows Ni(OH)_2(aq) + 2\ H^+$	**-21.188**	**120.943**	**125.613**	**17.058**
	± 8.786	± 15.481	± 41.840	± 62.760		**± 1.546**	**± 8.822**	**± 15.507**	**± 41.864**
	[2020JAE]	[2020JAE]	[2020JAE]	[2020JAE]					
β-$Ni(OH)_2$	-457.100	-542.300	80.000	82.010	$Ni^{2+} + 2\ H_2O(l) \rightleftarrows$ β-$Ni(OH)_2 + 2\ H^+$				
	± 1.400	± 1.500	± 0.800	± 0.300					
	[2005GAM/BUG]	[2005GAM/BUG]	[2005GAM/BUG]	[2005GAM/BUG]					
$Ni(OH)_3^-$	-590.519				$Ni^{2+} + 3\ H_2O(l) \rightleftarrows Ni(OH)_3^- + 3\ H^+$	-29.200	166.675		
	± 9.735					± 1.700	± 9.704		
	[2005GAM/BUG]					[2005GAM/BUG]	[2005GAM/BUG]		
$Ni(OH)_4^{2-}$	-742.978	-997.817	-22.912	77.504	$Ni^{2+} + 4\ H_2O(l) \rightleftarrows Ni(OH)_4^{2-} + 4\ H^+$	**-44.065**	**251.525**	**200.548**	**-170.804**
	[2020JAE]	[2020JAE]	[2020JAE]	[2020JAE]					
Ni_2OH^{3+}	**-268.224**	**-349.962**	**-242.663**		$2\ Ni^{2+} + H_2O(l) \rightleftarrows Ni_2OH^{3+} + H^+$	-10.600	60.505	45.900	-48.986
	± 5.913	**± 6.253**	**± 27.917**			± 1.000	± 5.708	± 6.000	± 27.776
						[2005GAM/BUG]	[2005GAM/BUG]	[2005GAM/BUG]	[2005GAM/BUG]
$Ni_4(OH)_4^{4+}$	**-974.737**	**-1173.401**	**-136.815**		$4\ Ni^{2+} + 4\ H_2O(l) \rightleftarrows Ni_4(OH)_4^{4+} + 4\ H^+$	-27.520	157.085	190.000	110.693
	± 3.226	**± 10.607**	**± 34.127**			± 0.150	± 0.856	± 10.000	± 33.663
						[2005GAM/BUG]	[2005GAM/BUG]	[2005GAM/BUG]	[2005GAM/BUG]
NiF^+	**-335.687**	**-380.860**	**-85.740**		$Ni^{2+} + F^- \rightleftarrows NiF^+$	1.430	-8.163	9.500	59.240
	± 1.119	**± 3.197**	**± 10.288**			± 0.080	± 0.457	± 3.000	± 10.178
						[2005GAM/BUG]	[2005GAM/BUG]	[2005GAM/BUG]	[2005GAM/BUG]

Table A3 Selected thermodynamic data for nickel (Ni) in JAEA-TDB-RN in 2020 (2/5)

Species / compound	$\Delta_f G^0_m$ (kJ.mol^{-1})	$\Delta_f H^0_m$ (kJ.mol^{-1})	S^0_m (J.K^{-1}.mol^{-1})	$C^0_{p,m}$ (J.K^{-1}.mol^{-1})	Reaction	$\log_{10} K°$	$\Delta_r G^0_m$ (kJ.mol^{-1})	$\Delta_r H^0_m$ (kJ.mol^{-1})	$\Delta_r S^0_m$ (J.K^{-1}.mol^{-1})
NiF_2(cr)	-609.852	-657.300	73.520	63.210	$Ni^{2+} + 2\ F^- \rightleftarrows NiF_2$(cr)	**0.101**	**-0.578**	**68.407**	**231.679**
	± 8.001	± 8.000	± 0.400	± 2.000		**± 1.428**	**± 8.149**	**± 8.159**	**± 1.818**
	[2005GAM/BUG]	[2005GAM/BUG]	[2005GAM/BUG]	[2005GAM/BUG]					
$NiCl^+$	**-177.520**				$Ni^{2+} + Cl^- \rightleftarrows NiCl^+$	0.080	-0.457		
	± 3.512					± 0.600	± 3.425		
						[2005GAM/BUG]	[2005GAM/BUG]		
$NiCl_2$(cr)	-258.743	-304.900	98.140	71.670	$Ni^{2+} + 2\ Cl^- \rightleftarrows NiCl_2$(cr)	**-8.691**	**49.609**	**84.271**	**116.470**
	± 0.154	± 0.110	± 0.300	± 0.300		**± 0.142**	**± 0.81**	**± 0.902**	**± 1.470**
	[2005GAM/BUG]	[2005GAM/BUG]	[2005GAM/BUG]	[2005GAM/BUG]					
$NiCl_2{\cdot}2H_2O$(cr)	**-756.578**	-913.374	186.200	230.000	$NiCl_2{\cdot}4H_2O$(cr) $\rightleftarrows NiCl_2{\cdot}2H_2O$(cr) + 2 H_2O(g)	-4.099	23.400		
		± 1.653	± 3.600	± 15.000		± 0.123	± 0.700		
		[2005GAM/BUG]	[2005GAM/BUG]	[2005GAM/BUG]		[2005GAM/BUG]	[2005GAM/BUG]		
					$Ni^{2+} + 2\ Cl^- + 2\ H_2O$(l) $\rightleftarrows NiCl_2{\cdot}2H_2O$(cr)	**-4.580**	**26.140**	**47.474**	**64.684**
								± 1.892	**± 3.881**
$NiCl_2{\cdot}4H_2O$(cr)	**-1236.243**	**-1512.900**	**252.954**		$NiCl_2{\cdot}6H_2O$(cr) $\rightleftarrows NiCl_2{\cdot}4H_2O$(cr) + 2 H_2O(g)	-3.777	21.560	107.000	286.567
						± 0.105	± 0.600	± 9.000	± 30.253
						[2005GAM/BUG]	[2005GAM/BUG]	[2005GAM/BUG]	[2005GAM/BUG]
					$Ni^{2+} + 2\ Cl^- + 4\ H_2O$(l) $\rightleftarrows NiCl_2{\cdot}4H_2O$(cr)	**-3.651**	**20.840**	**19.625**	**-8.408**
						± 0.156	**± 0.892**	**± 0.988**	**± 1.478**
$NiCl_2{\cdot}6H_2O$(cr)	**-1714.068**	-2104.700	340.964		$Ni^{2+} + 2\ Cl^- + 6\ H_2O$(l) $\rightleftarrows NiCl_2{\cdot}6H_2O$(cr)	-3.045	17.380	**-0.499**	**-60.244**
	± 1.002	± 1.800	± 6.673			± 0.014	± 0.080	**± 2.106**	**± 6.845**
		[2005GAM/BUG]	[2005GAM/BUG]			[2005GAM/BUG]	[2005GAM/BUG]		
$NiBr_2$(cr)	-195.408	-213.500	121.400	75.400	$Ni^{2+} + 2\ Br^- \rightleftarrows NiBr_2$(cr)	**-10.240**	**58.452**	**84.519**	**87.514**
	± 2.421	± 2.400	± 1.000	± 1.000		**± 0.449**	**± 2.563**	**± 2.573**	**± 1.771**
	[2005GAM/BUG]	[2005GAM/BUG]	[2005GAM/BUG]	[2005GAM/BUG]					
NiI_2(cr)	-94.360	-96.420	139.100	77.280	$Ni^{2+} + 2\ I^- \rightleftarrows NiI_2$(cr)	**-9.681**	**55.260**	**72.397**	**57.516**
	± 0.898	± 0.840	± 1.000	± 1.000		**± 0.359**	**± 2.050**	**± 2.068**	**± 1.771**
	[2005GAM/BUG]	[2005GAM/BUG]	[2005GAM/BUG]	[2005GAM/BUG]					
β-$Ni(IO_3)_2$	**-327.121**	**-490.379**	**214.310**		$Ni^{2+} + 2\ IO_3^- \rightleftarrows$ β-$Ni(IO_3)_2$	4.430	-25.287	7.300	109.296
	± 16.754	**± 17.230**	**± 21.499**			± 0.020	± 0.114	± 4.000	± 13.422
						[2005GAM/BUG]	[2005GAM/BUG]	[2005GAM/BUG]	[2005GAM/BUG]
$Ni(IO_3)_2{\cdot}2H_2O$(cr)	**-805.538**	**-1090.956**	**270.818**		$Ni^{2+} + 2\ IO_3^- + 2\ H_2O$(l) $\rightleftarrows Ni(IO_3)_2{\cdot}2H_2O$(cr)	5.140	-29.339	-21.600	25.958
	± 16.765	**± 17.490**	**± 23.811**			± 0.100	± 0.571	± 5.000	± 16.879
						[2005GAM/BUG]	[2005GAM/BUG]	[2005GAM/BUG]	[2005GAM/BUG]
NiS(aq)	**-37.934**				$Ni^{2+} + HS^- \rightleftarrows NiS(aq) + H^+$	0.723	**-4.127**		
	± 11.524					± 2.013	**± 11.490**		
						[2009KIT/KIR]			
β-NiS	-91.330	-94.000	52.970	47.080	$Ni^{2+} + HS^- \rightleftarrows$ β-$NiS + H^+$	**10.078**	**-57.523**	**-22.880**	**116.571**
	± 1.007	± 1.000	± 0.330	± 0.300		**± 0.234**	**± 1.335**		
	[2005GAM/BUG]	[2005GAM/BUG]	[2005GAM/BUG]	[2005GAM/BUG]					

Table A3 Selected thermodynamic data for nickel (Ni) in JAEA-TDB-RN in 2020 (3/5)

Species / compound	$\Delta_f G^0_m$ (kJ.mol^{-1})	$\Delta_f H^0_m$ (kJ.mol^{-1})	S^0_m (J.K^{-1}.mol^{-1})	$C^0_{p,m}$ (J.K^{-1}.mol^{-1})	Reaction	$\log_{10} K°$	$\Delta_r G^0_m$ (kJ.mol^{-1})	$\Delta_r H^0_m$ (kJ.mol^{-1})	$\Delta_r S^0_m$ (J.K^{-1}.mol^{-1})
NiS_2(cr)	-123.832	-128.000	80.000		$Ni^{2+} + 2\ HS^- \rightleftarrows NiS_2(cr) + 2\ H^+ + 2\ e^-$	**17.868**	**-101.991**	**-40.771**	**206.080**
	± 7.396	± 7.000	± 8.000			**± 1.311**	**± 7.483**		
	[2005GAM/BUG]	[2005GAM/BUG]	[2005GAM/BUG]						
Ni_3S_2(cr)	-211.172	-217.200	133.500	118.200	$3\ Ni^{2+} + 2\ HS^- + 2\ e^- \rightleftarrows Ni_3S_2(cr) + 2\ H^+$	**17.131**	**-97.785**	**-19.947**	**261.823**
	± 1.624	± 1.600	± 0.700	± 0.800		**± 0.516**	**± 2.947**		
	[2005GAM/BUG]	[2005GAM/BUG]	[2005GAM/BUG]	[2005GAM/BUG]					
Ni_9S_8(cr)	-746.803	-760.000	481.000	407.000	$9\ Ni^{2+} + 8\ HS^- + 2\ e^- \rightleftarrows Ni_9S_8(cr) + 8\ H^+$	**75.433**	**-430.576**	**-136.025**	**990.928**
	± 9.255	± 9.000	± 7.000	± 5.000		**± 2.110**	**± 12.042**		
	[2005GAM/BUG]	[2005GAM/BUG]	[2005GAM/BUG]	[2005GAM/BUG]					
$NiHS^+$	**-63.375**				$Ni^{2+} + HS^- \rightleftarrows NiHS^+$	5.180	-29.568		
	± 1.440					± 0.200	± 1.142		
						[2005GAM/BUG]	[2005GAM/BUG]		
$NiSO_4$(cr)	-762.688	-873.280	101.300	97.600	$Ni^{2+} + SO_4^{2-} \rightleftarrows NiSO_4(cr)$	**-4.825**	**27.544**	**91.334**	**214.272**
	± 1.572	± 1.570	± 0.200	± 0.100		**± 0.317**	**± 1.810**	**± 1.847**	**± 1.501**
	[2005GAM/BUG]	[2005GAM/BUG]	[2005GAM/BUG]	[2005GAM/BUG]					
α-$NiSO_4.6H_2O$	-2225.467	**-2684.129**	334.450	327.900	$Ni^{2+} + SO_4^{2-} + 6\ H_2O(l) \rightleftarrows$ α-$NiSO_4.6H_2O$	**2.127**	**-12.139**	-4.485	**27.884**
	± 1.059	**± 1.175**	± 1.000	± 1.000		**± 0.265**	**± 1.514**	± 0.200	**± 1.861**
	[2005GAM/BUG]		[2005GAM/BUG]	[2005GAM/BUG]					
β-$NiSO_4.6H_2O$	-2224.915	-2677.287	354.500		$Ni^{2+} + SO_4^{2-} + 6\ H_2O(l) \rightleftarrows$ β-$NiSO_4.6H_2O$	**2.030**	**-11.587**	**2.357**	**47.934**
	± 1.815	± 1.034	± 5.000			**± 0.370**	**± 2.113**	**± 1.552**	**± 5.241**
	[2005GAM/BUG]	[2005GAM/BUG]	[2005GAM/BUG]						
$NiSO_4 \cdot 7H_2O$(cr)	**-2463.450**	**-2977.649**	**379.082**	364.600	$Ni^{2+} + SO_4^{2-} + 7\ H_2O(l) \rightleftarrows NiSO_4 \cdot 7H_2O(cr)$	2.267	-12.940	-12.167	2.593
	± 1.146	**± 1.238**	**± 1.807**	± 4.000		± 0.019	± 0.110	± 0.226	± 0.843
				[2005GAM/BUG]		[2005GAM/BUG]	[2005GAM/BUG]	[2005GAM/BUG]	[2005GAM/BUG]
$NiSO_4$(aq)	**-803.646**	**-958.954**	**-48.998**		$Ni^{2+} + SO_4^{2-} \rightleftarrows NiSO_4(aq)$	2.350	-13.414	5.660	63.974
	± 0.914	**± 1.266**	**± 3.150**			± 0.030	± 0.171	± 0.810	± 2.777
						[2005GAM/BUG]	[2005GAM/BUG]	[2005GAM/BUG]	[2005GAM/BUG]
$Ni(SO_4)_2^{2-}$	**-1551.222**				$Ni^{2+} + 2\ SO_4^{2-} \rightleftarrows Ni(SO_4)_2^{2-}$	-16.530	**-16.530**		
	± 1.201					± 0.011	**± 0.011**		
						[2009KIT/KIR]			
$Ni(NO_3)_2 \cdot 2H_2O$(cr)		-1012.732			$Ni^{2+} + 2\ NO_3^- + 2\ H_2O(l) \rightleftarrows Ni(NO_3)_2 \cdot 2H_2O(cr)$			27.640	
		± 0.156						± 1.000	
		[2005GAM/BUG]						[2005GAM/BUG]	
$Ni(NO_3)_2 \cdot 4H_2O$(cr)		-1620.392			$Ni^{2+} + 2\ NO_3^- + 4\ H_2O(l) \rightleftarrows Ni(NO_3)_2 \cdot 4H_2O(cr)$			-8.360	
		± 1.441						± 0.800	
		[2005GAM/BUG]						[2005GAM/BUG]	
$Ni(NO_3)_2 \cdot 6H_2O$(cr)		-2214.452		463.000	$Ni^{2+} + 2\ NO_3^- + 6\ H_2O(l) \rightleftarrows Ni(NO_3)_2 \cdot 6H_2O(cr)$			-30.760	
		± 1.571		± 2.000				± 1.000	
		[2005GAM/BUG]		[2005GAM/BUG]				[2005GAM/BUG]	
$NiNO_3^+$	**-159.545**				$Ni^{2+} + NO_3^- \rightleftarrows NiNO_3^+$	0.500	-2.854		
	± 6.283					± 1.000	± 5.708		
						[2005GAM/BUG]	[2005GAM/BUG]		

Table A3 Selected thermodynamic data for nickel (Ni) in JAEA-TDB-RN in 2020 (4/5)

Species / compound	$\Delta_f G^0_m$ (kJ.mol^{-1})	$\Delta_f H^0_m$ (kJ.mol^{-1})	S^0_m (J.K^{-1}.mol^{-1})	$C^0_{p,m}$ (J.K^{-1}.mol^{-1})	Reaction	$\log_{10} K°$	$\Delta_r G^0_m$ (kJ.mol^{-1})	$\Delta_r H^0_m$ (kJ.mol^{-1})	$\Delta_r S^0_m$ (J.K^{-1}.mol^{-1})
$NiNH_3^{2+}$	**-32.438**				$Ni^{2+} + NH_4^+ \rightleftarrows NiNH_3^{2+} + H^+$	-16.530	**40.042**		
	± 0.919					± 0.011	**± 0.371**		
						[2009KIT/KIR]			
$Ni(NH_3)_2^{2+}$	**-16.180**				$Ni^{2+} + 2\ NH_4^+ \rightleftarrows Ni(NH_3)_2^{2+} + 2\ H^+$	-16.530	**83.006**		
	± 1.318					± 0.011	**± 0.833**		
						[2009KIT/KIR]			
$Ni(NH_3)_3^{2+}$	**1.231**				$Ni^{2+} + 3\ NH_4^+ \rightleftarrows Ni(NH_3)_3^{2+} + 3\ H^+$	-16.530	**127.124**		
	± 2.255					± 0.011	**± 1.867**		
						[2009KIT/KIR]			
$Ni(NH_3)_4^{2+}$	**21.508**				$Ni^{2+} + 4\ NH_4^+ \rightleftarrows Ni(NH_3)_4^{2+} + 4\ H^+$	-16.530	**174.107**		
	± 2.384					± 0.011	**± 1.815**		
						[2009KIT/KIR]			
$Ni(NH_3)_5^{2+}$	**45.803**				$Ni^{2+} + 5\ NH_4^+ \rightleftarrows Ni(NH_3)_5^{2+} + 5\ H^+$	-16.530	**225.108**		
	± 2.599					± 0.011	**± 1.832**		
						[2009KIT/KIR]			
$Ni(NH_3)_6^{2+}$	**76.416**				$Ni^{2+} + 6\ NH_4^+ \rightleftarrows Ni(NH_3)_6^{2+} + 6\ H^+$	-16.530	**282.428**		
	± 2.897					± 0.011	**± 1.941**		
						[2009KIT/KIR]			
$NiHPO_4$(aq)	**-1152.320**				$Ni^{2+} + HPO_4^{2-} \rightleftarrows NiHPO_4$(aq)	3.050	-17.410		
	± 1.249					± 0.090	± 0.514		
						[2005GAM/BUG]	[2005GAM/BUG]		
$NiP_2O_7^{2-}$	-2031.107				$Ni^{2+} + P_2O_7^{4-} \rightleftarrows NiP_2O_7^{2-}$	8.730	-49.831	30.600	269.768
	± 4.843					± 0.250	± 1.427	± 10.000	± 33.880
	[2005GAM/BUG]					[2005GAM/BUG]	[2005GAM/BUG]	[2005GAM/BUG]	[2005GAM/BUG]
$NiHP_2O_7^-$	-2064.270				$Ni^{2+} + HP_2O_7^{3-} \rightleftarrows NiHP_2O_7^-$	5.140	-29.339	47.900	259.062
	± 4.766					± 0.250	± 1.427	± 15.000	± 50.537
	[2005GAM/BUG]					[2005GAM/BUG]	[2005GAM/BUG]	[2005GAM/BUG]	[2005GAM/BUG]
NiAs(cr)	-66.583	-70.820	50.760	50.800	$Ni^{2+} + AsO_4^{3-} + 8\ H^+ + 7\ e^- \rightleftarrows$ NiAs(cr) $+ 4\ H_2O$(l)	**56.268**	**-321.180**	**-271.021**	**167.676**
	± 4.606	± 4.240	± 6.000	± 4.000		**± 1.080**	**± 6.167**	**± 5.910**	**± 6.200**
	[2005GAM/BUG]	[2005GAM/BUG]	[2005GAM/BUG]	[2005GAM/BUG]					
$NiAs_2$(cr)		-90.100			$Ni^{2+} + 2\ AsO_4^{3-} + 16\ H^+ + 12\ e^- \rightleftarrows NiAs_2$(cr) $+ 8\ H_2O$(l)			**-545.515**	
		± 8.000						**± 11.379**	
		[2005GAM/BUG]							
Ni_5As_2(cr)	-237.638	-244.600	196.200		$5\ Ni^{2+} + 2\ AsO_4^{3-} + 16\ H^+ + 20\ e^- \rightleftarrows Ni_5As_2$(cr) $+ 8\ H_2O$(l)	**106.782**	**-609.514**	**-479.967**	**433.395**
	± 21.914	± 20.000	± 30.000			**± 4.146**	**± 23.664**	**± 21.999**	**± 30.838**
	[2005GAM/BUG]	[2005GAM/BUG]	[2005GAM/BUG]						
$Ni_{11}As_8$(cr)	-715.758	-743.000	518.000	490.000	$11\ Ni^{2+} + 8\ AsO_4^{3-} + 64\ H^+ + 62\ e^-$	**458.164**	**-2615.218**	**-2179.574**	**1456.691**
	± 39.338	± 35.000	± 60.000	± 40.000	$\rightleftarrows Ni_{11}As_8$(cr) $+ 32\ H_2O$(l)	**± 9.032**	**± 51.554**	**± 48.513**	**± 62.197**
	[2005GAM/BUG]	[2005GAM/BUG]	[2005GAM/BUG]	[2005GAM/BUG]					
$Ni_3(AsO_3)_2$(cr,hyd)	**-1253.713**				$3\ Ni^{2+} + 2\ HAsO_2$(aq) $+ 2\ H_2O$(l)	-28.700	163.821		
	± 9.253				$\rightleftarrows Ni_3(AsO_3)_2$(cr,hyd) $+ 6\ H^+$	± 0.700	± 3.996		
						[2005GAM/BUG]	[2005GAM/BUG]		

Table A3 Selected thermodynamic data for nickel (Ni) in JAEA-TDB-RN in 2020 (5/5)

Species / compound	$\Delta_f G^0_m$ (kJ.mol^{-1})	$\Delta_f H^0_m$ (kJ.mol^{-1})	S^0_m (J.K^{-1}.mol^{-1})	$C^0_{p,m}$ (J.K^{-1}.mol^{-1})	Reaction	$\log_{10} K°$	$\Delta_r G^0_m$ (kJ.mol^{-1})	$\Delta_r H^0_m$ (kJ.mol^{-1})	$\Delta_r S^0_m$ (J.K^{-1}.mol^{-1})
$Ni_3(AsO_4)_2.8H_2O$(cr)	**-3491.896**	-4179.000	540.771		3 Ni^{2+} + 2 AsO_4^{3-} + 8 H_2O(l) ⇄ $Ni_3(AsO_4)_2.8H_2O$(cr)	28.100	-160.396	**49.023**	**702.387**
	± 8.854	± 20.000 [2005GAM/BUG]	± 73.331 [2005GAM/BUG]			± 0.500 [2005GAM/BUG]	± 2.854 [2005GAM/BUG]	**± 21.717**	**± 73.464**
$NiHAsO_4$(aq)	-776.918				Ni^{2+} + $HAsO_4^{2-}$ ⇄ $NiHAsO_4$(aq)	2.900	-16.553		
	± 4.426 [2005GAM/BUG]					± 0.300 [2005GAM/BUG]	± 1.712 [2005GAM/BUG]		
$NiCO_3$(cr)	**-636.444**	-713.320	85.400	90.300	Ni^{2+} + H_2O(l) + CO_2(g) ⇄ $NiCO_3$(cr) + 2 H^+	-7.160	40.870	**21.040**	**-66.484**
	± 1.291	± 1.424	± 2.000	± 4.100		± 0.180 [2005GAM/BUG]	± 1.027 [2005GAM/BUG]	**± 1.678**	**± 2.582**
$NiCO_3.5.5H_2O$(cr)	**-1921.143**	-2312.992	311.100	405.400	Ni^{2+} + 6.5 H_2O(l) + CO_2(g) ⇄ $NiCO_3.5.5H_2O$(cr) + 2 H^+	-10.630	60.676	**-6.521**	**-225.360**
	± 1.163	± 3.147 [2005GAM/BUG]	± 10.000 [2005GAM/BUG]	± 50.000 [2005GAM/BUG]		± 0.100 [2005GAM/BUG]	± 0.571 [2005GAM/BUG]	**± 3.338**	**± 10.147**
$NiCO_3$(aq)	**-597.730**				Ni^{2+} + CO_3^{2-} ⇄ $NiCO_3$(aq)	4.200	-23.974		
	± 2.427					± 0.400 [2005GAM/BUG]	± 2.283 [2005GAM/BUG]		
$NiHCO_3^+$	**-640.801**				Ni^{2+} + HCO_3^- ⇄ $NiHCO_3^+$	1.417	**-8.088**		
	± 1.268					± 0.175 [2009KIT/KIR]	**± 0.999**		
$Ni(CN)_4^{2-}$	**471.367**	**366.784**	**216.864**		Ni^{2+} + 4 CN^- ⇄ $Ni(CN)_4^{2-}$	30.200	-172.383	-180.700	-27.896
	± 33.488	**± 33.722**	**± 36.161**			± 0.120 [2005GAM/BUG]	± 0.685 [2005GAM/BUG]	± 4.000 [2005GAM/BUG]	± 13.611 [2005GAM/BUG]
$Ni(CN)_5^{3-}$	**653.452**	**507.008**	**243.576**		Ni^{2+} + 5 CN^- ⇄ $Ni(CN)_5^{3-}$	28.500	-162.679	-191.100	-95.324
	± 41.944	**± 42.607**	**± 50.638**			± 0.500 [2005GAM/BUG]	± 2.854 [2005GAM/BUG]	± 8.000 [2005GAM/BUG]	± 28.489 [2005GAM/BUG]
$NiSCN^+$	**36.780**	**9.755**	**7.623**		Ni^{2+} + SCN^- ⇄ $NiSCN^+$	1.810	-10.332	-11.800	-4.925
	± 8.407	**± 9.787**	**± 18.810**			± 0.040 [2005GAM/BUG]	± 0.228 [2005GAM/BUG]	± 5.000 [2005GAM/BUG]	± 16.788 [2005GAM/BUG]
$Ni(SCN)_2$(aq)	**124.642**	**77.122**	**137.961**		Ni^{2+} + 2 SCN^- ⇄ $Ni(SCN)_2$(aq)	2.690	-15.355	-21.000	-18.935
	± 16.759	**± 18.571**	**± 31.683**			± 0.070 [2005GAM/BUG]	± 0.400 [2005GAM/BUG]	± 8.000 [2005GAM/BUG]	± 26.866 [2005GAM/BUG]
$Ni(SCN)_3^-$	**215.643**	**145.690**	**261.795**		Ni^{2+} + 3 SCN^- ⇄ $Ni(SCN)_3^-$	3.020	-17.238	-29.000	-39.449
	± 25.137	**± 27.037**	**± 42.060**			± 0.180 [2005GAM/BUG]	± 1.027 [2005GAM/BUG]	± 10.000 [2005GAM/BUG]	± 33.717 [2005GAM/BUG]
Ni_2SiO_4(oliv)	-1288.441	-1396.000	128.100	123.200	2 Ni^{2+} + H_4SiO_4(aq) ⇄ Ni_2SiO_4(oliv) + 4 H^+	**-19.425**	**110.877**	**170.948**	**201.903**
	± 5.002 [2005GAM/BUG]	± 5.000 [2005GAM/BUG]	± 0.200 [2005GAM/BUG]	± 0.500 [2005GAM/BUG]		**± 0.971**	**± 5.541**	**± 6.319**	**± 10.622**

[2005GAM/BUG] Gamsjäger et al. [A6)]
[2009KIT/KIR] Kitamura et al. [A4)]
[2020JAE] Japan Atomic Energy Agency [A1)].

Table A4 Selected thermodynamic data for selenium (Se) in JAEA-TDB-RN in 2020 (1/17)

Values indicated by **boldface** are calculated and selected in the present report.

Species / compound	$\Delta_f G^0_m$ (kJ.mol^{-1})	$\Delta_f H^0_m$ (kJ.mol^{-1})	S^0_m (J.K^{-1}.mol^{-1})	$C^0_{p,m}$ (J.K^{-1}.mol^{-1})	Reaction	$\log_{10} K°$	$\Delta_r G^0_m$ (kJ.mol^{-1})	$\Delta_r H^0_m$ (kJ.mol^{-1})	$\Delta_r S^0_m$ (J.K^{-1}.mol^{-1})
Se(cr)	0.000	0.000	42.090	25.090	$SeO_3^{2-} + 6\ H^+ + 4\ e^- \rightleftarrows Se(cr) + 3\ H_2O(l)$	**61.169**	**-349.156**	**-350.355**	**-4.444**
	[2005OLI/NOL]	[2005OLI/NOL]	[2005OLI/NOL]	[2005OLI/NOL]		**± 0.312**	**± 1.782**	**± 1.173**	**± 7.024**
Se(mono)	1.281	2.140	44.970	25.090	$SeO_3^{2-} + 6\ H^+ + 4\ e^- \rightleftarrows Se(mono) + 3\ H_2O(l)$	**60.945**	**-347.875**	**-348.215**	**-1.564**
	± 0.184	± 0.100	± 0.400	± 0.800		**± 0.314**	**± 1.791**	**± 1.177**	**± 7.027**
	[2005OLI/NOL]	[2005OLI/NOL]	[2005OLI/NOL]	[2005OLI/NOL]					
Se(am)	**5.969**				$HSe^- \rightleftarrows Se(am) + H^+ + 2\ e^-$	6.570	-37.502		
	± 2.199					± 0.150	± 0.862		
						[2010IID/YAM]	[2010IID/YAM]		
Se(g)	195.927	236.070	176.729	20.819	$SeO_3^{2-} + 6\ H^+ + 4\ e^- \rightleftarrows Se(g) + 3\ H_2O(l)$	**26.844**	**-153.229**	**-114.285**	**130.195**
	± 1.524	± 1.521	± 0.006	± 0.001		**± 0.411**	**± 2.345**	**± 1.921**	**± 7.016**
	[2005OLI/NOL]	[2005OLI/NOL]	[2005OLI/NOL]	[2005OLI/NOL]					
Se^{2-}	**128.602**				$Se(cr) + 2\ e^- \rightleftarrows Se^{2-}$	-22.530	128.602		
	± 3.004					± 0.526	± 3.004		
						[2005OLI/NOL]	[2005OLI/NOL]		
$Se_2(g)$	92.442	141.100	247.380	41.710	$2\ SeO_3^{2-} + 12\ H^+ + 8\ e^- \rightleftarrows Se_2(g) + 6\ H_2O(l)$	**106.143**	**-605.870**	**-559.610**	**154.313**
	± 3.009	± 3.000	± 0.400	± 0.200		**± 0.817**	**± 4.664**	**± 3.808**	**± 14.037**
	[2005OLI/NOL]	[2005OLI/NOL]	[2005OLI/NOL]	[2005OLI/NOL]					
Se_2^{2-}	**112.672**				$2\ Se^{2-} \rightleftarrows Se_2^{2-} + 2\ e^-$	25.320	-144.528		
	± 6.295					± 0.333	± 1.903		
						[2005OLI/NOL]	[2005OLI/NOL]		
$Se_3(g)$	123.549	178.000	308.900		$3\ SeO_3^{2-} + 18\ H^+ + 12\ e^- \rightleftarrows Se_3(g) + 9\ H_2O(l)$	**161.863**	**-923.918**	**-873.065**	**169.299**
	± 10.439	± 10.000	± 10.000			**± 2.055**	**± 11.728**	**± 10.601**	**± 23.302**
	[2005OLI/NOL]	[2005OLI/NOL]	[2005OLI/NOL]						
Se_3^{2-}	**25.148**				$3\ Se^{2-} \rightleftarrows Se_3^{2-} + 4\ e^-$	49.966	-285.208		
	± 2.300					± 0.333	± 1.903		
						[2005OLI/NOL]	[2005OLI/NOL]		
$Se_4(g)$	111.647	163.000	340.600		$4\ SeO_3^{2-} + 24\ H^+ + 16\ e^- \rightleftarrows Se_4(g) + 12\ H_2O(l)$	**225.117**	**-1284.976**	**-1238.420**	**154.465**
	± 13.406	± 12.000	± 20.000			**± 2.660**	**± 15.183**	**± 12.884**	**± 34.461**
	[2005OLI/NOL]	[2005OLI/NOL]	[2005OLI/NOL]						
Se_4^{2-}	**95.153**				$4\ Se(cr) + 2\ e^- \rightleftarrows Se_4^{2-}$	-16.670	95.153		
	± 0.198					± 0.030	± 0.198		
						[2010IID/YAM]	[2010IID/YAM]		
$Se_5(g)$	88.393	144.400	398.300		$5\ SeO_3^{2-} + 30\ H^+ + 20\ e^- \rightleftarrows Se_5(g) + 15\ H_2O(l)$	**290.360**	**-1657.386**	**-1607.375**	**165.631**
	± 5.256	± 4.300	± 10.000			**± 1.812**	**± 10.343**	**± 7.271**	**± 36.477**
	[2005OLI/NOL]	[2005OLI/NOL]	[2005OLI/NOL]						
$Se_6(g)$	83.638	136.100	428.500		$6\ SeO_3^{2-} + 36\ H^+ + 24\ e^- \rightleftarrows Se_6(g) + 18\ H_2O(l)$	**352.362**	**-2011.297**	**-1966.030**	**149.298**
	± 4.866	± 3.800	± 10.000			**± 2.058**	**± 11.745**	**± 7.997**	**± 43.266**
	[2005OLI/NOL]	[2005OLI/NOL]	[2005OLI/NOL]						

Table A4 Selected thermodynamic data for selenium (Se) in JAEA-TDB-RN in 2020 (2/17)

Species / compound	$\Delta_f G^0_m$ (kJ.mol^{-1})	$\Delta_f H^0_m$ (kJ.mol^{-1})	S^0_m (J.K^{-1}.mol^{-1})	$C^0_{p,m}$ (J.K^{-1}.mol^{-1})	Reaction	$\log_{10} K°$	$\Delta_r G^0_m$ (kJ.mol^{-1})	$\Delta_r H^0_m$ (kJ.mol^{-1})	$\Delta_r S^0_m$ (J.K^{-1}.mol^{-1})
Se_7(g)	92.845	150.200	487.000		7 SeO_3^{2-} + 42 H^+ + 28 e^- ⇄ Se_7(g) + 21 H_2O(l)	**411.918**	**-2351.245**	**-2302.285**	**161.264**
	± 4.891	± 4.500	± 6.000			**± 2.347**	**± 13.396**	**± 9.362**	**± 49.476**
	[2005OLI/NOL]	[2005OLI/NOL]	[2005OLI/NOL]						
Se_8(g)	100.307	156.800	526.200		8 SeO_3^{2-} + 48 H^+ + 32 e^- ⇄ Se_8(g) + 24 H_2O(l)	**471.780**	**-2692.939**	**-2646.040**	**153.930**
	± 3.580	± 3.000	± 6.000			**± 2.575**	**± 14.696**	**± 9.850**	**± 56.446**
	[2005OLI/NOL]	[2005OLI/NOL]	[2005OLI/NOL]						
SeO(g)	30.855	57.400	233.700	32.520	SeO_3^{2-} + 4 H^+ + 2 e^- ⇄ SeO(g) + 2 H_2O(l)	**14.211**	**-81.118**	**-7.117**	**247.922**
	± 6.218	± 6.210	± 1.000	± 0.250		**± 1.132**	**± 6.464**	**± 6.315**	**± 7.084**
	[2005OLI/NOL]	[2005OLI/NOL]	[2005OLI/NOL]	[2005OLI/NOL]					
SeO_2(cr)	-171.797	-225.390	67.490	58.230	SeO_3^{2-} + 2 H^+ ⇄ SeO_2(cr) + H_2O(l)	**8.162**	**-46.588**	**-4.068**	**142.468**
	± 0.620	± 0.600	± 0.400	± 0.180		**± 0.327**	**± 1.865**	**± 1.284**	**± 7.023**
	[2005OLI/NOL]	[2005OLI/NOL]	[2005OLI/NOL]	[2005OLI/NOL]					
SeO_2(g)	-115.166	-110.590	262.590	43.360	SeO_3^{2-} + 2 H^+ ⇄ SeO_2(g) + H_2O(l)	**-1.760**	**10.043**	**110.732**	**337.568**
	± 2.600	± 2.571	± 1.250	± 0.150		**± 0.550**	**± 3.139**	**± 2.810**	**± 7.122**
	[2005OLI/NOL]	[2005OLI/NOL]	[2005OLI/NOL]	[2005OLI/NOL]					
SeO_3(cr)	-86.154	-163.100	91.740	77.240	SeO_4^{2-} + 2 H^+ ⇄ SeO_3(cr) + H_2O(l)	**-20.348**	**116.148**	**154.562**	**128.698**
	± 2.222	± 2.200	± 1.000	± 0.790		**± 0.463**	**± 2.645**	**± 4.135**	**± 12.727**
	[2005OLI/NOL]	[2005OLI/NOL]	[2005OLI/NOL]	[2005OLI/NOL]					
SeO_3^{2-}	-362.392	-507.160	-5.055		$HSeO_3^{2-}$ ⇄ SeO_3^{2-} + H^+	-8.360	47.719		
	± 1.756	± 1.130	± 7.011			± 0.230	± 1.317		
	[2005OLI/NOL]	[2005OLI/NOL]	[2005OLI/NOL]			[2005OLI/NOL]	[2005OLI/NOL]		
SeO_4^{2-}	-439.485	-603.500	32.965		$HSeO_4^{2-}$ ⇄ SeO_4^{2-} + H^+	-1.750	9.989	-20.800	-103.267
	± 1.431	± 3.500	± 12.687			± 0.100	± 0.579	± 3.200	± 10.902
	[2005OLI/NOL]	[2005OLI/NOL]	[2005OLI/NOL]			[2005OLI/NOL]	[2005OLI/NOL]	[2005OLI/NOL]	[2005OLI/NOL]
					SeO_3^{2-} + 2 H_2O(l) ⇄ SeO_4^{2-} + 2 H^+ + 2 e^-	**-28.046**	**160.090**	**189.498**	**98.776**
						± 0.397	**± 2.267**	**± 3.679**	**± 14.496**
Se_2O_3(cr)		-414.590			2 SeO_3^{2-} + 6 H^+ + 2 e^- ⇄ Se_2O_3(cr) + 3 H_2O(l)			**-257.785**	
		± 2.577						**± 3.442**	
		[2005OLI/NOL]							
HSe^-	**43.471**				H_2Se(aq) ⇄ HSe^- + H^+	-3.850	21.976		
	± 2.023					± 0.050	± 0.285		
						[2005OLI/NOL]	[2005OLI/NOL]		
					SeO_3^{2-} + 3 H^+ + 2 e^- ⇄ HSe^- + 3 H_2O(l)	**53.553**	**-305.685**		
						± 0.472	**± 2.696**		
H_2Se(g)	15.217	29.000	219.000	34.700	SeO_3^{2-} + 8 H^+ + 6 e^- ⇄ H_2Se(g) + 3 H_2O(l)	**58.503**	**-333.939**	**-321.355**	**41.787**
	± 2.003	± 2.000	± 0.100	± 0.100		**± 0.470**	**± 2.681**	**± 2.318**	**± 7.017**
	[2005OLI/NOL]	[2005OLI/NOL]	[2005OLI/NOL]	[2005OLI/NOL]					
H_2Se(aq)	**21.496**	14.300	148.637		SeO_3^{2-} + 8 H^+ + 6 e^- ⇄ H_2Se(aq) + 3 H_2O(l)	**57.403**	**-327.661**	**-336.055**	**-28.576**
	± 2.004	± 2.022	± 1.029			**± 0.470**	**± 2.681**	**± 2.337**	**± 7.091**
		[2005OLI/NOL]	[2005OLI/NOL]						

Table A4 Selected thermodynamic data for selenium (Se) in JAEA-TDB-RN in 2020 (3/17)

Species / compound	$\Delta_f G^0_m$ (kJ.mol^{-1})	$\Delta_f H^0_m$ (kJ.mol^{-1})	S^0_m (J.K^{-1}.mol^{-1})	$C^0_{p,m}$ (J.K^{-1}.mol^{-1})	Reaction	$\log_{10} K°$	$\Delta_r G^0_m$ (kJ.mol^{-1})	$\Delta_r H^0_m$ (kJ.mol^{-1})	$\Delta_r S^0_m$ (J.K^{-1}.mol^{-1})
$HSeO_3^-$	-410.112 ± 1.166 [2005OLI/NOL]	-512.330 ± 1.010 [2005OLI/NOL]	137.656 ± 5.184 [2005OLI/NOL]		$H_2SeO_3(aq) \rightleftarrows HSeO_3^- + H^+$	-2.640 ± 0.140 [2005OLI/NOL]	15.069 ± 0.799 [2005OLI/NOL]		
$HSeO_4^-$	**-449.517 ± 1.316**	-582.700 ± 4.700 [2005OLI/NOL]	136.232 ± 16.370 [2005OLI/NOL]		$H_2SeO_3(aq) + H_2O(l) \rightleftarrows HSeO_4^- + 3\ H^+ + 2\ e^-$	-37.289 ± 0.175 [2005OLI/NOL]	212.847 ± 1.000 [2005OLI/NOL]		
$H_2SeO_3(cr)$		**-524.728 ± 0.635**			$SeO_2(cr) + H_2O(l) \rightleftarrows H_2SeO_3(cr)$			-13.500 ± 0.180 [2005OLI/NOL]	
$H_2SeO_3(aq)$	**-425.308 ± 0.892**	-505.320 ± 0.650 [2005OLI/NOL]	211.710 ± 3.601 [2005OLI/NOL]		$Se(cr) + 3\ H_2O(l) \rightleftarrows H_2SeO_3(aq) + 2\ H_2(g)$	-50.147 ± 0.147 [2005OLI/NOL]	286.240 ± 0.840 [2005OLI/NOL]		
$H_2SeO_4(cr)$		-530.500 ± 1.880 [2005OLI/NOL]			$2\ SeO_4^{2-} + 2\ H^+ \rightleftarrows H_2SeO_4(cr) + 2\ e^-$			**676.500 ± 7.248**	
$SeF_2(g)$			271.280 ± 0.050 [2005OLI/NOL]	47.660 ± 0.040 [2005OLI/NOL]					
$SeF_4(l)$	-775.070 ± 24.067 [2005OLI/NOL]	-851.000 ± 24.000 [2005OLI/NOL]	193.000 ± 6.000 [2005OLI/NOL]						
$SeF_4(g)$	-765.549 ± 24.047 [2005OLI/NOL]	-806.000 ± 24.047 [2005OLI/NOL]	312.000 ± 0.100 [2005OLI/NOL]	82.030 ± 0.090 [2005OLI/NOL]	$SeO_3^{2-} + 4\ F^- + 6\ H^+ \rightleftarrows SeF_4(g) + 3\ H_2O(l)$	**-2.154 ± 4.250**	**12.297 ± 24.261**	**185.035 ± 24.224**	**579.542 ± 7.346**
$SeF_6(g)$	-1017.445 ± 0.438 [2005OLI/NOL]	-1118.000 ± 0.400 [2005OLI/NOL]	313.200 ± 0.500 [2005OLI/NOL]	110.440 ± 0.050 [2005OLI/NOL]	$SeO_3^{2-} + 6\ F^- + 8\ H^+ \rightleftarrows SeF_6(g) + 4\ H_2O(l)$	**-28.699 ± 0.754**	**163.813 ± 4.305**	**354.232 ± 5.359**	**639.005 ± 13.114**
$SeOF_2(l)$	-526.563 ± 16.006 [2005OLI/NOL]	-575.000 ± 16.000 [2005OLI/NOL]	185.000 ± 1.000 [2005OLI/NOL]						
$SeOF_2(g)$	-515.418 ± 16.032 [2005OLI/NOL]	-530.700 ± 16.031 [2005OLI/NOL]	296.200 ± 0.100 [2005OLI/NOL]	63.330 ± 0.050 [2005OLI/NOL]	$SeO_3^{2-} + 2\ F^- + 4\ H^+ \rightleftarrows SeOF_2(g) + 2\ H_2O(l)$	**11.193 ± 2.835**	**-63.890 ± 16.185**	**75.479 ± 16.128**	**467.460 ± 7.098**
$Se_2F_2(g)$			331.120 ± 0.100 [2005OLI/NOL]	72.230 ± 0.040 [2005OLI/NOL]					
$SeF_5Cl(g)$			341.000 ± 0.200 [2005OLI/NOL]	116.300 ± 0.100 [2005OLI/NOL]					
$SeCl_2(g)$	**-25.869 ± 5.602**	-17.000 ± 4.472 [2005OLI/NOL]	295.180 ± 0.060 [2005OLI/NOL]	53.570 ± 0.030 [2005OLI/NOL]	$SeO_3^{2-} + 2\ Cl^- + 6\ H^+ + 2\ e^- \rightleftarrows SeCl_2(g) + 3\ H_2O(l)$	**19.713 ± 0.844**	**-112.523 ± 4.819**	**-33.196 ± 4.627**	**265.855 ± 7.024**

Table A4 Selected thermodynamic data for selenium (Se) in JAEA-TDB-RN in 2020 (4/17)

Species / compound	$\Delta_f G^0_m$ (kJ.mol^{-1})	$\Delta_f H^0_m$ (kJ.mol^{-1})	S^0_m (J.K^{-1}.mol^{-1})	$C^0_{p,m}$ (J.K^{-1}.mol^{-1})	Reaction	$\log_{10} K°$	$\Delta_r G^0_m$ (kJ.mol^{-1})	$\Delta_r H^0_m$ (kJ.mol^{-1})	$\Delta_r S^0_m$ (J.K^{-1}.mol^{-1})
$SeCl_4$(cr)	-85.902	-179.000	176.000		SeO_3^{2-} + 4 Cl^- + 6 H^+ ⇄ $SeCl_4$(cr) + 3 H_2O(l)	**-15.785**	**90.101**	**138.964**	**163.884**
	± 3.114	± 2.000	± 8.000			**± 0.632**	**± 3.610**	**± 2.345**	**± 10.661**
	[2005OLI/NOL]	[2005OLI/NOL]	[2005OLI/NOL]						
Se_2Cl_2(l)	**-43.927**	-82.000	186.000		$SeCl_2$(g) + Se(cr) ⇄ Se_2Cl_2(l)	3.150	-17.980	-63.000	-151.000
	± 5.122	± 4.000	± 5.000			± 0.437	± 2.494	± 2.000	± 5.000
		[2005OLI/NOL]	[2005OLI/NOL]			[2005OLI/NOL]	[2005OLI/NOL]	[2005OLI/NOL]	[2005OLI/NOL]
Se_2Cl_2(g)	-34.935	-21.000	354.000	77.600	2 SeO_3^{2-} + 2 Cl^- + 12 H^+ + 6 e^- ⇄ Se_2Cl_2(g) + 6 H_2O(l)	**82.457**	**-470.667**	**-387.551**	**278.141**
	± 10.002	± 10.000	± 0.200	± 0.100		**± 1.860**	**± 10.620**	**± 10.273**	**± 14.037**
	[2005OLI/NOL]	[2005OLI/NOL]	[2005OLI/NOL]	[2005OLI/NOL]					
$SeOCl_2$(l)	-132.107	-180.600	205.100						
	± 2.089	± 2.000	± 2.000						
	[2005OLI/NOL]	[2005OLI/NOL]	[2005OLI/NOL]						
$SeOCl_2$(g)	-114.223	-128.000	321.540	70.200	SeO_3^{2-} + 2 Cl^- + 4 H^+ ⇄ $SeOCl_2$(g) + 2 H_2O(l)	**-6.374**	**36.383**	**141.643**	**352.971**
	± 2.502	± 2.500	± 0.100	± 0.050		**± 0.538**	**± 3.070**	**± 2.757**	**± 7.022**
	[2005OLI/NOL]	[2005OLI/NOL]	[2005OLI/NOL]	[2005OLI/NOL]					
$SeBr_2$(g)	-4.583	32.000	317.000	55.420	SeO_3^{2-} + 2 Br^- + 6 H^+ + 2 e^- ⇄ $SeBr_2$(g) + 3 H_2O(l)	**25.517**	**-145.652**	**-75.348**	**235.459**
	± 20.226	± 20.224	± 1.000	± 0.500		**± 3.558**	**± 20.307**	**± 20.260**	**± 7.099**
	[2005OLI/NOL]	[2005OLI/NOL]	[2005OLI/NOL]	[2005OLI/NOL]					
$SeBr_4$(cr)		-70.000			SeO_3^{2-} + 4 Br^- + 6 H^+ ⇄ $SeBr_4$(cr) + 3 H_2O(l)			**65.658**	
		± 5.000						**± 5.171**	
		[2005OLI/NOL]							
Se_2Br_2(l)		-31.000							
		± 3.000							
		[2005OLI/NOL]							
Se_2Br_2(g)			377.400	79.500					
			± 0.200	± 0.100					
			[2005OLI/NOL]	[2005OLI/NOL]					
$SeOBr_2$(cr)		-140.000			SeO_3^{2-} + 2 Br^- + 4 H^+ ⇄ $SeOBr_2$(cr) + 2 H_2O(l)			**38.490**	
		± 5.000						**± 5.139**	
		[2005OLI/NOL]							
SeS(g)	92.356	143.327	245.100	35.800	0.5 S_2(g) + 0.5 Se_2(g) ⇄ SeS(g)	-1.104	6.300	8.476	7.300
	± 6.871	± 6.869	± 0.500	± 0.100		± 1.174	± 6.700	± 6.702	± 0.500
	[2005OLI/NOL]	[2005OLI/NOL]	[2005OLI/NOL]	[2005OLI/NOL]		[2005OLI/NOL]	[2005OLI/NOL]	[2005OLI/NOL]	[2005OLI/NOL]
TeSe(g)			257.900	37.800	0.5 S_2(g) + 0.5 Te_2(g) ⇄ TeSe(g)	0.140	-0.800	-2.200	-4.700
			± 0.500	± 0.100		± 0.543	± 3.100	± 3.000	± 1.000
			[2005OLI/NOL]	[2005OLI/NOL]		[2005OLI/NOL]	[2005OLI/NOL]	[2005OLI/NOL]	[2005OLI/NOL]
Se_4N_4(cr)		679.000			4 SeO_3^{2-} + 4 NO_3^{2-} + 48 H^+ + 36 e^- ⇄ Se_4N_4(cr) + 24 H_2O(l)			**-3324.885**	
		± 35.000						**± 35.419**	
		[2005OLI/NOL]							
α-P_4Se_3			239.600	166.200					
			± 1.200	± 1.000					
			[2005OLI/NOL]	[2005OLI/NOL]					

Table A4 Selected thermodynamic data for selenium (Se) in JAEA-TDB-RN in 2020 (5/17)

Species / compound	$\Delta_f G^0_m$ (kJ.mol^{-1})	$\Delta_f H^0_m$ (kJ.mol^{-1})	S^0_m (J.K^{-1}.mol^{-1})	$C^0_{p,m}$ (J.K^{-1}.mol^{-1})	Reaction	$\log_{10} K°$	$\Delta_r G^0_m$ (kJ.mol^{-1})	$\Delta_r H^0_m$ (kJ.mol^{-1})	$\Delta_r S^0_m$ (J.K^{-1}.mol^{-1})
As_2Se_3(cr)			206.000 ± 3.000 [2005OLI/NOL]	121.400 ± 3.000 [2005OLI/NOL]					
As_4Se_3(cr)				172.500 ± 4.000 [2005OLI/NOL]					
As_4Se_4(cr)				196.600 ± 4.000 [2005OLI/NOL]					
SbSe(g)	134.874 ± 20.020 [2005OLI/NOL]	177.000 ± 20.000 [2005OLI/NOL]	228.900 ± 3.000 [2005OLI/NOL]		SeO_3^{2-} + $Sb(OH)_3$(aq) + 9 H^+ + 7 e^- ⇄ SbSe(g) + 6 H_2O(l)	**49.530**	**-282.721**		
Sb_2Se_3(cr)	-127.415 ± 3.723 [2005OLI/NOL]	-128.700 ± 3.600 [2005OLI/NOL]	213.000 ± 3.000 [2005OLI/NOL]	124.900 ± 1.500 [2005OLI/NOL]	3 SeO_3^{2-} + 2 $Sb(OH)_3$(aq) + 24 H^+ + 18 e^- ⇄ Sb_2Se_3(cr) + 13 H_2O(l)	**229.809**	**-1311.761**		
BiSe(cr)	-46.807 ± 5.720 [2005OLI/NOL]	-46.100 ± 5.700 [2005OLI/NOL]	101.200 ± 1.500 [2005OLI/NOL]	55.500 ± 0.900 [2005OLI/NOL]	SeO_3^{2-} + Bi^{3+} + 6 H^+ + 7 e^- ⇄ BiSe(cr) + 3 H_2O(l)	**86.109**	**-491.515**		
BiSe(g)			263.900 ± 6.000 [2005OLI/NOL]	36.460 ± 0.500 [2005OLI/NOL]					
Bi_2Se_3(cr)	-146.618 ± 10.065 [2005OLI/NOL]	-145.500 ± 10.000 [2005OLI/NOL]	243.500 ± 3.600 [2005OLI/NOL]	132.600 ± 2.100 [2005OLI/NOL]	3 SeO_3^{2-} + 2 Bi^{3+} + 18 H^+ + 18 e^- ⇄ Bi_2Se_3(cr) + 9 H_2O(l)	**242.674**	**-1385.191**		
CSe(g)	309.848 ± 9.202 [2005OLI/NOL]	362.000 ± 9.200 [2005OLI/NOL]	222.750 ± 0.500 [2005OLI/NOL]	30.580 ± 0.200 [2005OLI/NOL]	SeO_3^{2-} + HCO_3^- + 11 H^+ + 8 e^- ⇄ CSe(g) + 6 H_2O(l)	**28.717 ± 1.645**	**-163.916 ± 9.388**	**-155.937 ± 9.293**	**26.178 ± 7.066**
CSe_2(l)	196.020 ± 8.820 [2005OLI/NOL]	219.300 ± 7.600 [2005OLI/NOL]	168.000 ± 15.000 [2005OLI/NOL]	88.530 ± 0.900 [2005OLI/NOL]					
CSe_2(g)	203.937 ± 7.611 [2005OLI/NOL]	255.600 ± 7.603 [2005OLI/NOL]	263.200 ± 1.000 [2005OLI/NOL]	49.900 ± 0.100 [2005OLI/NOL]	2 SeO_3^{2-} + HCO_3^- + 17 H^+ + 12 e^- ⇄ CSe_2(g) + 9 H_2O(l)	**108.440 ± 1.477**	**-618.982 ± 8.432**	**-612.692 ± 7.990**	**20.094 ± 14.088**
$SeCN^-$	**141.344 ± 8.838**				Se(mono) + CN^- ⇄ $SeCN^-$	-3.574 ± 0.497 [2005OLI/NOL]	20.401 ± 2.837 [2005OLI/NOL]		
SiSe(g)	98.119 ± 10.501 [2005OLI/NOL]	150.200 ± 10.500 [2005OLI/NOL]	235.580 ± 0.200 [2005OLI/NOL]	33.620 ± 0.100 [2005OLI/NOL]	SeO_3^{2-} + $Si(OH)_4$(aq) + 10 H^+ + 8 e^- ⇄ SiSe(g) + 7 H_2O(l)	**-18.922 ± 1.896**	**108.005 ± 10.824**	**113.416 ± 11.131**	**17.584 ± 12.430**
$SiSe_2$(cr)		-177.600 ± 3.200 [2005OLI/NOL]			2 SeO_3^{2-} + $Si(OH)_4$(aq) + 16 H^+ + 12 e^- ⇄ $SiSe_2$(cr) + 10 H_2O(l)			**-564.739 ± 5.318**	

Table A4 Selected thermodynamic data for selenium (Se) in JAEA-TDB-RN in 2020 (6/17)

Species / compound	$\Delta_f G^0_m$ (kJ.mol^{-1})	$\Delta_f H^0_m$ (kJ.mol^{-1})	S^0_m (J.K^{-1}.mol^{-1})	$C^0_{p,m}$ (J.K^{-1}.mol^{-1})	Reaction	$\log_{10} K°$	$\Delta_r G^0_m$ (kJ.mol^{-1})	$\Delta_r H^0_m$ (kJ.mol^{-1})	$\Delta_r S^0_m$ (J.K^{-1}.mol^{-1})
GeSe(cr)	-52.226 ± 1.473 [2005OLI/NOL]	-50.300 ± 1.449 [2005OLI/NOL]	79.640 ± 0.800 [2005OLI/NOL]	49.880 ± 0.500 [2005OLI/NOL]					
GeSe(g)	70.450 ± 1.770 [2005OLI/NOL]	122.400 ± 1.761 [2005OLI/NOL]	247.420 ± 0.500 [2005OLI/NOL]	35.250 ± 0.200 [2005OLI/NOL]					
$GeSe_2$(cr)	-93.239 ± 12.007 [2005OLI/NOL]	-93.200 ± 12.000 [2005OLI/NOL]	115.400 ± 1.200 [2005OLI/NOL]	71.700 ± 0.700 [2005OLI/NOL]					
$GeSe_2$(g)		124.800 ± 21.633 [2005OLI/NOL]							
α-SnSe		-109.500 ± 15.000 [2005OLI/NOL]		51.910 ± 2.000 [2005OLI/NOL]	$SeO_3^{2-} + Sn^{2+} + 6\ H^+ + 6\ e^- \rightleftarrows$ α-SnSe + 3 H_2O(l)			**-450.238 ± 15.096**	
SnSe(g)	61.861 ± 15.693 [2005OLI/NOL]	110.200 ± 15.689 [2005OLI/NOL]	255.400 ± 1.000 [2005OLI/NOL]	35.930 ± 0.500 [2005OLI/NOL]	$SeO_3^{2-} + Sn^{2+} + 6\ H^+ + 6\ e^- \rightleftarrows$ SnSe(g) + 3 H_2O(l)			**-230.538 ± 15.781**	
$SnSe_2$(cr)		-114.900 ± 10.000 [2005OLI/NOL]		76.700 ± 0.500 [2005OLI/NOL]	2 $SeO_3^{2-} + Sn^{2+} + 12\ H^+ + 10\ e^- \rightleftarrows SnSe_2$(cr) + 6 H_2O(l)			**-805.993 ± 10.345**	
$SnSe_2$(g)		78.000 ± 16.100 [2005OLI/NOL]			2 $SeO_3^{2-} + Sn^{2+} + 12\ H^+ + 10\ e^- \rightleftarrows SnSe_2$(g) + 6 H_2O(l)			**-613.093 ± 16.317**	
PbSe(cr)	-97.936 ± 7.694 [2005OLI/NOL]	-98.500 ± 7.600 [2005OLI/NOL]	105.000 ± 4.000 [2005OLI/NOL]	50.610 ± 1.000 [2005OLI/NOL]	$SeO_3^{2-} + Pb^{2+} + 6\ H^+ + 6\ e^- \rightleftarrows$ PbSe(cr) + 3 H_2O(l)	**74.134 ± 1.384**	**-423.159 ± 7.900**	**-449.775 ± 7.694**	**-89.785 ± 8.173**
PbSe(g)	82.866 ± 8.689 [2005OLI/NOL]	129.500 ± 8.683 [2005OLI/NOL]	263.300 ± 1.000 [2005OLI/NOL]	36.360 ± 0.500 [2005OLI/NOL]	$SeO_3^{2-} + Pb^{2+} + 6\ H^+ + 6\ e^- \rightleftarrows$ PbSe(g) + 3 H_2O(l)	**42.459 ± 1.554**	**-242.357 ± 8.872**	**-221.775 ± 8.765**	**68.515 ± 7.197**
$PbSeO_3$(cr)	**-457.675 ± 5.976**	-532.080 ± 1.800 [2005OLI/NOL]	166.087 ± 20.968 [2005OLI/NOL]		$SeO_3^{2-} + Pb^{2+} \rightleftarrows PbSeO_3$(cr)	12.500 ± 1.000 [2005OLI/NOL]	-71.351 ± 5.708 [2005OLI/NOL]	**-25.840 ± 2.140**	**153.569 ± 22.145**
$PbSeO_4$(cr)	**-503.317 ± 2.032**	-607.300 ± 4.326 [2005OLI/NOL]	167.734 ± 16.027 [2005OLI/NOL]		$SeO_4^{2-} + Pb^{2+} \rightleftarrows PbSeO_4$(cr)	6.990 ± 0.250 [2005OLI/NOL]	-39.899 ± 1.427 [2005OLI/NOL]	-4.720 ± 2.530 [2005OLI/NOL]	116.269 ± 9.742 [2005OLI/NOL]
BSe_2(g)	131.400 ± 20.871 [2005OLI/NOL]	187.100 ± 20.000 [2005OLI/NOL]	276.900 ± 20.000 [2005OLI/NOL]		2 SeO_3^{2-} + $B(OH)_3$(aq) + 15 H^+ + 11 $e^- \rightleftarrows BSe_2$(g) + 9 H_2O(l)	**54.256 ± 3.715**	**-309.696 ± 21.207**	**-296.590 ± 20.174**	**35.286 ± 25.711**
AlSe(g)	206.569 ± 35.000 [2005OLI/NOL]	258.000 ± 35.000 [2005OLI/NOL]	242.890 ± 0.500 [2005OLI/NOL]	34.750 ± 0.200 [2005OLI/NOL]	$SeO_3^{2-} + Al^{3+} + 6\ H^+ + 7\ e^- \rightleftarrows$ AlSe(g) + 3 H_2O(l)	**-60.446 ± 6.144**	**345.029 ± 35.069**	**446.046 ± 35.052**	**338.405 ± 9.711**

Table A4 Selected thermodynamic data for selenium (Se) in JAEA-TDB-RN in 2020 (7/17)

Species / compound	$\Delta_f G^0_m$ (kJ.mol^{-1})	$\Delta_f H^0_m$ (kJ.mol^{-1})	S^0_m (J.K^{-1}.mol^{-1})	$C^0_{p,m}$ (J.K^{-1}.mol^{-1})	Reaction	$\log_{10} K°$	$\Delta_r G^0_m$ (kJ.mol^{-1})	$\Delta_r H^0_m$ (kJ.mol^{-1})	$\Delta_r S^0_m$ (J.K^{-1}.mol^{-1})
Al_2Se_3(cr)		-532.000 ± 40.000 [2005OLI/NOL]			3 SeO_3^{2-} + 2 Al^{3+} + 12 H^+ + 12 e^- ⇄ Al_2Se_3(cr) + 9 H_2O(l)			**-506.262** **± 40.267**	
GaSe(cr)		-145.000 ± 10.000 [2005OLI/NOL]	70.400 ± 0.700 [2005OLI/NOL]	48.600 ± 0.900 [2005OLI/NOL]					
Ga_2Se_3(cr)		-384.000 ± 40.000 [2005OLI/NOL]							
$Ga_2(SeO_3)_3 \cdot 6H_2O$(cr)					3 SeO_3^{2-} + 2 Ga^{3+} + 6 H_2O(l) ⇄ $Ga_2(SeO_3)_3 \cdot 6H_2O$(cr)	37.000 ± 2.000 [2005OLI/NOL]	-211.198 ± 11.416 [2005OLI/NOL]		
InSe(cr)			83.890 ± 0.900 [2005OLI/NOL]	49.750 ± 1.060 [2005OLI/NOL]					
α-In_2Se_3		-318.000 ± 20.000 [2005OLI/NOL]	203.100 ± 2.000 [2005OLI/NOL]	124.100 ± 4.100 [2005OLI/NOL]					
$In_2(SeO_3)_3 \cdot 6H_2O$(cr)					3 SeO_3^{2-} + 2 In^{3+} + 6 H_2O(l) ⇄ $In_2(SeO_3)_3 \cdot 6H_2O$(cr)	39.000 ± 2.000 [2005OLI/NOL]	-222.614 ± 11.416 [2005OLI/NOL]		
α-TlSe			103.000 ± 1.300 [2005OLI/NOL]	50.100 ± 0.800 [2005OLI/NOL]					
Tl_2Se(cr)			174.800 ± 3.000 [2005OLI/NOL]	82.200 ± 2.500 [2005OLI/NOL]					
Tl_2SeO_4(cr)	**-526.546** **± 1.772**	**-646.500** **± 6.103**	**-36.593** **± 21.223**		SeO_4^{2-} + 2 Tl^+ ⇄ Tl_2SeO_4(cr)	3.900 ± 0.150 [2005OLI/NOL]	-22.261 ± 0.856 [2005OLI/NOL]	-43.000 ± 5.000 [2005OLI/NOL]	-69.558 ± 17.014 [2005OLI/NOL]
TlSeCN(aq)	93.662 ± 4.156 [2005OLI/NOL]				$SeCN^-$ + Tl^+ ⇄ TlSeCN(aq)	1.750 ± 0.290 [2005OLI/NOL]	-9.989 ± 1.655 [2005OLI/NOL]		
α-ZnSe	-172.488 ± 4.013 [2005OLI/NOL]	-176.000 ± 4.000 [2005OLI/NOL]	71.940 ± 1.000 [2005OLI/NOL]	47.740 ± 1.500 [2005OLI/NOL]	SeO_3^{2-} + Zn^{2+} + 6 H^+ + 6 e^- ⇄ α-ZnSe + 3 H_2O(l)	**65.586** **± 0.771**	**-374.367** **± 4.400**	**-372.970** **± 4.174**	**4.348** **± 7.136**
ZnSe(g)		239.300 ± 20.000 [2005OLI/NOL]			SeO_3^{2-} + Zn^{2+} + 6 H^+ + 6 e^- ⇄ ZnSe(g) + 3 H_2O(l)			**42.330** **± 20.035**	
α-$ZnSeO_3$		-636.800 ± 11.300 [2005OLI/NOL]			SeO_3^{2-} + Zn^{2+} ⇄ α-$ZnSeO_3$			**23.745** **± 11.358**	

Table A4 Selected thermodynamic data for selenium (Se) in JAEA-TDB-RN in 2020 (8/17)

Species / compound	$\Delta_f G^0_m$ (kJ.mol^{-1})	$\Delta_f H^0_m$ (kJ.mol^{-1})	S^0_m (J.K^{-1}.mol^{-1})	$C^0_{p,m}$ (J.K^{-1}.mol^{-1})	Reaction	$\log_{10} K°$	$\Delta_r G^0_m$ (kJ.mol^{-1})	$\Delta_r H^0_m$ (kJ.mol^{-1})	$\Delta_r S^0_m$ (J.K^{-1}.mol^{-1})
β-$ZnSeO_3$		-652.700 ± 10.900 [2005OLI/NOL]			$SeO_3^{2-} + Zn^{2+} \rightleftarrows$ β-$ZnSeO_3$			**7.845** **± 10.960**	
$ZnSeO_4$(cr)		-664.730 ± 5.600 [2005OLI/NOL]			$SeO_4^{2-} + Zn^{2+} \rightleftarrows ZnSeO_4$(cr)			**92.155** **± 6.607**	
$ZnSeO_4$(aq)	**-599.091** **± 1.500**	**-752.285** **± 5.319**	**-19.875** **± 18.519**		$SeO_4^{2-} + Zn^{2+} \rightleftarrows ZnSeO_4$(aq)	2.160 ± 0.060 [2005OLI/NOL]	-12.329 ± 0.342 [2005OLI/NOL]	4.600 ± 4.000 [2005OLI/NOL]	56.781 ± 13.465 [2005OLI/NOL]
$ZnSeO_4 \cdot H_2O$(cr)		-983.070 ± 5.600 [2005OLI/NOL]			$SeO_4^{2-} + Zn^{2+} + H_2O(l) \rightleftarrows ZnSeO_4 \cdot H_2O$(cr)			**59.654** **± 6.608**	
$ZnSeO_4 \cdot 6H_2O$(cr)	**-2018.636** **± 1.627**	-2458.540 ± 5.610 [2005OLI/NOL]	417.016 ± 19.502 [2005OLI/NOL]		$SeO_4^{2-} + Zn^{2+} + 6\ H_2O(l) \rightleftarrows ZnSeO_4 \cdot 6H_2O$(cr)	1.538 ± 0.068 [2005OLI/NOL]	-8.779 ± 0.388 [2005OLI/NOL]		
$ZnSe_2O_5$(cr)		-888.300 ± 25.000 [2005OLI/NOL]			$2\ SeO_3^{2-} + Zn^{2+} + 4\ H^+ + 2\ e^- \rightleftarrows ZnSe_2O_5$(cr) + H_2O(l)			**-6.433** **± 25.103**	
$Zn(HSeO_3)_2 \cdot 2H_2O$(cr)		-1775.300 ± 25.000 [2005OLI/NOL]			$2\ SeO_3^{2-} + Zn^{2+} + 2\ H_2O(l) + 2\ H^+ \rightleftarrows Zn(HSeO_3)_2 \cdot 2H_2O$(cr)			**-35.918** **± 25.104**	
$ZnSeCN^+$	**-18.133** **± 3.827**				$SeCN^- + Zn^{2+} \rightleftarrows ZnSeCN^+$	1.210 ± 0.060 [2005OLI/NOL]	-6.907 ± 0.342 [2005OLI/NOL]	-5.950 ± 0.340 [2005OLI/NOL]	3.209 ± 1.619 [2005OLI/NOL]
$Zn(SeCN)_2$(aq)	**115.236** **± 7.632**				$2\ SeCN^- + Zn^{2+} \rightleftarrows Zn(SeCN)_2$(aq)	1.680 ± 0.110 [2005OLI/NOL]	-9.590 ± 0.628 [2005OLI/NOL]	-6.350 ± 1.200 [2005OLI/NOL]	10.865 ± 4.542 [2005OLI/NOL]
α-CdSe	-140.897 ± 1.918 [2005OLI/NOL]	-143.100 ± 1.900 [2005OLI/NOL]	86.500 ± 0.800 [2005OLI/NOL]	49.430 ± 0.480 [2005OLI/NOL]	$SeO_3^{2-} + Cd^{2+} + 6\ H^+ + 6\ e^- \rightleftarrows$ α-CdSe + 3 H_2O(l)	**72.235** **± 0.477**	**-412.320** **± 2.723**	**-417.535** **± 2.312**	**-17.913** **± 7.219**
$CdSeO_3$(cr)	-493.432 ± 6.467 [2005OLI/NOL]	-576.800 ± 2.500 [2005OLI/NOL]	122.000 ± 20.000 [2005OLI/NOL]		$SeO_3^{2-} + Cd^{2+} \rightleftarrows CdSeO_3$(cr)	**9.339** **± 1.181**	**-53.307** **± 6.743**	**6.280** **± 2.808**	**199.855** **± 21.246**
$CdSeO_4$(cr)		-634.100 ± 5.630 [2005OLI/NOL]			$SeO_4^{2-} + Cd^{2+} \rightleftarrows CdSeO_4$(cr)			**45.320** **± 6.656**	
$CdSeO_4$(aq)	-530.175 ± 1.652 [2005OLI/NOL]	-671.120 ± 5.349 [2005OLI/NOL]	31.463 ± 18.561 [2005OLI/NOL]		$SeO_4^{2-} + Cd^{2+} \rightleftarrows CdSeO_4$(aq)	2.270 ± 0.060 [2005OLI/NOL]	-12.957 ± 0.342 [2005OLI/NOL]	8.300 ± 4.000 [2005OLI/NOL]	71.297 ± 13.465 [2005OLI/NOL]
$CdSeO_4 \cdot H_2O$(cr)		-943.050 ± 5.620 [2005OLI/NOL]			$SeO_4^{2-} + Cd^{2+} + H_2O(l) \rightleftarrows CdSeO_4 \cdot H_2O$(cr)			**22.208** **± 6.649**	

Table A4 Selected thermodynamic data for selenium (Se) in JAEA-TDB-RN in 2020 (9/17)

Species / compound	$\Delta_f G^0_m$ (kJ.mol^{-1})	$\Delta_f H^0_m$ (kJ.mol^{-1})	S^0_m (J.K^{-1}.mol^{-1})	$C^0_{p,m}$ (J.K^{-1}.mol^{-1})	Reaction	$\log_{10} K°$	$\Delta_r G^0_m$ (kJ.mol^{-1})	$\Delta_r H^0_m$ (kJ.mol^{-1})	$\Delta_r S^0_m$ (J.K^{-1}.mol^{-1})
$CdSe_2O_5$(cr)		-828.000 ± 17.000 [2005OLI/NOL]			2 SeO_4^{2-} + Cd^{2+} + 6 H^+ + 2 e^- ⇄ $CdSe_2O_5$(cr) + 6 H_2O(l)			**-23.598 ± 17.160**	
$Cd_3H_2(SeO_3)_4$(cr)		-2306.000 ± 45.000 [2005OLI/NOL]			4 SeO_3^{2-} + 3 Cd^{2+} + 2 H^+ ⇄ $Cd_3H_2(SeO_3)_4$(cr)			**-49.600 ± 45.262**	
$CdSeCN^+$	**45.532 ± 3.888**				$SeCN^-$ + Cd^{2+} ⇄ $CdSeCN^+$	2.240 ± 0.060 [2005OLI/NOL]	-12.786 ± 0.342 [2005OLI/NOL]	-10.050 ± 0.200 [2005OLI/NOL]	9.177 ± 1.330 [2005OLI/NOL]
$Cd(SeCN)_2$(cr)	**161.833 ± 8.153**				Cd^{2+}+ 2 SCN^- ⇄ $Cd(SeCN)_2$(cr)	5.700 ± 0.500 [2005OLI/NOL]	-32.536 ± 2.854 [2005OLI/NOL]		
$Cd(SeCN)_2$(aq)	**175.304 ± 7.668**				2 $SeCN^-$ + Cd^{2+} ⇄ $Cd(SeCN)_2$(aq)	3.340 ± 0.120 [2005OLI/NOL]	-19.065 ± 0.685 [2005OLI/NOL]	-26.350 ± 2.000 [2005OLI/NOL]	-24.434 ± 7.091 [2005OLI/NOL]
$Cd(SeCN)_3^-$	**308.672 ± 11.487**				3 $SeCN^-$ + Cd^{2+} ⇄ $Cd(SeCN)_3^-$	3.810 ± 0.210 [2005OLI/NOL]	-21.748 ± 1.199 [2005OLI/NOL]	-3.350 ± 14.000 [2005OLI/NOL]	61.706 ± 47.128 [2005OLI/NOL]
$Cd(SeCN)_4^{-2}$	**440.214 ± 15.231**				4 $SeCN^-$ + Cd^{2+} ⇄ $Cd(SeCN)_4^{2-}$	4.600 ± 0.110 [2005OLI/NOL]	-26.257 ± 0.628 [2005OLI/NOL]	-40.000 ± 14.000 [2005OLI/NOL]	-46.094 ± 47.003 [2005OLI/NOL]
α-HgSe	-51.200 ± 4.000 [2005OLI/NOL]	-57.011 ± 4.100 [2005OLI/NOL]	98.500 ± 3.000 [2005OLI/NOL]	54.400 ± 0.700 [2005OLI/NOL]	SeO_3^{2-} + Hg^{2+} + 6 H^+ + 6 e^- ⇄ α-HgSe + 3 H_2O(l)	**98.987 ± 0.769**	**-565.023 ± 4.390**	**-577.576 ± 4.269**	**-42.523 ± 7.672**
$HgSe_2^{2-}$	65.334 ± 5.641 [2005OLI/NOL]				α-HgSe + HSe^- ⇄ $HgSe_2^{2-}$ + H^+	-12.800 ± 0.600 [2005OLI/NOL]	73.063 ± 3.425 [2005OLI/NOL]		
$HgSeO_3$(cr)	-290.195 ± 5.980 [2005OLI/NOL]	-373.600 ± 5.000 [2005OLI/NOL]	151.732 ± 26.108 [2005OLI/NOL]		SeO_3^{2-} + Hg^{2+} ⇄ $HgSeO_3$(cr)	16.200 ± 1.000 [2005OLI/NOL]	-92.470 ± 5.708 [2005OLI/NOL]		
$Hg(SeO_3)_2^{2-}$	-644.882 ± 6.291 [2005OLI/NOL]				SeO_3^{2-} + $HgSeO_3$(cr) ⇄ $Hg(SeO_3)_2^{2-}$	-1.350 ± 0.150 [2005OLI/NOL]	7.706 ± 0.856 [2005OLI/NOL]		
Hg_2SeO_3(cr)	-295.587 ± 5.998 [2005OLI/NOL]				SeO_3^{2-} + Hg_2^{2+} ⇄ Hg_2SeO_3(cr)	15.200 ± 1.000 [2005OLI/NOL]	-86.762 ± 5.708 [2005OLI/NOL]		
$Hg_3H_2(SeO_3)_4$(cr)		-1652.800 ± 32.500 [2005OLI/NOL]			4 SeO_3^{2-} + 3 Hg^{2+} + 2 H^+ ⇄ $Hg_3H_2(SeO_3)_4$(cr)			**-134.790 ± 32.818**	
$Hg(SeCN)_2$(aq)	**309.480 ± 9.510**				2 $SeCN^-$ + Hg^{2+} ⇄ $Hg(SeCN)_2$(aq)	22.300 ± 1.000 [2005OLI/NOL]	-127.289 ± 5.708 [2005OLI/NOL]		

Table A4 Selected thermodynamic data for selenium (Se) in JAEA-TDB-RN in 2020 (10/17)

Species / compound	$\Delta_f G^0_m$ (kJ.mol^{-1})	$\Delta_f H^0_m$ (kJ.mol^{-1})	S^0_m (J.K^{-1}.mol^{-1})	$C^0_{p,m}$ (J.K^{-1}.mol^{-1})	Reaction	$\log_{10} K°$	$\Delta_r G^0_m$ (kJ.mol^{-1})	$\Delta_r H^0_m$ (kJ.mol^{-1})	$\Delta_r S^0_m$ (J.K^{-1}.mol^{-1})
$Hg(SeCN)_3^-$	**419.844 ± 12.753**				$3\ SeCN^- + Hg^{2+} \rightleftarrows Hg(SeCN)_3^-$	26.800 ± 1.000 [2005OLI/NOL]	-152.976 ± 5.708 [2005OLI/NOL]		
$Hg(SeCN)_4^{-2}$	**541.625 ± 15.469**				$4\ SeCN^- + Hg^{2+} \rightleftarrows Hg(SeCN)_4^{2-}$	29.300 ± 0.500 [2005OLI/NOL]	-167.246 ± 2.854 [2005OLI/NOL]	-193.000 ± 3.000 [2005OLI/NOL]	-86.381 ± 13.888 [2005OLI/NOL]
α-CuSe	-36.835 ± 0.563 [2005OLI/NOL]	-39.500 ± 0.500 [2005OLI/NOL]	66.300 ± 0.800 [2005OLI/NOL]	50.300 ± 0.600 [2005OLI/NOL]	$SeO_3^{2-} + Cu^{2+} + 6\ H^+ + 6\ e^- \rightleftarrows$ α-CuSe $+ 3\ H_2O(l)$	**79.112 ± 0.329**	**-451.575 ± 1.880**	**-455.544 ± 1.502**	**-13.844 ± 7.172**
β-CuSe	-34.910 ± 0.563 [2005OLI/NOL]	-36.800 ± 0.500 [2005OLI/NOL]	68.900 ± 0.800 [2005OLI/NOL]		$SeO_3^{2-} + Cu^{2+} + 6\ H^+ + 6\ e^- \rightleftarrows$ β-CuSe $+ 3\ H_2O(l)$	**78.775 ± 0.329**	**-449.650 ± 1.880**	**-452.844 ± 1.502**	**-11.244 ± 7.172**
CuSe(g)		320.800 ± 15.000 [2005OLI/NOL]			$SeO_3^{2-} + Cu^{2+} + 6\ H^+ + 6\ e^- \rightleftarrows CuSe(g) + 3\ H_2O(l)$			**-95.244 ± 15.067**	
α-Cu_2Se		-59.300 ± 0.500 [2005OLI/NOL]			$SeO_3^{2-} + 2\ Cu^{2+} + 6\ H^+ + 8\ e^- \rightleftarrows$ α-$Cu_2Se + 3\ H_2O(l)$			**-541.033 ± 2.038**	
$CuSe_2$(cr)		-41.200 ± 5.900 [2005OLI/NOL]			$2\ SeO_3^{2-} + Cu^{2+} + 12\ H^+ + 10\ e^- \rightleftarrows CuSe_2(cr) + 6\ H_2O(l)$			**-807.599 ± 6.399**	
Cu_3Se_2(cr)		-96.800 ± 7.100 [2005OLI/NOL]			$2\ SeO_3^2 + 3\ Cu^{2+-} + 12\ H^+ + 14\ e^- \rightleftarrows Cu_3Se_2(cr) + 6\ H_2O(l)$			**-994.576 ± 7.849**	
$CuSeO_3$(cr)		-386.900 ± 1.520 [2005OLI/NOL]			$SeO_3^{2-} + Cu^{2+} \rightleftarrows CuSeO_3(cr)$			**54.571 ± 2.054**	
$CuSeO_3 \cdot 2H_2O$(cr)		-998.600 ± 1.510 [2005OLI/NOL]			$SeO_3^{2-} + Cu^{2+} + 2\ H_2O(l) \rightleftarrows CuSeO_3 \cdot 2H_2O(cr)$			**14.548 ± 2.057**	
$CuSeO_4$(cr)		-480.330 ± 2.810 [2005OLI/NOL]			$SeO_4^{2-} + Cu^{2+} \rightleftarrows CuSeO_4(cr)$			**57.481 ± 4.558**	
$CuSeO_4 \cdot 5H_2O$(cr)	**-1573.741 ± 1.910**	-1973.330 ± 2.830 [2005OLI/NOL]	312.800 ± 12.494 [2005OLI/NOL]		$SeO_4^{2-} + Cu^{2+} + 5\ H_2O(l) \rightleftarrows CuSeO_4 \cdot 5H_2O(cr)$	2.440 ± 0.200 [2005OLI/NOL]	-13.928 ± 1.142 [2005OLI/NOL]		
AgSe(g)		309.000 ± 6.000 [2005OLI/NOL]			$SeO_3^{2-} + Ag^+ + 6\ H^+ + 5\ e^- \rightleftarrows AgSe(g) + 3\ H_2O(l)$			**-147.145 ± 6.114**	
α-Ag_2Se	-46.900 ± 1.300 [2005OLI/NOL]	-40.129 ± 1.318 [2005OLI/NOL]	149.900 ± 0.500 [2005OLI/NOL]	81.150 ± 0.900 [2005OLI/NOL]	$SeO_3^{2-} + 2\ Ag^+ + 6\ H^+ + 6\ e^- \rightleftarrows$ α-$Ag_2Se + 3\ H_2O(l)$	**96.399 ± 0.390**	**-550.248 ± 2.227**	**-602.064 ± 1.771**	**-174.213 ± 7.079**

Table A4 Selected thermodynamic data for selenium (Se) in JAEA-TDB-RN in 2020 (11/17)

Species / compound	$\Delta_f G^0_m$ (kJ.mol^{-1})	$\Delta_f H^0_m$ (kJ.mol^{-1})	S^0_m (J.K^{-1}.mol^{-1})	$C^0_{p,m}$ (J.K^{-1}.mol^{-1})	Reaction	$\log_{10} K°$	$\Delta_r G^0_m$ (kJ.mol^{-1})	$\Delta_r H^0_m$ (kJ.mol^{-1})	$\Delta_r S^0_m$ (J.K^{-1}.mol^{-1})
Ag_2SeO_3(cr)	**-298.387**	-363.440	216.773		$SeO_3^{2-} + 2\ Ag^+ \rightleftarrows Ag_2SeO_3$(cr)	15.800	-90.187		
	± 2.472	± 1.020	± 8.885			± 0.300	± 1.712		
		[2005OLI/NOL]	[2005OLI/NOL]			[2005OLI/NOL]	[2005OLI/NOL]		
Ag_2SeO_4(cr)	**-330.158**	-422.510	227.717		$SeO_4^{2-} + 2\ Ag^+ \rightleftarrows Ag_2SeO_4$(cr)	7.860	-44.865		
	± 3.208	± 2.120	± 12.885			± 0.500	± 2.854		
		[2005OLI/NOL]	[2005OLI/NOL]			[2005OLI/NOL]	[2005OLI/NOL]		
AgSeCN(cr)	**133.246**				$SeCN^- + Ag^+ \rightleftarrows AgSeCN$(cr)	13.998	-79.901	-108.100	-94.583
	± 4.783					± 0.508	± 2.900	± 1.700	± 11.275
						[2005OLI/NOL]	[2005OLI/NOL]	[2005OLI/NOL]	[2005OLI/NOL]
$Ag(SeCN)_3^{2-}$	406.193				$3\ SeCN^- + Ag^+ \rightleftarrows Ag(SeCN)_3^{2-}$	13.850	-79.056		
	± 11.529					± 0.300	± 1.712		
	[2005OLI/NOL]					[2005OLI/NOL]	[2005OLI/NOL]		
$Ni_{0.88}Se$(cr)	-69.628	-69.800	67.800	48.260	$SeO_3^{2-} + 0.88\ Ni^{2+} + 6\ H^+ + 5.76\ e^- \rightleftarrows Ni_{0.88}Se$(cr) + 3 H_2O(l)	**66.311**	**-378.504**	**-371.744**	**22.253**
	± 1.621	± 1.600	± 0.800	± 0.500		**± 0.438**	**± 2.502**	**± 2.129**	**± 7.168**
	[2005OLI/NOL]	[2005OLI/NOL]	[2005OLI/NOL]	[2005OLI/NOL]					
$NiSe_2$(cr)	-112.355	-115.500	103.500	74.500	$2\ SeO_3^{2-} + Ni^{2+} + 12\ H^+ + 10\ e^- \rightleftarrows NiSe_2$(cr) + 6 H_2O(l)	**134.003**	**-764.894**	**-761.198**	**11.554**
	± 7.017	± 7.000	± 1.500	± 1.000		**± 1.385**	**± 7.908**	**± 7.435**	**± 14.181**
	[2005OLI/NOL]	[2005OLI/NOL]	[2005OLI/NOL]	[2005OLI/NOL]					
Ni_3Se_2(cr)		-179.500			$2\ SeO_3^{2-} + 3\ Ni^{2+} + 12\ H^+ + 14\ e^- \rightleftarrows Ni_3Se_2$(cr) + 6 H_2O(l)			**-715.174**	
		± 6.000						**± 6.960**	
		[2005OLI/NOL]							
$NiSeO_3 \cdot 2H_2O$(cr)	**-915.637**	-1109.330	196.268		$SeO_3^{2-} + Ni^{2+} + 2\ H_2O$(l) $\rightleftarrows NiSeO_3 \cdot 2H_2O$(cr)	5.800	-33.107		
	± 6.025	± 2.830	± 22.320			± 1.000	± 5.708		
		[2005OLI/NOL]	[2005OLI/NOL]			[2005OLI/NOL]	[2005OLI/NOL]		
$NiSeO_4$(aq)	**-500.498**				$SeO_4^{2-} + Ni^{2+} \rightleftarrows NiSeO_4$(aq)	2.670	-15.240		
	± 1.650					± 0.050	± 0.285		
						[2005OLI/NOL]	[2005OLI/NOL]		
$NiSeO_4 \cdot 6H_2O$(cr)	**-1916.236**				$SeO_4^{2-} + Ni^{2+} + 6\ H_2O$(l) $\rightleftarrows NiSeO_4 \cdot 6H_2O$(cr)	1.381	-7.883		
	± 1.752					± 0.045	± 0.257		
						[2005OLI/NOL]	[2005OLI/NOL]		
$NiSeCN^+$	80.175				$SeCN^- + Ni^{2+} \rightleftarrows NiSeCN^+$	1.770	-10.103	-12.800	-9.045
	± 3.893					± 0.060	± 0.342	± 4.000	± 1.766
	[2005OLI/NOL]					[2005OLI/NOL]	[2005OLI/NOL]	[2005OLI/NOL]	[2005OLI/NOL]
$Ni(SeCN)_2$(aq)	**213.543**				$2\ SeCN^- + Ni^{2+} \rightleftarrows Ni(SeCN)_2$(aq)	2.240	-12.786	-25.000	-40.966
	± 7.681					± 0.140	± 0.799	± 4.000	± 13.681
						[2005OLI/NOL]	[2005OLI/NOL]	[2005OLI/NOL]	[2005OLI/NOL]
$Co_{0.84}Se$(cr)	-56.300	-55.400			$SeO_3^{2-} + 0.84\ Co^{2+} + 6\ H^+ + 5.68\ e^- \rightleftarrows Co_{0.84}Se$(cr) + 3 H_2O(l)	**63.027**	**-359.762**		
	± 6.500	± 6.000				**± 1.190**	**± 6.792**		
	[2005OLI/NOL]	[2005OLI/NOL]							
$CoSe_2$(cr)		-105.500	97.200	75.600					
		± 15.000	± 2.000	± 1.000					
		[2005OLI/NOL]	[2005OLI/NOL]	[2005OLI/NOL]					

Table A4 Selected thermodynamic data for selenium (Se) in JAEA-TDB-RN in 2020 (12/17)

Species / compound	$\Delta_f G^0_m$ (kJ.mol^{-1})	$\Delta_f H^0_m$ (kJ.mol^{-1})	S^0_m (J.K^{-1}.mol^{-1})	$C^0_{p,m}$ (J.K^{-1}.mol^{-1})	Reaction	$\log_{10} K°$	$\Delta_r G^0_m$ (kJ.mol^{-1})	$\Delta_r H^0_m$ (kJ.mol^{-1})	$\Delta_r S^0_m$ (J.K^{-1}.mol^{-1})
Co_9Se_8(cr)		-617.600 ± 40.000 [2005OLI/NOL]							
$CoSeO_3 \cdot 2H_2O$(cr)	**-936.248 ± 3.055**				$SeO_3^{2-} + Co^{2+} + 2\ H_2O(l) \rightleftarrows CoSeO_3 \cdot 2H_2O$(cr)	7.900 ± 0.400 [2005OLI/NOL]	-45.094 ± 2.283 [2005OLI/NOL]		
$CoSeO_4$(aq)	**-509.294 ± 1.768**				$SeO_4^{2-} + Co^{2+} \rightleftarrows CoSeO_4$(aq)	2.700 ± 0.050 [2005OLI/NOL]	-15.412 ± 0.285 [2005OLI/NOL]		
$CoSeO_4 \cdot 6H_2O$(cr)	**-503.923 ± 1.762**				$SeO_4^{2-} + Co^{2+} + 6\ H_2O(l) \rightleftarrows CoSeO_4 \cdot 6H_2O$(cr)	1.759 ± 0.043 [2005OLI/NOL]	-10.040 ± 0.245 [2005OLI/NOL]		
$CoSeCN^+$	**73.091 ± 4.286**				$SeCN^- + Co^{2+} \rightleftarrows CoSeCN^+$	1.500 ± 0.300 [2005OLI/NOL]	-8.562 ± 1.712 [2005OLI/NOL]	-6.000 ± 4.000 [2005OLI/NOL]	8.593 ± 14.594 [2005OLI/NOL]
$FeSe_{1.95}$ $Fe_{1.042}Se$(cr) Fe_7Se_8(cr,α) Fe_3Se_4(cr,γ) $FeSe_2$(cr) $FeSeO_3^+$ $Fe_2(SeO_3)_3 \cdot 3H_2O$(cr)	See Table A1								
Pd_4Se(cr)			200.100 ± 3.000 [2005OLI/NOL]	137.000 ± 2.000 [2005OLI/NOL]					
$RuSe_2$(cr)			80.800 ± 0.800 [2005OLI/NOL]	69.870 ± 1.000 [2005OLI/NOL]					
α-MnSe			90.800 ± 3.000 [2005OLI/NOL]	51.040 ± 0.300 [2005OLI/NOL]					
$MnSeO_3 \cdot 2H_2O$(cr)	**-1110.677 ± 6.655**				$SeO_3^{2-} + Mn^{2+} + 2\ H_2O(l) \rightleftarrows MnSeO_3 \cdot 2H_2O$(cr)	7.600 ± 1.000 [2005OLI/NOL]	-43.381 ± 5.708 [2005OLI/NOL]		
$MnSeO_4$(aq)	**-683.894 ± 3.272**				$SeO_4^{2-} + Mn^{2+} \rightleftarrows MnSeO_4$(aq)	2.430 ± 0.050 [2005OLI/NOL]	-13.871 ± 0.285 [2005OLI/NOL]		
α-Cr_2Se_3			187.700 ± 1.500 [2005OLI/NOL]	120.800 ± 0.900 [2005OLI/NOL]					

Table A4 Selected thermodynamic data for selenium (Se) in JAEA-TDB-RN in 2020 (13/17)

Species / compound	$\Delta_f G^0_m$ (kJ.mol^{-1})	$\Delta_f H^0_m$ (kJ.mol^{-1})	S^0_m (J.K^{-1}.mol^{-1})	$C^0_{p,m}$ (J.K^{-1}.mol^{-1})	Reaction	$\log_{10} K°$	$\Delta_r G^0_m$ (kJ.mol^{-1})	$\Delta_r H^0_m$ (kJ.mol^{-1})	$\Delta_r S^0_m$ (J.K^{-1}.mol^{-1})
γ-Cr_2Se_3			178.000 ± 6.000 [2005OLI/NOL]	122.900 ± 0.900 [2005OLI/NOL]					
$MoSe_2$(cr)			89.100 ± 0.500 [2005OLI/NOL]	70.584 ± 0.500 [2005OLI/NOL]					
WSe_2(cr)				72.600 ± 1.000 [2005OLI/NOL]					
$NbSe_2$(cr)			103.500 ± 0.600 [2005OLI/NOL]	73.520 ± 0.300 [2005OLI/NOL]					
EuSe(cr)				51.000 ± 3.000 [2005OLI/NOL]					
Sm_2Se_3(cr)			221.200 ± 3.000 [2005OLI/NOL]	128.200 ± 1.500 [2005OLI/NOL]					
Nd_2Se_3(cr)			224.100 ± 2.500 [2005OLI/NOL]	130.200 ± 2.000 [2005OLI/NOL]					
Nd_3Se_4(cr)			359.600 ± 5.800 [2005OLI/NOL]	187.060 ± 1.470 [2005OLI/NOL]					
Pr_3Se_4(cr)			371.000 ± 6.000 [2005OLI/NOL]	183.760 ± 1.450 [2005OLI/NOL]					
LaSe(cr)				49.200 ± 1.000 [2005OLI/NOL]					
La_2Se_3(cr)			202.200 ± 1.800 [2005OLI/NOL]	125.600 ± 1.000 [2005OLI/NOL]					
PuSe(cr)			92.100 ± 1.800 [2005OLI/NOL]	59.700 ± 1.200 [2005OLI/NOL]					
USe(cr)	-273.255 ± 18.006 [2005OLI/NOL]	-272.000 ± 18.000 [2005OLI/NOL]	96.500 ± 1.500 [2005OLI/NOL]	54.800 ± 0.300 [2005OLI/NOL]	$SeO_3^{2-} + U^{4+} + 6\ H^+ + 8\ e^- \rightleftarrows USe(cr) + 3\ H_2O(l)$	**16.214 ± 3.185**	**-92.551 ± 18.180**	**-31.155 ± 18.338**	**205.504 ± 14.459**
β-USe_2			133.800 ± 1.500 [2005OLI/NOL]	79.160 ± 0.300 [2005OLI/NOL]					

Table A4 Selected thermodynamic data for selenium (Se) in JAEA-TDB-RN in 2020 (14/17)

Species / compound	$\Delta_f G^0_m$ (kJ.mol^{-1})	$\Delta_f H^0_m$ (kJ.mol^{-1})	S^0_m (J.K^{-1}.mol^{-1})	$C^0_{p,m}$ (J.K^{-1}.mol^{-1})	Reaction	$\log_{10} K°$	$\Delta_r G^0_m$ (kJ.mol^{-1})	$\Delta_r H^0_m$ (kJ.mol^{-1})	$\Delta_r S^0_m$ (J.K^{-1}.mol^{-1})
U_3Se_4(cr)		-1023.000 ± 92.000 [2005OLI/NOL]			4 SeO_3^{2-} + 3 U^{4+} + 24 H^+ + 28 e^- ⇄ U_3Se_4(cr) + 12 H_2O(l)			**-650.820** **± 92.650**	
UO_2SeO_3(cr)		-1522.200 ± 1.100 [2005OLI/NOL]			SeO_3^{2-} + UO_2^{2+} ⇄ UO_2SeO_3(cr)			**3.960** **± 2.176**	
UO_2SeO_4(cr)		-1539.300 ± 3.300 [2005OLI/NOL]			SeO_4^{2-} + UO_2^{2+} ⇄ UO_2SeO_4(cr)			**83.200** **± 5.039**	
UO_2SeO_4(aq)	-1407.676 ± 2.672 [2005OLI/NOL]				SeO_4^{2-} + UO_2^{2+} ⇄ UO_2SeO_4(aq)	2.740 ± 0.250 [2005OLI/NOL]	-15.640 ± 1.427 [2005OLI/NOL]		
$MgSeO_3$(cr)		-900.300 ± 2.500 [2005OLI/NOL]			SeO_3^{2-} + Mg^{2+} ⇄ $MgSeO_3$(cr)			**72.820** **± 2.951**	
$MgSeO_3·6H_2O$(cr)	**-2272.693** **± 2.582**	-2707.210 ± 1.300 [2005OLI/NOL]	328.460 ± 9.756 [2005OLI/NOL]		SeO_3^{2-} + Mg^{2+} + 6 H_2O(l) ⇄ $MgSeO_3·6H_2O$(cr)	5.820 ± 0.250 [2005OLI/NOL]	-33.221 ± 1.427 [2005OLI/NOL]		
$MgSeO_4$(aq)	**-906.028** **± 2.129**				SeO_4^{2-} + Mg^{2+} ⇄ $MgSeO_4$(aq)	2.200 ± 0.200 [2005OLI/NOL]	-12.558 ± 1.142 [2005OLI/NOL]		
$MgSeO_4$(cr)		-971.320 ± 2.620 [2005OLI/NOL]			SeO_4^{2-} + Mg^{2+} ⇄ $MgSeO_4$(cr)			**98.140** **± 4.505**	
$MgSeO_4·H_2O$(cr)		-1298.240 ± 2.580 [2005OLI/NOL]			SeO_4^{2-} + Mg^{2+}+ H_2O(l) ⇄ $MgSeO_4·H_2O$(cr)			**57.058** **± 4.483**	
$MgSeO_4·4H_2O$(cr)		-2192.670 ± 2.650 [2005OLI/NOL]			SeO_4^{2-} + Mg^{2+}+ 4 H_2O(l) ⇄ $MgSeO_4·4H_2O$(cr)			**20.143** **± 4.542**	
$MgSeO_4·6H_2O$(cr)	**-2323.033** **± 1.912**	-2781.400 ± 2.400 [2005OLI/NOL]	351.144 ± 10.484 [2005OLI/NOL]		SeO_4^{2-} + Mg^{2+}+ 6 H_2O(l) ⇄ $MgSeO_4·6H_2O$(cr)	1.133 ± 0.044 [2005OLI/NOL]	-6.467 ± 0.251 [2005OLI/NOL]		
CaSe(cr)		-414.400 ± 35.000 [2005OLI/NOL]			SeO_3^{2-} + Ca^{2+} + 6 H^+ + 6 e^- ⇄ CaSe(cr) + 3 H_2O(l)			**-221.672** **± 35.029**	
$CaSeO_3·H_2O$(cr)	**-1188.896** **± 2.400**				SeO_3^{2-} + Ca^{2+} + H_2O(l) ⇄ $CaSeO_3·H_2O$(cr)	6.400 ± 0.250 [2005OLI/NOL]	-36.531 ± 1.427 [2005OLI/NOL]		
$CaSeO_4$(cr)		-1112.140 ± 2.580 [2005OLI/NOL]			SeO_4^{2-} + Ca^{2+} ⇄ $CaSeO_4$(cr)			**34.443** **± 4.420**	

Table A4 Selected thermodynamic data for selenium (Se) in JAEA-TDB-RN in 2020 (15/17)

Species / compound	$\Delta_f G^0_m$ (kJ.mol^{-1})	$\Delta_f H^0_m$ (kJ.mol^{-1})	S^0_m (J.K^{-1}.mol^{-1})	$C^0_{p,m}$ (J.K^{-1}.mol^{-1})	Reaction	$\log_{10} K°$	$\Delta_r G^0_m$ (kJ.mol^{-1})	$\Delta_r H^0_m$ (kJ.mol^{-1})	$\Delta_r S^0_m$ (J.K^{-1}.mol^{-1})
$CaSeO_4$(aq)	**-1003.691**				$SeO_4^{2-} + Ca^{2+} \rightleftarrows CaSeO_4$(aq)	2.000	-11.416		
	± 1.734					± 0.100 [2005OLI/NOL]	± 0.571 [2005OLI/NOL]		
$CaSeO_4 \cdot 2H_2O$(cr)	**-1481.938**	-1709.000	198.799		$SeO_4^{2-} + Ca^{2+} + 2\ H_2O$(l) $\rightleftarrows CaSeO_4 \cdot 2H_2O$(cr)	2.680	-15.298		
	± 2.181	± 2.600 [2005OLI/NOL]	± 11.654 [2005OLI/NOL]			± 0.250 [2005OLI/NOL]	± 1.427 [2005OLI/NOL]		
SrSe(cr)		-406.000			$SeO_3^{2-} + Sr^{2+} + 6\ H^+ + 6\ e^- \rightleftarrows$ SrSe(cr) + 3 H_2O(l)			**-205.448**	
		± 35.000 [2005OLI/NOL]						**± 35.023**	
$SrSeO_3$(cr)	**-962.189**	-1051.900	104.663		$SeO_3^{2-} + Sr^{2+} \rightleftarrows SrSeO_3$(cr)	6.300	-35.961		
	± 3.444	± 2.700 [2005OLI/NOL]	± 14.567 [2005OLI/NOL]			± 0.500 [2005OLI/NOL]	± 2.854 [2005OLI/NOL]		
$BaSeO_3$(cr)	**-957.096**	-1036.700	145.594		$SeO_3^{2-} + Ba^{2+} \rightleftarrows BaSeO_3$(cr)	6.500	-37.102		
	± 2.814	± 2.900 [2005OLI/NOL]	± 15.016 [2005OLI/NOL]			± 0.250 [2005OLI/NOL]	± 1.427 [2005OLI/NOL]		
$BaSeO_4$(cr)	**-1040.239**	-1144.000	166.983		$SeO_4^{2-} + Ba^{2+} \rightleftarrows BaSeO_4$(cr)	7.560	-43.153		
	± 2.275	± 5.000 [2005OLI/NOL]	± 19.590 [2005OLI/NOL]			± 0.100 [2005OLI/NOL]	± 0.571 [2005OLI/NOL]		
NH_4HSe(cr)	**-24.170**	-132.040	102.770		$H_2Se(g) + NH_3(g) \rightleftarrows NH_4HSe$(cr)	4.024	-22.969	-115.100	-309.000
	± 5.344	± 4.046 [2005OLI/NOL]	± 11.702 [2005OLI/NOL]			± 0.866 [2005OLI/NOL]	± 4.943 [2005OLI/NOL]	± 3.500 [2005OLI/NOL]	± 11.700 [2005OLI/NOL]
$(NH_4)_2SeO_4$(cr)	**-593.193**	-878.450	209.654		$SeO_4^{2-} + 2\ NH_4^+ \rightleftarrows (NH_4)_2SeO_4$(cr)	-0.911	5.200		
	± 1.623	± 3.500 [2005OLI/NOL]	± 12.912 [2005OLI/NOL]			± 0.065 [2005OLI/NOL]	± 0.371 [2005OLI/NOL]		
Li_2Se(cr)		-434.100			$SeO_3^{2-} + 2\ Li^+ + 6\ H^+ + 6\ e^- \rightleftarrows Li_2Se$(cr) + 3 H_2O(l)			**-227.548**	
		± 15.000 [2005OLI/NOL]						**± 15.047**	
$Li_2Se_2O_5$(cr)		-1310.870			$2\ SeO_3^{2-} + 2\ Li^+ + 2\ H^+ \rightleftarrows Li_2Se_2O_5$(cr) + H_2O(l)			**-25.481**	
		± 4.700 [2005OLI/NOL]						**± 5.219**	
Li_2SeO_3(cr)		-1031.810			$SeO_3^{2-} + 2\ Li^+ \rightleftarrows Li_2SeO_3$(cr)			**32.257**	
		± 2.460 [2005OLI/NOL]						**± 2.712**	
$Li_2SeO_3 \cdot H_2O$(cr)		-1328.600			$SeO_3^{2-} + 2\ Li^+ + H_2O$(l) $\rightleftarrows Li_2SeO_3 \cdot H_2O$(cr)			**21.305**	
		± 2.430 [2005OLI/NOL]						**± 2.687**	
Li_2SeO_4(cr)		-1127.690			$SeO_4^{2-} + 2\ Li^+ \rightleftarrows Li_2SeO_4$(cr)			**32.717**	
		± 5.600 [2005OLI/NOL]						**± 6.606**	
$Li_2SeO_4 \cdot H_2O$(cr)	**-1251.826**	-1420.000	181.757		$SeO_4^{2-} + 2\ Li^+ + H_2O$(l) $\rightleftarrows Li_2SeO_4 \cdot H_2O$(cr)	-1.762	10.058		
	± 1.491	± 5.600 [2005OLI/NOL]	± 19.452 [2005OLI/NOL]			± 0.065 [2005OLI/NOL]	± 0.371 [2005OLI/NOL]		

Table A4 Selected thermodynamic data for selenium (Se) in JAEA-TDB-RN in 2020 (16/17)

Species / compound	$\Delta_f G^0_m$ (kJ.mol^{-1})	$\Delta_f H^0_m$ (kJ.mol^{-1})	S^0_m (J.K^{-1}.mol^{-1})	$C^0_{p,m}$ (J.K^{-1}.mol^{-1})	Reaction	$\log_{10} K°$	$\Delta_r G^0_m$ (kJ.mol^{-1})	$\Delta_r H^0_m$ (kJ.mol^{-1})	$\Delta_r S^0_m$ (J.K^{-1}.mol^{-1})
$LiHSeO_3$(cr)		-817.850 ± 1.840 [2005OLI/NOL]			$SeO_3^{2-} + Li^+ + H^+ \rightleftarrows LiHSeO_3$(cr)			**-32.236** **± 2.161**	
$LiH_3(SeO_3)_2$(cr)		-1371.700 ± 3.700 [2005OLI/NOL]			$2\ SeO_3^{2-} + Li^+ + 3\ H^+ \rightleftarrows LiH_3(SeO_3)_2$(cr)			**-78.926** **± 4.336**	
Na_2Se(cr)		-337.700 ± 10.000 [2005OLI/NOL]			$SeO_3^{2-} + 2\ Na^+ + 6\ H^+ + 6\ e^- \rightleftarrows Na_2Se$(cr) + 3 H_2O(l)			**-207.464** **± 10.070**	
Na_2SeO_3(cr)	-868.679 ± 0.967 [2005OLI/NOL]	-959.620 ± 0.950 [2005OLI/NOL]	147.400 ± 0.300 [2005OLI/NOL]	126.100 ± 0.300 [2005OLI/NOL]	$SeO_3^{2-} + 2\ Na^+ \rightleftarrows Na_2SeO_3$(cr)	**-3.061** **± 0.354**	**17.474** **± 2.020**	**28.131** **± 1.486**	**35.638** **± 7.030**
$Na_2SeO_3 \cdot 5H_2O$(cr)		-2404.670 ± 1.000 [2005OLI/NOL]			$SeO_3^{2-} + 2\ Na^+ + 5\ H_2O$(l) $\rightleftarrows Na_2SeO_3 \cdot 5H_2O$(cr)			**12.273** **± 1.606**	
Na_2SeO_4(cr)		-1076.500 ± 3.500 [2005OLI/NOL]			$SeO_4^{2-} + 2\ Na^+ \rightleftarrows Na_2SeO_4$(cr)			**7.591** **± 4.953**	
$Na_2SeO_4 \cdot 10H_2O$(cr)	**-3338.960** **± 1.835**	-4013.600 ± 3.600 [2005OLI/NOL]	623.928 ± 13.224 [2005OLI/NOL]		$SeO_4^{2-} + 2\ Na^+ + 10\ H_2O$(l) $\rightleftarrows Na_2SeO_4 \cdot 10H_2O$(cr)	0.681 ± 0.087 [2005OLI/NOL]	-3.887 ± 0.497 [2005OLI/NOL]		
$Na_2Se_2O_5$(cr)		-1219.640 ± 4.710 [2005OLI/NOL]			$2\ SeO_3^{2-} + 2\ Na^+ + 2\ H^+ \rightleftarrows Na_2Se_2O_5$(cr) + H_2O(l)			**-10.567** **± 5.228**	
$Na_2Se_2O_7$(cr)		-1322.000 ± 5.000 [2005OLI/NOL]			$2\ SeO_4^{2-} + 2\ Na^+ + 2\ H^+ \rightleftarrows Na_2Se_2O_7$(cr) + H_2O(l)			**79.753** **± 8.605**	
$NaHSeO_3$(cr)		-760.100 ± 2.500 [2005OLI/NOL]			$SeO_3^{2-} + Na^+ + H^+ \rightleftarrows NaHSeO_3$(cr)			**-12.645** **± 2.745**	
$NaHSeO_3 \cdot 3H_2O$(cr)		-1642.550 ± 2.500 [2005OLI/NOL]			$SeO_3^{2-} + Na^+ + H^+ + 3\ H_2O$(l) $\rightleftarrows NaHSeO_3 \cdot 3H_2O$(cr)			**-37.580** **± 2.763**	
$NaHSeO_4$(cr)		-822.230 ± 5.590 [2005OLI/NOL]			$SeO_4^{2-} + Na^+ + H^+ \rightleftarrows NaHSeO_4$(cr)			**261.861** **± 6.597**	
$NaH_3(SeO_3)_2$(cr)		-1316.640 ± 4.710 [2005OLI/NOL]			$2\ SeO_3^{2-} + Na^+ + 3\ H^+ \rightleftarrows NaH_3(SeO_3)_2$(cr)			**-62.025** **± 5.225**	
K_2Se(cr)		-398.700 ± 10.000 [2005OLI/NOL]			$SeO_3^{2-} + 2\ K^+ + 6\ H^+ + 6\ e^- \rightleftarrows K_2Se$(cr) + 3 H_2O(l)			**105.639** **± 10.001**	

Table A4 Selected thermodynamic data for selenium (Se) in JAEA-TDB-RN in 2020 (17/17)

Species / compound	$\Delta_f G^0_m$ (kJ.mol^{-1})	$\Delta_f H^0_m$ (kJ.mol^{-1})	S^0_m (J.K^{-1}.mol^{-1})	$C^0_{p,m}$ (J.K^{-1}.mol^{-1})	Reaction	$\log_{10} K°$	$\Delta_r G^0_m$ (kJ.mol^{-1})	$\Delta_r H^0_m$ (kJ.mol^{-1})	$\Delta_r S^0_m$ (J.K^{-1}.mol^{-1})
K_2SeO_3(cr)		-981.090 ± 2.360 [2005OLI/NOL]			$SeO_3^{2-} + 2\ K^+ \rightleftarrows K_2SeO_3$(cr)			**30.409 ± 2.622**	
K_2SeO_4(cr)	**-999.249 ± 1.499**	-1112.497 ± 1.537 [2005OLI/NOL]	202.900 ± 1.000 [2005OLI/NOL]	142.640 ± 1.000 [2005OLI/NOL]	$SeO_4^{2-} + 2\ K^+ \rightleftarrows K_2SeO_4$(cr)	-0.904 ± 0.065 [2005OLI/NOL]	5.160 ± 0.371 [2005OLI/NOL]		
$K_2Se_2O_5$(cr)		-1250.050 ± 4.720 [2005OLI/NOL]			$2\ SeO_3^{2-} + 2\ K^+ + 2\ H^+ \rightleftarrows K_2Se_2O_5$(cr) + H_2O(l)			**-17.229 ± 5.237**	
$KHSeO_3$(cr)		-773.490 ± 1.840 [2005OLI/NOL]			$SeO_3^{2-} + K^+ + H^+ \rightleftarrows KHSeO_3$(cr)			**-14.160 ± 2.161**	
$KH_3(SeO_3)_2$(cr)		-1329.800 ± 4.710 [2005OLI/NOL]			$2\ SeO_3^{2-} + K^+ + 3\ H^+ \rightleftarrows KH_3(SeO_3)_2$(cr)			**-63.310 ± 5.225**	
Rb_2Se(cr)				74.700 ± 2.000 [2005OLI/NOL]					
Rb_2SeO_3(cr)		-973.170 ± 2.400 [2005OLI/NOL]			$SeO_3^{2-} + 2\ Rb^+ \rightleftarrows Rb_2SeO_3$(cr)			**36.237 ± 2.665**	
Rb_2SeO_4(cr)	-1005.100 ± 1.500 [2005OLI/NOL]	-1116.500 ± 2.200 [2005OLI/NOL]	232.317 ± 8.957 [2005OLI/NOL]		$SeO_4^{2-} + 2\ Rb^+ \rightleftarrows Rb_2SeO_4$(cr)	**-0.304 ± 0.371**	**1.735 ± 2.115**	**-10.753 ± 4.142**	**-41.646 ± 15.536**
Cs_2Se(cr)				76.000 ± 2.000 [2005OLI/NOL]					
$Cs_2SeO_3 \cdot H_2O$(cr)		-1311.830 ± 2.550 [2005OLI/NOL]			$SeO_3^{2-} + 2\ Cs^+ + H_2O$(l) $\rightleftarrows Cs_2SeO_3 \cdot H_2O$(cr)			**-2.777 ± 2.802**	
Cs_2SeO_4(cr)	**-1019.188 ± 1.536**	-1138.700 ± 3.500 [2005OLI/NOL]	220.707 ± 13.229 [2005OLI/NOL]		$SeO_4^{2-} + 2\ Cs^+ \rightleftarrows Cs_2SeO_4$(cr)	-0.636 ± 0.065 [2005OLI/NOL]	3.630 ± 0.371 [2005OLI/NOL]		

[2005OLI/NOL] Olin et al. [A7)]
[2010IID/YAM] Iida et al. [A8)]

Table A5 Selected thermodynamic data for zirconium (Zr) in JAEA-TDB-RN in 2020 (1/7)

Values indicated by **boldface** are calculated and selected in the present report.

Species / compound	$\Delta_f G^0_m$ (kJ.mol^{-1})	$\Delta_f H^0_m$ (kJ.mol^{-1})	S^0_m (J.K^{-1}.mol^{-1})	$C^0_{p,m}$ (J.K^{-1}.mol^{-1})	Reaction	$\log_{10} K°$	$\Delta_r G^0_m$ (kJ.mol^{-1})	$\Delta_r H^0_m$ (kJ.mol^{-1})	$\Delta_r S^0_m$ (J.K^{-1}.mol^{-1})
Zr(cr)	0.000	0.000	39.080 ± 0.100 [2005BRO/CUR]	26.080 ± 0.050 [2005BRO/CUR]	Zr(cr) ⇄ Zr^{4+} + 4 e^-	**92.590 ± 1.616**	**-528.509 ± 9.227**	**-608.500 ± 5.000**	**-268.291 ± 35.200**
Zr(omega)				29.000 ± 0.050 [2005BRO/CUR]					
Zr(g)	566.882 ± 1.400 [2005BRO/CUR]	609.800 ± 1.400 [2005BRO/CUR]	183.027 ± 0.010 [2005BRO/CUR]	24.775 ± 0.010 [2005BRO/CUR]	Zr(g) ⇄ Zr^{4+} + 4 e^-	**191.903 ± 1.635**	**-1095.391 ± 9.333**	**-1218.300 ± 5.192**	**-412.238 ± 35.200**
Zr^{4+}	**-528.425 ± 9.229**	-608.500 ± 5.000 [2005BRO/CUR]	-490.569 ± 35.200 [2005BRO/CUR]		ZrO_2(mono) + 4 H^+ ⇄ Zr^{4+} + 2 H_2O(l)	-7.000 ± 1.600 [2005BRO/CUR]	39.956 ± 9.133 [2005BRO/CUR]		
ZrO(g)	30.576 ± 27.124 [2005BRO/CUR]	56.200 ± 27.008 [2005BRO/CUR]	227.600 ± 8.400 [2005BRO/CUR]	30.800 ± 1.000 [2005BRO/CUR]	ZrO(g) + 2 H^+ ⇄ Zr^{4+} + H_2O(l) + 2 e^-	**139.499 ± 5.019**	**-796.268 ± 28.651**	**-950.538 ± 27.467**	**-517.567 ± 36.189**
ZrO_2(mono)	-1042.746 ± 1.313 [2005BRO/CUR]	-1100.600 ± 1.300 [2005BRO/CUR]	50.190 ± 0.620 [2005BRO/CUR]	55.960 ± 0.790 [2005BRO/CUR]					
ZrO_2(g)	-298.386 ± 47.042 [2005BRO/CUR]	-289.600 ± 47.018 [2005BRO/CUR]	273.700 ± 5.000 [2005BRO/CUR]	46.100 ± 1.000 [2005BRO/CUR]	ZrO_2(g) + 4 H^+ ⇄ Zr^{4+} + 2 H_2O(l)	**123.420 ± 8.398**	**-704.488 ± 47.939**	**-890.577 ± 47.284**	**-624.423 ± 35.554**
ZrH(cr)	-64.686 ± 0.801 [2005BRO/CUR]	-84.400 ± 0.800 [2005BRO/CUR]	38.300 ± 0.100 [2005BRO/CUR]	30.200 ± 0.100 [2005BRO/CUR]	ZrH(cr) ⇄ Zr^{4+} + H^+ + 5 e^-	**81.258 ± 1.623**	**-463.823 ± 9.262**	**-524.100 ± 5.064**	**-202.172 ± 35.200**
ε-ZrH_2	-124.281 ± 1.700 [2005BRO/CUR]	-164.400 ± 1.700 [2005BRO/CUR]	35.200 ± 0.080 [2005BRO/CUR]	30.930 ± 0.060 [2005BRO/CUR]	ε-ZrH_2 ⇄ Zr^{4+} + 2 H^+ + 6 e^-	**70.817 ± 1.644**	**-404.228 ± 9.382**	**-444.100 ± 5.281**	**-133.732 ± 35.200**
$ZrOH^{3+}$	**-767.518 ± 9.313**				Zr^{4+} + H_2O(l) ⇄ $ZrOH^{3+}$ + H^+	0.320 ± 0.220 [2005BRO/CUR]	-1.827 ± 1.256 [2005BRO/CUR]		
$Zr(OH)_2^{2+}$	**≥ -989.734**				Zr^{4+} + 2 H_2O(l) ⇄ $ZrOH)_2^{2+}$ + 2 H^+	≤ -2.302 [2018RAI/KIT]	**≥ 13.140**		
$Zr(OH)_4$(am)	**-1478.301 ± 9.244**				Zr^{4+} + 4 H_2O(l) ⇄ $Zr(OH)_4$(am) + 4 H^+	0.186 ± 0.067 [2018RAI/KIT]	**-1.062 ± 0.382**		
$Zr(OH)_4$(aq)	**> -1420.593**				Zr^{4+} + 4 H_2O(l) ⇄ $Zr(OH)_4$(aq) + 4 H^+	< -9.924 [2018RAI/KIT]	**> 56.647**		

Table A5 Selected thermodynamic data for zirconium (Zr) in JAEA-TDB-RN in 2020 (2/7)

Species / compound	$\Delta_f G^0_m$ (kJ.mol^{-1})	$\Delta_f H^0_m$ (kJ.mol^{-1})	S^0_m (J.K^{-1}.mol^{-1})	$C^0_{p,m}$ (J.K^{-1}.mol^{-1})	Reaction	$\log_{10} K°$	$\Delta_r G^0_m$ (kJ.mol^{-1})	$\Delta_r H^0_m$ (kJ.mol^{-1})	$\Delta_r S^0_m$ (J.K^{-1}.mol^{-1})
$Zr(OH)_5^-$	**-1602.230**				$Zr^{4+} + 5\ H_2O(l) \rightleftarrows Zr(OH)_5^- + 5\ H^+$	-19.655	**112.192**		
	± 9.343					± 0.242	**± 1.381**		
						[2018RAI/KIT]			
$Zr(OH)_6^{2-}$	**-1761.607**				$Zr^{4+} + 6\ H_2O(l) \rightleftarrows Zr(OH)_6^{2-} + 6\ H^+$	-33.286	**189.998**		
	± 9.361					± 0.256	**± 1.461**		
						[2018RAI/KIT]			
ZrF(g)	41.353	72.100	243.600	32.800	$ZrF(g) \rightleftarrows Zr^{4+} + F^- + 3\ e^-$	**149.195**	**-851.613**	**-1015.948**	**-551.330**
	± 1.165	± 1.000	± 2.000	± 1.000		**± 1.634**	**± 9.324**	**± 5.143**	**± 35.261**
	[2005BRO/CUR]	[2005BRO/CUR]	[2005BRO/CUR]	[2005BRO/CUR]					
ZrF^{3+}	**-868.025**	**-961.348**	**-368.698**		$Zr^{4+} + F^- \rightleftarrows ZrF^{3+}$	10.120	-57.765	-17.500	135.051
	± 9.260	**± 5.093**	**± 35.308**			± 0.070	± 0.400	± 0.700	± 2.703
						[2005BRO/CUR]	[2005BRO/CUR]	[2005BRO/CUR]	[2005BRO/CUR]
$ZrF_2(g)$	-492.769	-478.300	290.400	49.400	$ZrF_2(g) \rightleftarrows Zr^{4+} + 2\ F^- + 2\ e^-$	**104.982**	**-599.241**	**-800.895**	**-676.649**
	± 1.436	± 0.800	± 0.400	± 2.000		**± 1.653**	**± 9.434**	**± 5.238**	**± 35.219**
	[2005BRO/CUR]	[2005BRO/CUR]	[2005BRO/CUR]	[2005BRO/CUR]					
ZrF_2^{2+}	**-1197.894**	**-1295.995**	**-218.138**		$Zr^{4+} + 2\ F^- \rightleftarrows ZrF_2^{2+}$	18.550	-105.884	-16.800	298.790
	± 9.490	**± 5.272**	**± 35.871**			± 0.310	± 1.769	± 1.000	± 6.817
						[2005BRO/CUR]	[2005BRO/CUR]	[2005BRO/CUR]	[2005BRO/CUR]
$ZrF_3(g)$	-1065.713	-1075.900	309.100	68.400	$ZrF_3(g) \rightleftarrows Zr^{4+} + 3\ F^- + e^-$	**53.967**	**-308.048**	**-538.643**	**-773.868**
	± 1.692	± 1.200	± 4.000	± 2.000		**± 1.681**	**± 9.593**	**± 5.520**	**± 35.464**
	[2005BRO/CUR]	[2005BRO/CUR]	[2005BRO/CUR]	[2005BRO/CUR]					
ZrF_3^+	**-1514.863**	**-1625.743**	**-94.412**		$Zr^{4+} + 3\ F^- \rightleftarrows ZrF_3^+$	24.720	-141.103	-11.200	435.696
	± 9.689	**± 5.650**	**± 36.430**			± 0.380	± 2.169	± 1.700	± 9.243
						[2005BRO/CUR]	[2005BRO/CUR]	[2005BRO/CUR]	[2005BRO/CUR]
$ZrF_4(aq)$	**-1827.380**	**-1971.890**	**-40.623**		$Zr^{4+} + 4\ F^- \rightleftarrows ZrF_4(aq)$	30.110	-171.869	-22.000	502.664
	± 9.875	**± 6.282**	**± 37.208**			± 0.400	± 2.283	± 2.700	± 11.860
						[2005BRO/CUR]	[2005BRO/CUR]	[2005BRO/CUR]	[2005BRO/CUR]
β-ZrF_4	-1810.119	-1911.300	105.300	102.800	$\beta\text{-}ZrF_4 \rightleftarrows Zr^{4+} + 4\ F^-$	**-27.086**	**154.608**	**-38.590**	**-648.587**
	± 1.322	± 1.000	± 2.900	± 2.900		**± 1.699**	**± 9.698**	**± 5.759**	**± 35.386**
	[2005BRO/CUR]	[2005BRO/CUR]	[2005BRO/CUR]	[2005BRO/CUR]					
$ZrF_4(g)$	-1634.578	-1671.120	322.100	87.440	$ZrF_4(g) \rightleftarrows Zr^{4+} + 4\ F^-$	**3.667**	**-20.933**	**-278.770**	**-865.387**
	± 1.045	± 1.001	± 1.000	± 0.500		**± 1.693**	**± 9.664**	**± 5.760**	**± 35.281**
	[2005BRO/CUR]	[2005BRO/CUR]	[2005BRO/CUR]	[2005BRO/CUR]					
ZrF_5^-	**-2134.760**				$Zr^{4+} + 5\ F^- \rightleftarrows ZrF_5^-$	34.600	-197.498		
	± 10.104					± 0.420	± 2.397		
						[2005BRO/CUR]	[2005BRO/CUR]		
ZrF_6^{2-}	**-2436.546**				$Zr^{4+} + 6\ F^- \rightleftarrows ZrF_6^{2-}$	38.110	-217.533		
	± 10.358					± 0.430	± 2.454		
						[2005BRO/CUR]	[2005BRO/CUR]		
ZrCl(cr)	-264.480	-291.200	61.000	47.160	$ZrCl(cr) \rightleftarrows Zr^{4+} + Cl^- + 3\ e^-$	**69.256**	**-395.319**	**-484.380**	**-298.816**
	± 2.021	± 2.000	± 0.970	± 0.590		**± 1.655**	**± 9.446**	**± 5.386**	**± 35.214**
	[2005BRO/CUR]	[2005BRO/CUR]	[2005BRO/CUR]	[2005BRO/CUR]					

Table A5 Selected thermodynamic data for zirconium (Zr) in JAEA-TDB-RN in 2020 (3/7)

Species / compound	$\Delta_f G^0_m$ (kJ.mol^{-1})	$\Delta_f H^0_m$ (kJ.mol^{-1})	S^0_m (J.K^{-1}.mol^{-1})	$C^0_{p,m}$ (J.K^{-1}.mol^{-1})	Reaction	$\log_{10} K°$	$\Delta_r G^0_m$ (kJ.mol^{-1})	$\Delta_r H^0_m$ (kJ.mol^{-1})	$\Delta_r S^0_m$ (J.K^{-1}.mol^{-1})
ZrCl(g)	200.418 ± 23.580 [2005BRO/CUR]	231.837 ± 23.563 [2005BRO/CUR]	256.000 ± 3.000 [2005BRO/CUR]	35.700 ± 1.500 [2005BRO/CUR]	ZrCl(g) ⇄ Zr^{4+} + Cl^- + 3 e^-	**150.703 ± 4.436**	**-860.217 ± 25.321**	**-1007.417 ± 24.088**	**-493.816 ± 35.328**
$ZrCl_3^+$	**-668.875 ± 9.234**				Zr^{4+} + Cl^- ⇄ $ZrCl^{3+}$	1.590 ± 0.060 [2005BRO/CUR]	-9.076 ± 0.342 [2005BRO/CUR]		
$ZrCl_2$(cr)	-496.151 ± 13.023 [2005BRO/CUR]	-542.800 ± 13.000 [2005BRO/CUR]	105.700 ± 2.600 [2005BRO/CUR]	68.800 ± 1.600 [2005BRO/CUR]	$ZrCl_2$(cr) ⇄ Zr^{4+} + 2 Cl^- + 2 e^-	**51.671 ± 2.796**	**-294.937 ± 15.962**	**-399.859 ± 13.929**	**-352.120 ± 35.297**
$ZrCl_2$(g)	-154.311 ± 19.869 [2005BRO/CUR]	-145.385 ± 19.813 [2005BRO/CUR]	292.100 ± 5.000 [2005BRO/CUR]	58.300 ± 2.500 [2005BRO/CUR]	$ZrCl_2$(g) ⇄ Zr^{4+} + 2 Cl^- + 2 e^-	**111.558 ± 3.838**	**-636.777 ± 21.908**	**-797.274 ± 20.435**	**-538.520 ± 35.555**
$ZrCl_2^{2+}$	**-803.475 ± 9.330**				Zr^{4+} + 2 Cl^- ⇄ $ZrCl_2^{2+}$	2.170 ± 0.240 [2005BRO/CUR]	-12.386 ± 1.370 [2005BRO/CUR]		
$ZrCl_3$(cr)	-689.742 ± 3.013 [2005BRO/CUR]	-760.100 ± 3.000 [2005BRO/CUR]	137.720 ± 0.940 [2005BRO/CUR]	92.950 ± 0.620 [2005BRO/CUR]	$ZrCl_3$(cr) ⇄ Zr^{4+} + 3 Cl^- + e^-	**40.756 ± 1.701**	**-232.636 ± 9.711**	**-349.639 ± 5.837**	**-392.744 ± 35.216**
$ZrCl_3$(g)	-510.571 ± 9.196 [2005BRO/CUR]	-520.143 ± 9.074 [2005BRO/CUR]	341.600 ± 5.000 [2005BRO/CUR]	76.100 ± 2.500 [2005BRO/CUR]	$ZrCl_3$(g) ⇄ Zr^{4+} + 3 Cl^- + e^-	**72.145 ± 2.283**	**-411.807 ± 13.031**	**-589.596 ± 10.364**	**-596.624 ± 35.557**
$ZrCl_4$(cr)	-890.150 ± 1.188 [2005BRO/CUR]	-980.800 ± 0.900 [2005BRO/CUR]	181.200 ± 2.600 [2005BRO/CUR]	117.500 ± 1.600 [2005BRO/CUR]	$ZrCl_4$(cr) ⇄ Zr^{4+} + 4 Cl^-	**28.647 ± 1.631**	**-163.518 ± 9.312**	**-296.019 ± 5.092**	**-444.829 ± 35.302**
$ZrCl_4$(g)	-836.425 ± 0.949 [2005BRO/CUR]	-871.500 ± 0.901 [2005BRO/CUR]	367.600 ± 1.000 [2005BRO/CUR]	98.200 ± 1.000 [2005BRO/CUR]	$ZrCl_4$(g) ⇄ Zr^{4+} + 4 Cl^-	**38.059 ± 1.627**	**-217.243 ± 9.284**	**-405.319 ± 5.093**	**-631.229 ± 35.221**
ZrBr(cr)		218.900 ± 3.500 [2005BRO/CUR]			ZrBr(cr) ⇄ Zr^{4+} + Br^- + 3 e^-			**-948.903 ± 6.105**	
ZrBr(g)			268.200 ± 3.000 [2005BRO/CUR]	36.700 ± 1.500 [2005BRO/CUR]					
$ZrBr_2$(cr)		-399.200 ± 13.000 [2005BRO/CUR]			$ZrBr_2$(cr) ⇄ Zr^{4+} + 2 Br^- + 2 e^-			**-452.307 ± 13.932**	
$ZrBr_2$(g)			318.900 ± 5.000 [2005BRO/CUR]	60.400 ± 2.500 [2005BRO/CUR]					
$ZrBr_3$(cr)		-599.800 ± 13.000 [2005BRO/CUR]			$ZrBr_3$(cr) ⇄ Zr^{4+} + 3 Br^- + e^-			**-373.210 ± 13.936**	

Table A5 Selected thermodynamic data for zirconium (Zr) in JAEA-TDB-RN in 2020 (4/7)

Species / compound	$\Delta_f G^0_m$ (kJ.mol^{-1})	$\Delta_f H^0_m$ (kJ.mol^{-1})	S^0_m (J.K^{-1}.mol^{-1})	$C^0_{p,m}$ (J.K^{-1}.mol^{-1})	Reaction	$\log_{10} K°$	$\Delta_r G^0_m$ (kJ.mol^{-1})	$\Delta_r H^0_m$ (kJ.mol^{-1})	$\Delta_r S^0_m$ (J.K^{-1}.mol^{-1})
$ZrBr_3$(g)			379.300 ± 5.000 [2005BRO/CUR]	79.400 ± 2.500 [2005BRO/CUR]					
$ZrBr_4$(cr)		-759.500 ± 3.300 [2005BRO/CUR]			$ZrBr_4$(cr) ⇄ Zr^{4+} + 4 Br^-			**-335.013 ± 6.021**	
$ZrBr_4$(g)	-664.669 ± 3.775 [2005BRO/CUR]	-643.500 ± 3.759 [2005BRO/CUR]	414.500 ± 1.000 [2005BRO/CUR]	102.700 ± 1.000 [2005BRO/CUR]	$ZrBr_4$(g) ⇄ Zr^{4+} + 4 Br^-	**49.056 ± 1.750**	**-280.014 ± 9.992**	**-451.013 ± 6.284**	**-573.696 ± 35.224**
ZrI(cr)	-150.417 ± 1.205 [2005BRO/CUR]	-152.400 ± 1.200 [2005BRO/CUR]	90.500 ± 0.300 [2005BRO/CUR]	50.800 ± 0.100 [2005BRO/CUR]	ZrI(cr) ⇄ Zr^{4+} + I^- + 3 e^-	**75.335 ± 1.637**	**-430.015 ± 9.343**	**-513.002 ± 5.210**	**-278.359 ± 35.202**
ZrI(g)	349.318 ± 11.036 [2005BRO/CUR]	403.000 ± 11.000 [2005BRO/CUR]	277.200 ± 3.000 [2005BRO/CUR]	37.200 ± 1.500 [2005BRO/CUR]	ZrI(g) ⇄ Zr^{4+} + I^- + 3 e^-	**162.884 ± 2.524**	**-929.750 ± 14.409**	**-1068.402 ± 12.112**	**-465.059 ± 35.328**
ZrI_2(cr)	-273.799 ± 10.001 [2005BRO/CUR]	-277.800 ± 10.000 [2005BRO/CUR]	141.800 ± 0.300 [2005BRO/CUR]	75.500 ± 0.200 [2005BRO/CUR]	ZrI_2(cr) ⇄ Zr^{4+} + 2 I^- + 2 e^-	**62.816 ± 2.402**	**-358.557 ± 13.710**	**-444.505 ± 11.305**	**-288.306 ± 35.204**
ZrI_2(g)	77.761 ± 16.070 [2005BRO/CUR]	135.000 ± 16.000 [2005BRO/CUR]	347.200 ± 5.000 [2005BRO/CUR]	61.400 ± 2.500 [2005BRO/CUR]	ZrI_2(g) ⇄ Zr^{4+} + 2 I^- + 2 e^-	**124.406 ± 3.260**	**-710.117 ± 18.606**	**-857.305 ± 16.846**	**-493.706 ± 35.556**
ZrI_3(cr)	-385.580 ± 15.001 [2005BRO/CUR]	-391.600 ± 15.000 [2005BRO/CUR]	193.100 ± 0.400 [2005BRO/CUR]	100.300 ± 0.200 [2005BRO/CUR]	ZrI_3(cr) ⇄ Zr^{4+} + 3 I^- + e^-	**52.330 ± 3.117**	**-298.699 ± 17.790**	**-387.607 ± 16.009**	**-298.254 ± 35.208**
ZrI_3(g)	-185.876 ± 4.365 [2005BRO/CUR]	-130.000 ± 4.100 [2005BRO/CUR]	400.700 ± 5.000 [2005BRO/CUR]	80.900 ± 2.500 [2005BRO/CUR]	ZrI_3(g) ⇄ Zr^{4+} + 3 I^- + e^-	**87.316 ± 1.842**	**-498.403 ± 10.512**	**-649.207 ± 6.936**	**-505.854 ± 35.559**
ZrI_4(cr)	-480.862 ± 3.714 [2005BRO/CUR]	-488.900 ± 3.700 [2005BRO/CUR]	244.400 ± 0.900 [2005BRO/CUR]	125.100 ± 0.500 [2005BRO/CUR]	ZrI_4(cr) ⇄ Zr^{4+} + 4 I^-	**44.734 ± 1.839**	**-255.341 ± 10.495**	**-347.210 ± 7.064**	**-308.201 ± 35.221**
ZrI_4(g)	-405.959 ± 3.732 [2005BRO/CUR]	-355.500 ± 3.712 [2005BRO/CUR]	440.600 ± 1.140 [2005BRO/CUR]	104.590 ± 0.250 [2005BRO/CUR]	ZrI_4(g) ⇄ Zr^{4+} + 4 I^-	**57.856 ± 1.840**	**-330.244 ± 10.501**	**-480.610 ± 7.070**	**-504.401 ± 35.228**
$ZrS_{1.5}$(cr)	-502.107 ± 3.886 [2005BRO/CUR]	-509.400 ± 1.100 [2005BRO/CUR]	62.700 ± 12.500 [2005BRO/CUR]		$ZrS_{1.5}$(cr) + 1.5 H^+ ⇄ Zr^{4+} + 1.5 HS^- + e^-	**1.481 ± 1.757**	**-8.453 ± 10.032**	**-123.263**	**-385.631**
ZrS_2(cr)	-565.750 ± 12.015 [2005BRO/CUR]	-573.200 ± 12.000 [2005BRO/CUR]	78.200 ± 2.000 [2005BRO/CUR]	56.400 ± 2.000 [2005BRO/CUR]	ZrS_2(cr) + 2 H^+ ⇄ Zr^{4+} + 2 HS^-	**-10.717 ± 2.658**	**61.173 ± 15.172**	**-67.517**	**-432.371**
ZrS_3(cr)	-601.920 ± 4.836 [2005BRO/CUR]	-615.200 ± 4.600 [2005BRO/CUR]	90.700 ± 5.000 [2005BRO/CUR]		ZrS_3(cr) + 3 H^+ + 2 e^- ⇄ Zr^{4+} + 3 HS^-	**-19.150 ± 1.838**	**109.310 ± 10.493**	**-41.625**	**-507.350**

Table A5 Selected thermodynamic data for zirconium (Zr) in JAEA-TDB-RN in 2020 (5/7)

Species / compound	$\Delta_f G^0_m$ (kJ.mol^{-1})	$\Delta_f H^0_m$ (kJ.mol^{-1})	S^0_m (J.K^{-1}.mol^{-1})	$C^0_{p,m}$ (J.K^{-1}.mol^{-1})	Reaction	$\log_{10} K°$	$\Delta_r G^0_m$ (kJ.mol^{-1})	$\Delta_r H^0_m$ (kJ.mol^{-1})	$\Delta_r S^0_m$ (J.K^{-1}.mol^{-1})
$Zr(SO_3)_2$(cr)	-1834.870	-2011.000	127.900		$Zr(SO_3)_2$(cr) ⇄ Zr^{4+} + 2 SO_3^{2-}	**-58.367**	**333.163**	**131.401**	**-677.045**
	± 10.032	± 10.000	± 2.700			**± 3.781**	**± 21.584**	**± 20.127**	**± 171.043**
	[2005BRO/CUR]	[2005BRO/CUR]	[2005BRO/CUR]						
$ZrSO_4^{2+}$	**-1313.153**	-1480.900	-213.393		Zr^{4+} + SO_4^{2-} ⇄ $ZrSO_4^{2+}$	7.040	-40.185	**37.202**	**258.348**
	± 9.253	± 5.100	± 35.431			± 0.090	± 0.514	**± 7.154**	**± 49.946**
		[2005BRO/CUR]	[2005BRO/CUR]			[2005BRO/CUR]	[2005BRO/CUR]		
$Zr(SO_4)_2$(cr)	-2009.454	-2245.200	133.100	185.100	$Zr(SO_4)_2$(cr) ⇄ Zr^{4+} + 2 SO_4^{2-}	**1.397**	**-7.973**	**-182.503**	**-586.013**
	± 2.183	± 2.100	± 2.000	± 10.000		**± 1.669**	**± 9.526**	**± 5.487**	**± 35.271**
	[2005BRO/CUR]	[2005BRO/CUR]	[2005BRO/CUR]	[2005BRO/CUR]					
$Zr(SO_4)_2$(aq)	**-2083.298**	-2359.800	**-3.622**		Zr^{4+} + 2 SO_4^{2-} ⇄ $Zr(SO_4)_2$(aq)	11.540	-65.871	**67.903**	**449.291**
	± 9.350	± 5.200	**± 35.884**			± 0.210	± 1.199	**± 7.262**	**± 50.276**
		[2005BRO/CUR]				[2005BRO/CUR]	[2005BRO/CUR]		
$Zr(SO_4)_3^{2-}$	**-2843.511**				Zr^{4+} + 3 SO_4^{2-} ⇄ $Zr(SO_4)_3^{2-}$	14.300	-81.625		
	± 9.757					± 0.500	± 2.854		
						[2005BRO/CUR]	[2005BRO/CUR]		
$Zr(SO_4)_2 \cdot 4H_2O$(cr)	-3008.762	-3470.900	306.800	321.300	$Zr(SO_4)_2 \cdot 4H_2O$(cr) ⇄ Zr^{4+} + 2 SO_4^{2-} + 4 H_2O(l)	**-7.464**	**42.604**	**-100.157**	**-480.021**
	± 2.607	± 2.600	± 0.600	± 0.300		**± 1.689**	**± 9.641**	**± 5.713**	**± 35.221**
	[2005BRO/CUR]	[2005BRO/CUR]	[2005BRO/CUR]	[2005BRO/CUR]					
$Zr(SeO_3)_2$(cr)		-1609.550			$Zr(SeO_3)_2$(cr) ⇄ Zr^{4+} + 2 SeO_3^{2-}			**-13.270**	
		± 2.689						**± 6.111**	
		[2005BRO/CUR]							
$ZrTe_{1.843}$(cr)	-291.328	-295.000	117.480	70.590					
	± 7.000	± 7.000	± 0.120	± 0.280					
	[2005BRO/CUR]	[2005BRO/CUR]	[2005BRO/CUR]	[2005BRO/CUR]					
$ZrTe_2$(cr)	-290.037	-294.000	124.230						
	± 7.000	± 7.000	± 0.100						
	[2005BRO/CUR]	[2005BRO/CUR]	[2005BRO/CUR]						
Zr_5Te_4(cr)	-810.430	-829.000	330.000	222.000					
	± 44.000	± 44.000	± 0.400	± 0.300					
	[2005BRO/CUR]	[2005BRO/CUR]	[2005BRO/CUR]	[2005BRO/CUR]					
$ZrTe_3O_8$(cr)		-2119.200							
		± 9.600							
		[2005BRO/CUR]							
ZrN(cr)	-341.852	-370.500	38.800	39.700	ZrN(cr) + 3 H_2O(l) ⇄ Zr^{4+} + NO_3^- + 6 H^+ + 9 e^-	**-72.525**	**413.973**	**412.616**	**-4.141**
	± 1.952	± 1.389	± 4.600	± 1.400		**± 1.711**	**± 9.764**	**± 5.216**	**± 35.510**
	[2005BRO/CUR]	[2005BRO/CUR]	[2005BRO/CUR]	[2005BRO/CUR]					
$ZrNO_3^{3+}$	**-648.503**				Zr^{4+} + NO_3^- ⇄ $ZrNO_3^{3+}$	1.590	-9.076		
	± 9.573					± 0.080	± 0.457		
						[2005BRO/CUR]	[2005BRO/CUR]		
$Zr(NO_3)_2^{2+}$	**-765.414**				Zr^{4+} + 2 NO_3^- ⇄ $Zr(NO_3)_2^{2+}$	2.640	-15.069		
	± 10.549					± 0.170	± 0.970		
						[2005BRO/CUR]	[2005BRO/CUR]		

Table A5 Selected thermodynamic data for zirconium (Zr) in JAEA-TDB-RN in 2020 (6/7)

Species / compound	$\Delta_f G^0_m$ (kJ.mol^{-1})	$\Delta_f H^0_m$ (kJ.mol^{-1})	S^0_m (J.K^{-1}.mol^{-1})	$C^0_{p,m}$ (J.K^{-1}.mol^{-1})	Reaction	$\log_{10} K°$	$\Delta_r G^0_m$ (kJ.mol^{-1})	$\Delta_r H^0_m$ (kJ.mol^{-1})	$\Delta_r S^0_m$ (J.K^{-1}.mol^{-1})
ZrP_2O_7(cr)			188.800 ± 2.000 [2005BRO/CUR]	150.700 ± 1.500 [2005BRO/CUR]					
α-$Zr(HPO_4)_2$	-2987.000 ± 23.000 [2005BRO/CUR]	-3166.200 ± 6.000 [2005BRO/CUR]	471.508 ± 79.726 [2005BRO/CUR]		α-$Zr(HPO_4)_2 \rightleftarrows Zr^{4+} + 2\ PO_4^{3-} + 2\ H^+$	**-73.735 ± 5.239**	**420.883 ± 29.904**	**2.950 ± 18.469**	**-1405.581 ± 188.692**
β-$Zr(HPO_4)_2$		-3159.100 ± 6.000 [2005BRO/CUR]			β-$Zr(HPO_4)_2 \rightleftarrows Zr^{4+} + 2\ PO_4^{3-} + 2\ H^+$			**-4.150 ± 18.469**	
$Zr(HPO_4)_2 \cdot H_2O$(cr)	**-3181.136 ± 20.026**	-3466.100 ± 1.600 [2005BRO/CUR]	**350.001 ± 67.385**		$Zr^{4+} + 2\ H_3PO_4$(aq) + H_2O(l) $\rightleftarrows Zr(HPO_4)_2 \cdot H_2O$(cr) + $4\ H^+$	22.800 ± 3.100 [2005BRO/CUR]	-130.143 ± 17.695 [2005BRO/CUR]	**4.913 ± 5.511**	**452.663 ± 77.845**
$Zr(HPO_4)_2 \cdot 2H_2O$(cr)		-3742.100 ± 13.300 [2005BRO/CUR]			$Zr(HPO_4)_2 \cdot 2H_2O$(cr) $\rightleftarrows Zr^{4+} + 2\ PO_4^{3-} + 2\ H^+ + 2\ H_2O$(l)			**7.173 ± 21.955**	
α-$Zr(HAsO_4)_2$		-2364.700 ± 12.100 [2005BRO/CUR]			α-$Zr(HAsO_4)_2 \rightleftarrows Zr^{4+} + 2\ AsO_4^{3-} + 2\ H^+$			**-20.080 ± 15.343**	
β-$Zr(HAsO_4)_2$		-2360.900 ± 12.000 [2005BRO/CUR]			β-$Zr(HAsO_4)_2 \rightleftarrows Zr^{4+} + 2\ AsO_4^{3-} + 2\ H^+$			**-23.880 ± 15.264**	
$Zr(HAsO_4)_2 \cdot H_2O$(cr)		-2659.300 ± 13.100 [2005BRO/CUR]			$Zr(HAsO_4)_2 \cdot H_2O$(cr) $\rightleftarrows Zr^{4+} + 2\ AsO_4^{3-} + 2\ H^+ + H_2O$(l)			**-11.318 ± 16.144**	
ZrC(cr)	-203.476 ± 2.585 [2005BRO/CUR]	-207.000 ± 2.500 [2005BRO/CUR]	33.000 ± 2.200 [2005BRO/CUR]	37.280 ± 0.750 [2005BRO/CUR]	ZrC(cr) + $3\ H_2O$(l) $\rightleftarrows Zr^{4+} + HCO_3^{2-} + 5\ H^+ + 8\ e^-$	**35.113 ± 1.680**	**-200.425 ± 9.588**	**-233.918 ± 5.603**	**-112.173 ± 35.273**
$Zr(CO_3)_4^{4-}$	**-2878.182 ± 9.326**				$Zr^{4+} + 4\ CO_3^{2-} \rightleftarrows Zr(CO_3)_4^{4-}$	0.334 ± 0.144 [2017KOB/SAS]	**-1.906 ± 0.823**		
$Zr(CO_3)_5^{6-}$	**-3401.598 ± 9.420**				$Zr^{4+} + 5\ CO_3^{2-} \rightleftarrows Zr(CO_3)_5^{6-}$	-10.795 ± 0.233 [2017KOB/SAS]	**61.618 ± 1.333**		
$Zr(CO_3)_2(OH)_2^{2-}$	**-2162.430 ± 9.275**				$Zr^{4+} + 2\ H_2O$(l) + $2\ HCO_3^- \rightleftarrows Zr(CO_3)_2(OH)_2^{2-} + 4\ H^+$	-2.510 ± 0.130 [2017KOB/SAS]	**14.327 ± 0.744**		
$ZrSiO_4$(cr)	-1919.712 ± 3.115 [2005BRO/CUR]	-2034.200 ± 3.100 [2005BRO/CUR]	84.200 ± 1.000 [2005BRO/CUR]	98.200 ± 0.600 [2005BRO/CUR]	$ZrSiO_4$(cr) + $4\ H^+ \rightleftarrows Zr^{4+} + Si(OH)_4$(aq)	**-14.616 ± 1.736**	**83.431 ± 9.907**	**-31.224 ± 6.816**	**-384.972 ± 36.674**
$Ca_2[Zr(OH)_6]^{2+}$	**-2910.716 ± 9.575**				$Zr^{4+} + 2\ Ca^{2+} + 6\ H_2O$(l) $\rightleftarrows Ca_2[Zr(OH)_6]^{2+} + 6\ H^+$	-25.660 ± 0.335 [2009ALT/NEC]	**146.468 ± 1.912**		

Table A5 Selected thermodynamic data for zirconium (Zr) in JAEA-TDB-RN in 2020 (7/7)

Species / compound	$\Delta_f G^0_m$ (kJ.mol^{-1})	$\Delta_f H^0_m$ (kJ.mol^{-1})	S^0_m (J.K^{-1}.mol^{-1})	$C^0_{p,m}$ (J.K^{-1}.mol^{-1})	Reaction	$\log_{10} K°$	$\Delta_r G^0_m$ (kJ.mol^{-1})	$\Delta_r H^0_m$ (kJ.mol^{-1})	$\Delta_r S^0_m$ (J.K^{-1}.mol^{-1})
$Ca_3[Zr(OH)_6]^{4+}$	**-3455.823**				$Zr^{4+} + 3\ Ca^{2+} + 6\ H_2O(l) \rightleftarrows Ca_3[Zr(OH)_6]^{4+} + 6\ H^+$	-27.006	**154.151**		
	± 9.645					± 0.238	**± 1.359**		
						[2009ALT/NEC]			
$Ca_2ZrSi_3O_{12}$(cr)	-5951.457	-6283.000	297.600	252.500	$Ca_2ZrSi_3O_{12}$(cr) + 12 H^+ + 4 e^-	**-69.034**	**394.052**	**217.561**	**-593.104**
	± 15.076	± 15.000	± 5.000	± 2.500	$\rightleftarrows Zr^{4+} + 2\ Ca^{2+} + 3\ Si(OH)_4$(aq)	**± 3.253**	**± 18.567**	**± 18.951**	**± 47.004**
	[2005BRO/CUR]	[2005BRO/CUR]	[2005BRO/CUR]	[2005BRO/CUR]					
$Ca_3ZrSi_2O_9$(cr)	-4769.295	-5029.000	253.600	238.100	$Ca_3ZrSi_2O_9$(cr) + 10 H^+	**47.356**	**-270.311**	**-408.436**	**-464.104**
	± 10.046	± 10.000	± 3.000	± 1.500	$\rightleftarrows 3\ Ca^{2+} + Zr^{4+} + 2\ Si(OH)_4$(aq) + H_2O(l)	**± 2.508**	**± 14.318**	**± 13.345**	**± 40.859**
	[2005BRO/CUR]	[2005BRO/CUR]	[2005BRO/CUR]	[2005BRO/CUR]					
$SrZrSi_2O_7$(cr)	-3443.991	-3640.800	190.330	187.810	$SrZrSi_2O_7$(cr) + H_2O(l) + 6 $H^+ \rightleftarrows Zr^{4+} + Sr^{2+} + 2\ Si(OH)_4$(aq)	**4.680**	**-26.715**	**-146.617**	**-402.734**
	± 4.203	± 4.200	± 0.480	± 0.380		**± 1.892**	**± 10.802**	**± 9.502**	**± 40.781**
	[2005BRO/CUR]	[2005BRO/CUR]	[2005BRO/CUR]	[2005BRO/CUR]					
$Sr_6ZrSi_5O_{18}$(cr)		-9867.900			$Sr_6ZrSi_5O_{18}$(cr) + 2 H_2O(l) + 16 H^+			**-758.988**	
		± 8.600			$\rightleftarrows Zr^{4+} + 6\ Sr^{2+} + 2\ Si(OH)_4$(aq)			**± 20.105**	
		[2005BRO/CUR]							
Na_2ZrSiO_5(cr)	-2523.498	-2670.000	182.000	172.400	Na_2ZrSiO_5(cr) + 6 $H^+ \rightleftarrows Zr^{4+} + 2\ Na^+ + Si(OH)_4$(aq) + H_2O(l)	**12.916**	**-73.727**	**-161.854**	**-296.032**
	± 20.003	± 20.000	± 1.000	± 2.000		**± 3.873**	**± 22.105**	**± 20.902**	**± 36.677**
	[2005BRO/CUR]	[2005BRO/CUR]	[2005BRO/CUR]	[2005BRO/CUR]					
$Na_2ZrSi_2O_7$(cr)	-3412.402	-3606.000	248.000	211.000	$Na_2ZrSi_2O_7$(cr) + H_2O(l) + 6 H^+	**3.194**	**-18.230**	**-111.101**	**-312.081**
	± 10.019	± 10.000	± 2.000	± 5.000	$\rightleftarrows Zr^{4+} + 2\ Na^+ + 2\ Si(OH)_4$(aq)	**± 2.470**	**± 14.101**	**± 13.131**	**± 40.780**
	[2005BRO/CUR]	[2005BRO/CUR]	[2005BRO/CUR]	[2005BRO/CUR]					
$Na_2ZrSi_3O_9 \cdot 2H_2O$(cr)	-4654.000				$Na_2ZrSi_3O_9 \cdot 2H_2O$(cr) + H_2O(l) + 6 H^+	**14.787**	**-84.404**		
	± 20.000				$\rightleftarrows Zr^{4+} + 2\ Na^+ + 3\ Si(OH)_4$(aq)	**± 3.976**	**± 22.693**		
	[2005BRO/CUR]								
$Na_2ZrSi_4O_{11}$(cr)	-5181.000				$Na_2ZrSi_4O_{11}$(cr) + 5 H_2O(l) + 6 H^+	**-14.638**	**83.554**		
	± 20.000				$\rightleftarrows Zr^{4+} + 2\ Na^+ + 4\ Si(OH)_4$(aq)	**± 4.065**	**± 23.203**		
	[2005BRO/CUR]								
$Na_2ZrSi_6O_{15} \cdot 3H_2O$(cr)	-7391.000				$Na_2ZrSi_6O_{15} \cdot 3H_2O$(cr) + 6 H_2O(l) + 6 H^+	**14.857**	**-84.807**		
	± 30.000				$\rightleftarrows Zr^{4+} + 2\ Na^+ + 6\ Si(OH)_4$(aq)	**± 5.823**	**± 33.237**		
	[2005BRO/CUR]								
$Na_4Zr_2Si_3O_{12}$(cr)	-5944.005	-6285.000	427.000	365.000	$Na_4Zr_2Si_3O_{12}$(cr) + 12 $H^+ \rightleftarrows 2\ Zr^{4+} + 4\ Na^+ + 3\ Si(OH)_4$(aq)	**14.690**	**-83.852**	**-263.955**	**-605.113**
	± 20.057	± 20.000	± 5.000	± 5.000		**± 4.870**	**± 27.800**	**± 24.632**	**± 76.983**
	[2005BRO/CUR]	[2005BRO/CUR]	[2005BRO/CUR]	[2005BRO/CUR]					
$NaZr_2P_3O_{12}$(cr)	-4556.968	-4889.000	370.000	310.000	$NaZr_2P_3O_{12}$(cr) $\rightleftarrows 2\ Zr^{4+} + Na^+ + 3\ PO_4^{3-}$	**-31.825**	**181.657**	**-400.421**	
	± 20.222	± 20.000	± 10.000	± 10.000		**± 6.507**	**± 37.144**	**± 33.619**	
	[2005BRO/CUR]	[2005BRO/CUR]	[2005BRO/CUR]	[2005BRO/CUR]					
$Cs_2ZrSi_2O_7$(cr)		-3587.000			$Cs_2ZrSi_2O_7$(cr) + H_2O(l) + 6 H^+			**-165.565**	
		± 10.000			$\rightleftarrows Zr^{4+} + 2\ Cs^+ + 2\ Si(OH)_4$(aq)			**± 13.132**	
		[2005BRO/CUR]							

[2005BRO/CUR] Brown et al. [A9)]
[2009ALT/NEC] Altmaier et al. [A10)]
[2017KOB/SAS] Kobayashi and Sasaki [A11)].
[2018RAI/KIT] Rai et al. [A12)]

Table A6 Selected thermodynamic data for niobium (Nb) in JAEA-TDB-RN in 2020

Values indicated by **boldface** are calculated and selected in the present report.

Species / compound	$\Delta_f G^0_m$ (kJ.mol^{-1})	$\Delta_f H^0_m$ (kJ.mol^{-1})	S^0_m (J.K^{-1}.mol^{-1})	$C^0_{p,m}$ (J.K^{-1}.mol^{-1})	Reaction	$\log_{10} K°$	$\Delta_r G^0_m$ (kJ.mol^{-1})	$\Delta_r H^0_m$ (kJ.mol^{-1})	$\Delta_r S^0_m$ (J.K^{-1}.mol^{-1})
$Nb(OH)_6^-$					$Nb(OH)_5(aq) + H_2O(l) \rightleftarrows Nb(OH)_6^- + H^+$	> -6.758	**< 38.575**		
						[2010KIT/FUJ]			
$Nb_2O_5(s)$					$Nb_2O_5(s) + 7\ H_2O(l) \rightleftarrows 2\ Nb(OH)_6^- + 2\ H^+$	-28.913	**165.037**		
						± 0.507	**± 2.894**		
						[2010KIT/FUJ]			

[2010KIT/FUJ] Kitamura et al. [A13)]

Table A7 Selected thermodynamic data for molybdenum (Mo) in JAEA-TDB-RN in 2020

Values indicated by **boldface** are calculated and selected in the present report.

Species / compound	$\Delta_f G^0_m$ (kJ.mol^{-1})	$\Delta_f H^0_m$ (kJ.mol^{-1})	S^0_m (J.K^{-1}.mol^{-1})	$C^0_{p,m}$ (J.K^{-1}.mol^{-1})	Reaction	$\log_{10} K°$	$\Delta_r G^0_m$ (kJ.mol^{-1})	$\Delta_r H^0_m$ (kJ.mol^{-1})	$\Delta_r S^0_m$ (J.K^{-1}.mol^{-1})
Mo(cr)	0.000	0.000	28.660	24.060					
	[1982WAG/EVA]	[1982WAG/EVA]	[1982WAG/EVA]	[1982WAG/EVA]					
MoO_2(cr)	**-533.101**				MoO_2(cr) + 2 H_2O(l) ⇄ MoO_4^{2-} + 4 H^+ + 2 e^-	-29.570	**168.787**		
						[2010KIT/KIR]			
MoO_4^{2-}	**-838.679**				Mo(metal) + 4 H_2O(l) ⇄ MoO_4^{2-} + 8 H^+ + 6 e^-	-19.280	**110.051**		
						[2010KIT/KIR]			
Mo^{3+}	**-57.708**				MoO_4^{2-} + 8 H^+ + 3 e^- ⇄ Mo^{3+} + 4 H_2O(l)	29.390	**-167.759**		
						[2010KIT/KIR]			
$HMoO_4^-$	**-862.082**				MoO_4^{2-} + H^+ ⇄ $HMoO_4^-$	4.100	**-23.403**		
						± 0.100	**± 0.571**		
						[2010KIT/KIR]			
H_2MoO_4(aq)	**-876.923**				MoO_4^{2-} + 2 H^+ ⇄ H_2MoO_4(aq)	6.700	**-38.244**		
						± 0.200	**± 1.142**		
						[2010KIT/KIR]			
$Mo_7O_{24}^{6-}$	**-5224.551**				7 MoO_4^{2-} + 8 H^+ ⇄ $Mo_7O_{24}^{6-}$ + 4 H_2O(l)	53.000	**-302.526**		
						± 0.200	**± 1.142**		
						[2010KIT/KIR]			
$HMo_7O_{24}^{5-}$	**-5263.366**				7 MoO_4^{2-} + 9 H^+ ⇄ $HMo_7O_{24}^{5-}$ + 4 H_2O(l)	59.800	**-341.341**		
						± 0.500	**± 2.854**		
						[2010KIT/KIR]			
$PbMoO_4$(cr)	**-936.702**				$PbMoO_4$(cr) ⇄ MoO_4^{2-} + Pb^{2+}	-12.980	**74.090**		
						± 0.050	**± 0.285**		
						[2010KIT/KIR]			
$Sm(MoO_4)_2^-$					Sm^{3+}+ 2 MoO_4^{2-} ⇄ $Sm(MoO_4)_2^-$	11.200	**-63.930**		
						± 0.300	**± 1.712**		
						[2010KIT/KIR]			
$Sm_2(MoO_4)_3 \cdot xH_2O$(cr)					$Sm_2(MoO_4)_3 \cdot xH_2O$(cr) ⇄ 3 MoO_4^{2-} + 2 Sm^{3+} + x H_2O(l)	-26.100	**148.980**		
						± 0.300	**± 1.712**		
						[2010KIT/KIR]			
$CaMoO_4$(cr)	**-1436.848**				$CaMoO_4$(cr) ⇄ MoO_4^{2-} + Ca^{2+}	-7.950	**45.379**		
						± 0.050	**± 0.285**		
						[2010KIT/KIR]			

[1982WAG/EVA] Wagman et al.[A5)]
[2010KIT/KIR] Kitamura et al. [A14)]

Table A8 Selected thermodynamic data for technetium (Tc) in JAEA-TDB-RN in 2020 (1/3)

Values indicated by **boldface** are calculated and selected in the present report.

Species / compound	$\Delta_f G^0_m$ (kJ.mol^{-1})	$\Delta_f H^0_m$ (kJ.mol^{-1})	S^0_m (J.K^{-1}.mol^{-1})	$C^0_{p,m}$ (J.K^{-1}.mol^{-1})	Reaction	$\log_{10} K°$	$\Delta_r G^0_m$ (kJ.mol^{-1})	$\Delta_r H^0_m$ (kJ.mol^{-1})	$\Delta_r S^0_m$ (J.K^{-1}.mol^{-1})
Tc(cr)	0.000	0.000	32.506	24.879	Tc(cr) + 4 H_2O(l) ⇄ TcO_4^- + 8 H^+ + 7 e^-	**-54.541**	**311.324**	**413.953**	**344.778**
			± 0.700	± 1.000		**± 1.336**	**± 7.627**	**± 7.612**	**± 1.693**
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]					
Tc(g)	630.711	675.000	181.052	20.795	Tc(g) + 4 H_2O(l) ⇄ TcO_4^- + 8 H^+ + 7 e^-	**55.954**	**-319.387**	**-261.047**	**196.232**
	± 25.001	± 25.000	± 0.010	± 0.010		**± 4.579**	**± 26.138**	**± 26.133**	**± 1.541**
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]					
TcO(g)	357.494	390.000	244.109	31.256	TcO(g) + 3 H_2O(l) ⇄ TcO_4^- + 6 H^+ + 5 e^-	**49.641**	**-283.352**	**-261.885**	**72.419**
	± 57.001	± 57.000	± 0.600	± 0.750		**± 10.075**	**± 57.508**	**± 57.505**	**± 1.637**
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]					
TcO^{2+}	**-116.689**				$TcO(OH)_2$(aq) + 2 H^+ ⇄ TcO^{2+} + 2 H_2O(l)	< 4.000	> -22.832		
						[2003GUI/FAN]	[2003GUI/FAN]		
TcO_2(cr)	-401.850	-457.800	50.000		TcO_2(cr) + 2 H_2O(l) ⇄ TcO_4^- + 4 H^+ + 3 e^-	**-41.837**	**238.809**	**300.077**	**205.772**
	± 11.762	± 11.700	± 4.000			**± 2.455**	**± 14.014**	**± 13.953**	**± 4.276**
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]						
TcO_4^-	-637.406	-729.400	199.600	-15.000	$TcO(OH)_2$(aq) + H_2O(l) ⇄ TcO_4^- + 4 H^+ + 3 e^-	**-29.432**	**167.998**		
	± 7.616	± 7.600	± 1.500	± 8.000		**± 2.045**	**± 11.673**		
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]					
TcO_4^{2-}	**-575.759**				TcO_4^- + e^- ⇄ TcO_4^{2-}	-10.800	61.647		
	± 8.133					± 0.500	± 2.854		
						[2003GUI/FAN]	[2003GUI/FAN]		
Tc_2O_7(cr)	-950.280	-1126.500	192.000	160.400	Tc_2O_7(cr) + H_2O(l) ⇄ 2 TcO_4^- + 2 H^+	**15.303**	**-87.349**	**-46.462**	**137.277**
	± 15.562	± 14.900	± 15.000	± 15.000		**± 3.815**	**± 21.776**	**± 21.285**	**± 15.297**
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]					
Tc_2O_7(g)	-904.820	-1008.100	436.641	146.736	Tc_2O_7(g) + H_2O(l) ⇄ 2 TcO_4^- + 2 H^+	**23.267**	**-132.809**	**-164.862**	**-107.364**
	± 16.462	± 16.063	± 12.000	± 5.000		**± 3.929**	**± 22.428**	**± 22.115**	**± 12.370**
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]					
$TcO(OH)^+$	**-357.085**				$TcO(OH)_2$(aq) + H^+ ⇄ $TcO(OH)^+$ + H_2O(l)	4.563	**-26.046**		
	± 8.931					± 0.216	**± 1.233**		
						[2004HES/XIA]			
$TcO(OH)_2$(aq)	**-568.136**				TcO_2·1.6H_2O(s) ⇄ $TcO(OH)_2$(aq) + 0.6 H_2O(l)	-8.415	**48.033**		
	± 8.435					± 0.180	**± 1.027**		
						[2004HES/XIA]			
TcO_2·1.6H_2O(cr)	**-758.462**				TcO_4^- + 4 H^+ + 3 e^- ⇄ TcO_2·1.6H_2O(cr) + 0.4 H_2O(l)	37.829	-215.930		
	± 8.372					± 0.609	± 3.476		
						[2003GUI/FAN]	[2003GUI/FAN]		
$TcO(OH)_3^-$	**-743.187**				$TcO(OH)_2$(aq) + H_2O(l) ⇄ $TcO(OH)_3^-$ + H^+	-10.900	62.218		
	± 9.136					± 0.400	± 2.283		
						[2003GUI/FAN]	[2003GUI/FAN]		

Table A8 Selected thermodynamic data for technetium (Tc) in JAEA-TDB-RN in 2020 (2/3)

Species / compound	$\Delta_f G^0_m$ (kJ.mol^{-1})	$\Delta_f H^0_m$ (kJ.mol^{-1})	S^0_m (J.K^{-1}.mol^{-1})	$C^0_{p,m}$ (J.K^{-1}.mol^{-1})	Reaction	$\log_{10} K°$	$\Delta_r G^0_m$ (kJ.mol^{-1})	$\Delta_r H^0_m$ (kJ.mol^{-1})	$\Delta_r S^0_m$ (J.K^{-1}.mol^{-1})
$Tc_2O_7 \cdot H_2O$(s)	-1194.300 ± 15.500 [2003GUI/FAN]	-1414.146 ± 14.905 [2003GUI/FAN]	278.933 ± 72.138 [2003GUI/FAN]		$Tc_2O_7 \cdot H_2O(s) \rightleftarrows 2\ TcO_4^- + 2\ H^+$	**14.105 ± 3.807**	**-80.512 ± 21.732**	**-44.654 ± 21.288**	**120.267 ± 72.200**
TcF_6(cr,cubic)			253.520 ± 0.510 [2003GUI/FAN]	157.840 ± 0.320 [2003GUI/FAN]					
TcF_6(g)			359.136 ± 4.500 [2003GUI/FAN]	120.703 ± 2.629 [2003GUI/FAN]	TcF_6(cr,cubic) $\rightleftarrows$ TcF_6(g)	-0.535 ± 0.327 [2003GUI/FAN]	3.054 ± 1.867 [2003GUI/FAN]	34.540 ± 1.300 [2003GUI/FAN]	105.600 ± 4.500 [2003GUI/FAN]
TcO_3F(g)			306.879 ± 0.677 [2003GUI/FAN]	77.261 ± 0.308 [2003GUI/FAN]					
$TcO_2Cl_4^{3-}$					$TcOCl_5^{2-} + H_2O(l) \rightleftarrows TcO_2Cl_4^{3-} + Cl^- + 2\ H^+$	-2.950 ± 0.150 [2003GUI/FAN]	16.839 ± 0.856 [2003GUI/FAN]		
TcO_3Cl(g)			317.636 ± 0.797 [2003GUI/FAN]	80.365 ± 0.308 [2003GUI/FAN]					
TcS(g)	491.925 ± 65.001 [2003GUI/FAN]	549.000 ± 65.000 [2003GUI/FAN]	255.990 ± 1.000 [2003GUI/FAN]	34.474 ± 1.000 [2003GUI/FAN]	$TcS(g) + 4\ H_2O(l) \rightleftarrows TcO_4^- + HS^- + 7\ H^+ + 5\ e^-$	**29.543 ± 11.466**	**-168.634 ± 65.448**	**-151.155**	**58.814**
NH_4TcO_4(cr)	**-722.054 ± 7.634**				$TcO_4^- + NH_4^+ \rightleftarrows NH_4TcO_4$(cr)	0.910 ± 0.070 [2003GUI/FAN]	-5.194 ± 0.400 [2003GUI/FAN]		
$(NH_4)_2TcCl_6$(cr)					$TcCl_6^{2-} + 2\ NH_4^+ \rightleftarrows (NH_4)_2TcCl_6$(cr)	7.988 ± 1.000 [2003GUI/FAN]	-45.596 ± 5.708 [2003GUI/FAN]		
$(NH_4)_2TcBr_6$(cr)					$TcBr_6^{2-} + 2\ NH_4^+ \rightleftarrows (NH_4)_2TcBr_6$(cr)	6.680 ± 1.000 [2003GUI/FAN]	-38.130 ± 5.708 [2003GUI/FAN]		
TcC(g)	765.602 ± 40.250 [2003GUI/FAN]	826.500 ± 40.000 [2003GUI/FAN]	242.500 ± 15.000 [2003GUI/FAN]		$TcC(g) + 7\ H_2O(l) \rightleftarrows TcO_4^- + HCO_3^- + 13\ H^+ + 11\ e^-$	**57.755 ± 7.178**	**-329.670 ± 40.970**	**-244.965 ± 40.723**	**284.822 ± 15.096**
$TcCO_3(OH)_2$(aq)	**-968.859 ± 9.010**				$TcO(OH)_2(aq) + CO_2(g) \rightleftarrows TcCO_3(OH)_2$(aq)	1.100 ± 0.300 [2003GUI/FAN]	-6.279 ± 1.712 [2003GUI/FAN]		
$TcCO_3(OH)_3^-$	**-1158.665 ± 9.486**				$TcO(OH)_2(aq) + CO_2(g) + H_2O(l) \rightleftarrows TcCO_3(OH)_3^- + H^+$	-7.200 ± 0.600 [2003GUI/FAN]	41.098 ± 3.425 [2003GUI/FAN]		
$TlTcO_4$(cr)	**-700.173 ± 7.653**				$TcO_4^- + Tl^+ \rightleftarrows TlTcO_4$(cr)	5.320 ± 0.120 [2003GUI/FAN]	-30.367 ± 0.685 [2003GUI/FAN]		

Table A8 Selected thermodynamic data for technetium (Tc) in JAEA-TDB-RN in 2020 (3/3)

Species / compound	$\Delta_f G^0_m$ (kJ.mol^{-1})	$\Delta_f H^0_m$ (kJ.mol^{-1})	S^0_m (J.K^{-1}.mol^{-1})	$C^0_{p,m}$ (J.K^{-1}.mol^{-1})	Reaction	$\log_{10} K°$	$\Delta_r G^0_m$ (kJ.mol^{-1})	$\Delta_r H^0_m$ (kJ.mol^{-1})	$\Delta_r S^0_m$ (J.K^{-1}.mol^{-1})
$AgTcO_4$(cr)	**-578.975 ± 7.654**				$TcO_4^- + Ag^+ \rightleftarrows AgTcO_4$(cr)	3.270 ± 0.130 [2003GUI/FAN]	-18.665 ± 0.742 [2003GUI/FAN]		
$NaTcO_4 \cdot 4H_2O$(s)	**-1843.508 ± 7.631**				$TcO_4^- + 4\ H_2O(l) + Na^+ \rightleftarrows NaTcO_4 \cdot 4H_2O$(s)	-0.790 ± 0.040 [2003GUI/FAN]	4.509 ± 0.228 [2003GUI/FAN]		
$KTcO_4$(cr)	**-932.928 ± 7.618**	**-1035.190 ± 7.612**	**164.605 ± 2.132**	123.300 ± 0.250 [2003GUI/FAN]	$TcO_4^- + K^+ \rightleftarrows KTcO_4$(cr)	2.288 ± 0.026 [2003GUI/FAN]	-13.060 ± 0.148 [2003GUI/FAN]	-53.620 ± 0.420 [2003GUI/FAN]	-136.039 ± 1.494 [2003GUI/FAN]
K_2TcCl_6(cr)					$TcCl_6^{2-} + 2\ K^+ \rightleftarrows K_2TcCl_6$(cr)	9.610 ± 1.000 [2003GUI/FAN]	-54.854 ± 5.708 [2003GUI/FAN]		
K_2TcBr_6(cr)					$TcBr_6^{2-} + 2\ K^+ \rightleftarrows K_2TcBr_6$(cr)	6.920 ± 1.000 [2003GUI/FAN]	-39.500 ± 5.708 [2003GUI/FAN]		
Rb_2TcCl_6(cr)					$TcCl_6^{2-} + 2\ Rb^+ \rightleftarrows Rb_2TcCl_6$(cr)	11.120 ± 1.000 [2003GUI/FAN]	-63.473 ± 5.708 [2003GUI/FAN]		
Rb_2TcBr_6(cr)					$TcBr_6^{2-} + 2\ Rb^+ \rightleftarrows Rb_2TcBr_6$(cr)	9.470 ± 1.000 [2003GUI/FAN]	-54.055 ± 5.708 [2003GUI/FAN]		
$CsTcO_4$(cr)	**-949.719 ± 7.624**				$TcO_4^- + Cs^+ \rightleftarrows CsTcO_4$(cr)	3.617 ± 0.047 [2003GUI/FAN]	-20.646 ± 0.268 [2003GUI/FAN]		
Cs_2TcCl_6(cr)					$TcCl_6^{2-} + 2\ Cs^+ \rightleftarrows Cs_2TcCl_6$(cr)	11.430 ± 1.000 [2003GUI/FAN]	-65.243 ± 5.708 [2003GUI/FAN]		
Cs_2TcBr_6(cr)					$TcBr_6^{2-} + 2\ Cs^+ \rightleftarrows Cs_2TcBr_6$(cr)	11.240 ± 1.000 [2003GUI/FAN]	-64.158 ± 5.708 [2003GUI/FAN]		

[2003GUI/FAN] Guillaumont et al.[A15)]
[2004HES/XIA] Hess et al.[A16)]

Table A9 Selected thermodynamic data for palladium (Pd) in JAEA-TDB-RN in 2020 (1/2)

Values indicated by **boldface** are calculated and selected in the present report.

Species / compound	$\Delta_f G^0_m$ (kJ.mol^{-1})	$\Delta_f H^0_m$ (kJ.mol^{-1})	S^0_m (J.K^{-1}.mol^{-1})	$C^0_{p,m}$ (J.K^{-1}.mol^{-1})	Reaction	$\log_{10} K°$	$\Delta_r G^0_m$ (kJ.mol^{-1})	$\Delta_r H^0_m$ (kJ.mol^{-1})	$\Delta_r S^0_m$ (J.K^{-1}.mol^{-1})
Pd(cr)	0.000	0.000	37.570	25.980					
	[1982WAG/EVA]	[1982WAG/EVA]	[1982WAG/EVA]	[1982WAG/EVA]					
Pd(s)	**18.779**				$Pd^{2+} + 2\ e^- \rightleftarrows Pd(s)$	29.570	**-168.787**		
						± 1.120	**± 6.393**		
						[2012RAI/YUI]			
Pd^{2+}	**187.566**				$Pd(cr) \rightleftarrows Pd^{2+} + 2\ e^-$	-32.860	**187.566**		
						[1999LOT/OCH]			
$Pd(OH)_2(aq)$	**> -266.878**				$Pd^{2+} + 2\ H_2O(l) \rightleftarrows Pd(OH)_2(aq) + 2\ H^+$	< -3.490	**> 19.921**		
						[2012RAI/YUI]			
$Pd(OH)_2(am)$	**-307.234**				$Pd(OH)_2(am) + 2\ H^+ \rightleftarrows Pd^{2+} + 2\ H_2O(l)$	-3.580	**20.435**		
						± 0.360	**± 2.055**		
						[2012RAI/YUI]			
$Pd(OH)_2$(colloidal)	**-300.555**				$Pd(OH)_2$(colloidal) $+ 2\ H^+ \rightleftarrows Pd^{2+} + 2\ H_2O(l)$	-2.410	**13.756**		
						[2012RAI/YUI]			
$Pd(OH)_3^-$	**-435.621**				$Pd^{2+} + 3\ H_2O(l) \rightleftarrows Pd(OH)_3^- + 3\ H^+$	-15.480	**88.360**		
						± 0.350	**± 1.998**		
						[2012RAI/YUI]			
$PdCl^+$	**27.736**				$Pd^{2+} + Cl^- \rightleftarrows PdCl^+$	5.000	**-28.540**		
						± 0.240	**± 1.370**		
						[2012RAI/YUI]			
$PdCl_2(aq)$	**-123.075**				$Pd^{2+} + 2\ Cl^- \rightleftarrows PdCl_2(aq)$	8.420	**-48.062**		
						± 0.310	**± 1.769**		
						[2012RAI/YUI]			
$PdCl_3^-$	**-268.692**				$Pd^{2+} + 3\ Cl^- \rightleftarrows PdCl_3^-$	10.930	**-62.389**		
						± 0.380	**± 2.169**		
						[2012RAI/YUI]			
$PdCl_4^{2-}$	**-412.083**				$Pd^{2+} + 4\ Cl^- \rightleftarrows PdCl_4^{2-}$	13.050	**-74.490**		
						± 0.590	**± 3.368**		
						[2012RAI/YUI]			
$PdCl_3OH^{2-}$	**-465.005**				$Pd^{2+} + 3\ Cl^- + H_2O(l) \rightleftarrows PdCl_3OH^{2-} + H^+$	3.770	**-21.519**		
						± 0.626	**± 3.573**		
						[2012RAI/YUI]			
$PdNO_3^+$	**75.695**				$Pd^{2+} + NO_3^- \rightleftarrows PdNO_3^+$	0.167	**-0.953**		
						± 0.024	**± 0.137**		
						[1995FRI/PIT]			

Table A9 Selected thermodynamic data for palladium (Pd) in JAEA-TDB-RN in 2020 (2/2)

Species / compound	$\Delta_f G^0_m$ (kJ.mol^{-1})	$\Delta_f H^0_m$ (kJ.mol^{-1})	S^0_m (J.K^{-1}.mol^{-1})	$C^0_{p,m}$ (J.K^{-1}.mol^{-1})	Reaction	$\log_{10} K°$	$\Delta_r G^0_m$ (kJ.mol^{-1})	$\Delta_r H^0_m$ (kJ.mol^{-1})	$\Delta_r S^0_m$ (J.K^{-1}.mol^{-1})
$Pd(NO_3)_2(aq)$	**-29.920**				$Pd^{2+} + 2\ NO_3^- \rightleftarrows Pd(NO_3)_2(aq)$	-0.762 ± 0.039 [1995FRI/PIT]	**4.350 ± 0.223**		
$PdOHNO_3(aq)$	**-156.824**				$Pd^{2+} + NO_3^- + H_2O(l) \rightleftarrows PdOHNO_3(aq) + H^+$	-0.650 ± 0.036 [1995FRI/PIT]	**3.710 ± 0.205**		
$PdNH_3^{2+}$	**106.040**				$Pd^{2+} + NH_4^+ \rightleftarrows PdNH_3^{2+} + H^+$	0.363 [1999LOT/OCH]	**-2.072**		
$Pd(NH_3)_2^{2+}$	**28.510**				$Pd^{2+} + 2\ NH_4^+ \rightleftarrows Pd(NH_3)_2^{2+} + 2\ H^+$	0.026 [1999LOT/OCH]	**-0.148**		
$Pd(NH_3)_3^{2+}$	**-41.030**				$Pd^{2+} + 3\ NH_4^+ \rightleftarrows Pd(NH_3)_3^{2+} + 3\ H^+$	-1.711 [1999LOT/OCH]	**9.766**		
$Pd(NH_3)_4^{2+}$	**-106.573**				$Pd^{2+} + 4\ NH_4^+ \rightleftarrows Pd(NH_3)_4^{2+} + 4\ H^+$	-4.148 [1999LOT/OCH]	**23.677**		

[1982WAG/EVA] Wagman et al. [A5)]
[1995FRI/PIT] Frias et al. [A17)]
[1999LOT/OCH] Lothenbach et al. [A18)]
[2012RAI/YUI] Rai et al. [A19)]

Table A10 Selected thermodynamic data for tin (Sn) in JAEA-TDB-RN in 2020 (1/5)

Values indicated by **boldface** are calculated and selected in the present report.

Species / compound	$\Delta_f G^0_m$ (kJ.mol^{-1})	$\Delta_f H^0_m$ (kJ.mol^{-1})	S^0_m (J.K^{-1}.mol^{-1})	$C^0_{p,m}$ (J.K^{-1}.mol^{-1})	Reaction	$\log_{10} K°$	$\Delta_r G^0_m$ (kJ.mol^{-1})	$\Delta_r H^0_m$ (kJ.mol^{-1})	$\Delta_r S^0_m$ (J.K^{-1}.mol^{-1})
α-Sn	0.119	-1.980	44.140	25.800	α-Sn ⇄ Sn^{2+} + 2 e^-	**4.837**	**-27.608**	**-6.806**	**69.803**
	± 0.162	± 0.100	± 0.420	± 0.300		**± 0.265**	**± 1.515**	**± 0.843**	**± 4.205**
	[2012GAM/GAJ]	[2012GAM/GAJ]	[2012GAM/GAJ]	[2012GAM/GAJ]					
β-Sn	0.000	0.000	51.170						
			± 0.084						
	[2020JAE]	[2020JAE]	[2020JAE]						
Sn^{2+}	-27.489	-8.786	-16.736	-64.852	β-Sn ⇄ Sn^{2+} + 2 e^-	**4.816**	**-27.489**	**-8.786**	**62.763**
	± 1.506	± 0.837	± 4.184			**± 0.264**	**± 1.506**	**± 0.837**	**± 4.185**
	[2020JAE]	[2020JAE]	[2020JAE]	[2020JAE]					
Sn^{4+}	**46.613**				Sn^{2+} + 2 H^+ ⇄ Sn^{4+} + H_2(g)	-12.982	74.102		
	± 4.142					± 0.676	± 3.859		
						[2012GAM/GAJ]	[2012GAM/GAJ]		
					$Sn(OH)_4$(aq) + 4 H^+ ⇄ Sn^{4+} + 4 H_2O(l)	**-7.850**	**44.805**		
						± 0.892	**± 5.089**		
SnH_4(g)	188.065	162.800	227.800	50.316	Sn^{2+} + 4 H^+ + 6 e^- ⇄ SnH_4(g)	**-37.763**	**215.554**	**171.586**	**-147.501**
	± 2.183	± 2.100	± 2.000	± 0.300		**± 0.465**	**± 2.652**	**± 2.261**	**± 4.639**
	[2012GAM/GAJ]	[2012GAM/GAJ]	[2012GAM/GAJ]	[2012GAM/GAJ]					
SnO(romarchite)	-257.149	-285.935	57.153	47.999	Sn^{2+} + H_2O(l) ⇄ SnO(romarchite) + 2 H^+	**-1.641**	**9.365**	**10.385**	**3.993**
	± 0.837	± 0.711	± 0.293			**± 0.659**	**± 3.761**	**± 1.135**	**± 4.191**
	[2020JAE]	[2020JAE]	[2020JAE]	[2020JAE]					
SnO_2(am)	-513.879	-573.836	55.229	69.036	$Sn(OH)_4$(aq) ⇄ SnO_2(am) + 2 H_2O(l)	**7.239**	**-41.321**	**-42.610**	**-1.573**
	± 0.837	± 6.276	± 20.920	± 20.920		**± 0.535**	**± 3.053**	**± 14.035**	**± 46.779**
	[2020JAE]	[2020JAE]	[2020JAE]	[2020JAE]					
SnO_2(cass)	-519.950	-580.781	52.300	54.572	$Sn(OH)_4$(aq) ⇄ SnO_2(cass) + 2 H_2O(l)	**8.303**	**-47.392**	**-49.555**	**-4.502**
	± 0.544	± 0.418	± 1.255	± 0.879		**± 0.523**	**± 2.986**	**± 12.561**	**± 41.859**
	[2020JAE]	[2020JAE]	[2020JAE]	[2020JAE]					
$SnOH^+$	-245.182	-267.065	80.333	-53.974	Sn^{2+} + H_2O(l) ⇄ $SnOH^+$ + H^+	**-3.414**	**19.489**	**27.560**	**27.146**
	± 2.929					**± 0.577**	**± 3.295**		
	[2020JAE]	[2020JAE]	[2020JAE]	[2020JAE]					
$SnOH^{3+}$	-243.969	-282.043	-104.600	-36.401	$Sn(OH)_4$(aq) + 3 H^+ ⇄ $SnOH^{3+}$ + 3 H_2O(l)	**1.506**	**-8.594**	**-36.656**	**-91.479**
	± 1.172					**± 0.555**	**± 3.169**		
	[2020JAE]	[2020JAE]	[2020JAE]	[2020JAE]					
$Sn_3(OH)_4^{2+}$	**-999.232**				3 Sn^{2+} + 4 H_2O(l) ⇄ $Sn_3(OH)_4^{2+}$ + 4 H^+	-5.600	31.965		
	± 5.270					± 0.470	± 2.683		
						[2012GAM/GAJ]	[2012GAM/GAJ]		
$Sn(OH)_2$(aq)	**-458.016**				Sn^{2+} + 2 H_2O(l) ⇄ $Sn(OH)_2$(aq) + 2 H^+	-7.680	43.838		
	± 2.743					± 0.400	± 2.283		
						[2012GAM/GAJ]	[2012GAM/GAJ]		

Table A10 Selected thermodynamic data for tin (Sn) in JAEA-TDB-RN in 2020 (2/5)

Species / compound	$\Delta_f G^0_m$ (kJ.mol^{-1})	$\Delta_f H^0_m$ (kJ.mol^{-1})	S^0_m (J.K^{-1}.mol^{-1})	$C^0_{p,m}$ (J.K^{-1}.mol^{-1})	Reaction	$\log_{10} K°$	$\Delta_r G^0_m$ (kJ.mol^{-1})	$\Delta_r H^0_m$ (kJ.mol^{-1})	$\Delta_r S^0_m$ (J.K^{-1}.mol^{-1})
$Sn(OH)_2^{2+}$	-482.373 ± 2.929 [2020JAE]	-536.042 [2020JAE]	76.199 [2020JAE]	-186.180 [2020JAE]	$Sn(OH)_4(aq) + 2\ H^+ \rightleftarrows Sn(OH)_2^{2+} + 2\ H_2O(l)$	**1.720 ± 0.726**	**-9.816 ± 4.147**	**-4.816**	**19.397**
$Sn(OH)_3^-$	-482.373 ± 2.929 [2020JAE]	-796.621 [2020JAE]	109.253 [2020JAE]	-114.591 [2020JAE]	$Sn^{2+} + 3\ H_2O(l) \rightleftarrows Sn(OH)_3^- + 3\ H^+$	**-16.598 ± 0.398**	**94.742 ± 2.272**	**69.680**	**-83.780**
$Sn(OH)_3^+$	-482.373 ± 2.929 [2020JAE]	-806.704 [2020JAE]	178.707 [2020JAE]	-273.081 [2020JAE]	$Sn(OH)_4(aq) + H^+ \rightleftarrows Sn(OH)_3^+ + 3\ H_2O(l)$	**0.754 ± 0.779**	**-4.301 ± 4.449**	**10.360**	**51.982**
$Sn(OH)_4(aq)$	-482.373 ± 2.929 [2020JAE]	-482.373 ± 2.929 [2020JAE]	-482.373 ± 2.929 [2020JAE]	-57.572 [2020JAE]	$Sn^{2+} + 4\ H_2O(l) \rightleftarrows Sn(OH)_4(aq) + 4\ H^+ + 2\ e^-$	**-5.132 ± 0.581**	**29.296 ± 3.318**	**49.237 ± 12.587**	**64.371 ± 42.050**
$Sn(OH)_5^-$	-482.373 ± 2.929 [2020JAE]	-1379.607 [2020JAE]	144.030 [2020JAE]	40.769 [2020JAE]	$Sn(OH)_4(aq) + H_2O(l) \rightleftarrows Sn(OH)_5^- + H^+$	**-8.142 ± 0.895**	**46.476 ± 5.108**	**9.134**	**-122.541**
$Sn(OH)_6^{2-}$	-482.373 ± 2.929 [2020JAE]	-1689.838 [2020JAE]	-62.609 [2020JAE]	-62.337 [2020JAE]	$Sn(OH)_4(aq) + 2\ H_2O(l) \rightleftarrows Sn(OH)_6^{2-} + 2\ H^+$	**-18.329 ± 0.632**	**104.625 ± 3.605**	**-15.259**	**-399.103**
SnF^+	-339.205 ± 1.966 [2020JAE]	-365.096 ± 2.510 [2020JAE]	0.335 ± 4.602 [2020JAE]	15.899 ± 20.920 [2020JAE]	$Sn^{2+} + F^- \rightleftarrows SnF^+$	**5.250 ± 0.450**	**-29.966 ± 2.566**	**-20.962 ± 2.730**	**30.250 ± 6.244**
$SnF_2(aq)$	-641.742 ± 3.347 [2020JAE]	-725.296 ± 2.929 [2020JAE]	-26.317 ± 5.021 [2020JAE]	25.941 ± 20.920 [2020JAE]	$Sn^{2+} + 2\ F^- \rightleftarrows SnF_2(aq)$	**8.891 ± 0.684**	**-50.752 ± 3.907**	**-45.815 ± 3.327**	**16.778 ± 6.626**
$SnF_2(cr)$		-700.260 ± 2.169 [2012GAM/GAJ]			$Sn^{2+} + 2\ F^- \rightleftarrows SnF_2(cr)$			**-20.778 ± 2.683**	
$SnF_2(g)$	-543.387 ± 3.000 [2012GAM/GAJ]	-535.000 ± 3.000 [2012GAM/GAJ]	282.100 ± 0.100 [2012GAM/GAJ]	49.700 ± 0.100 [2012GAM/GAJ]	$Sn^{2+} + 2\ F^- \rightleftarrows SnF_2(g)$	**-8.340 ± 0.633**	**47.603 ± 3.614**	**144.482 ± 3.390**	**325.195 ± 4.324**
SnF_3^-	-938.388 ± 6.276 [2020JAE]	-1097.756 ± 6.276 [2020JAE]	-113.805 ± 5.439 [2020JAE]	-128.449 ± 29.288 [2020JAE]	$Sn^{2+} + 3\ F^- \rightleftarrows SnF_3^-$	**11.501 ± 1.184**	**-65.647 ± 6.759**	**-82.927 ± 6.642**	**-57.530 ± 7.054**
$BaSnF_4(cr)$			205.100 ± 0.300 [2012GAM/GAJ]	146.500 ± 1.600 [2012GAM/GAJ]	$Sn^{2+} + Ba^{2+} + 4\ F^- \rightleftarrows BaSnF_4(cr)$				
$PbSnF_4(cr)$			223.700 ± 0.300 [2012GAM/GAJ]	162.400 ± 0.800 [2012GAM/GAJ]	$Sn^{2+} + Pb^{2+} + 4\ F^- \rightleftarrows PbSnF_4(cr)$				
$SrSnF_4(cr)$			187.200 ± 0.300 [2012GAM/GAJ]	147.400 ± 7.600 [2012GAM/GAJ]	$Sn^{2+} + Sr^{2+} + 4\ F^- \rightleftarrows SrSnF_4(cr)$				

Table A10 Selected thermodynamic data for tin (Sn) in JAEA-TDB-RN in 2020 (3/5)

Species / compound	$\Delta_f G^0_m$ (kJ.mol^{-1})	$\Delta_f H^0_m$ (kJ.mol^{-1})	S^0_m (J.K^{-1}.mol^{-1})	$C^0_{p,m}$ (J.K^{-1}.mol^{-1})	Reaction	$\log_{10} K°$	$\Delta_r G^0_m$ (kJ.mol^{-1})	$\Delta_r H^0_m$ (kJ.mol^{-1})	$\Delta_r S^0_m$ (J.K^{-1}.mol^{-1})
$SnCl^+$	-166.816	-174.054	73.053	-2.929	$Sn^{2+} + Cl^- \rightleftarrows SnCl^+$	**1.408**	**-8.037**	**1.812**	**33.054**
	± 1.674	± 2.510	± 5.439	± 29.288		**± 0.395**	**± 2.254**	**± 2.648**	**± 6.864**
	[2020JAE]	[2020JAE]	[2020JAE]	[2020JAE]					
$SnCl_2$(aq)	-303.214	-344.343	136.273	-38.911	$Sn^{2+} + 2\ Cl^- \rightleftarrows SnCl_2$(aq)	**2.303**	**-13.146**	**-1.397**	**39.539**
	± 0.962	± 2.092	± 6.694	± 33.472		**± 0.315**	**± 1.799**	**± 2.260**	**± 7.901**
	[2020JAE]	[2020JAE]	[2020JAE]	[2020JAE]					
$SnCl_2$(cr)	-286.069	-327.900	133.960	77.960	$Sn^{2+} + 2\ Cl^- \rightleftarrows SnCl_2$(cr)	**-0.701**	**3.999**	**15.046**	**37.226**
	± 2.206	± 2.200	± 0.530	± 0.310		**± 0.469**	**± 2.679**	**± 2.360**	**± 4.231**
	[2012GAM/GAJ]	[2012GAM/GAJ]	[2012GAM/GAJ]	[2012GAM/GAJ]					
$SnCl_2$(g)	-206.933	-197.500	305.900	54.600	$Sn^{2+} + 2\ Cl^- \rightleftarrows SnCl_2$(g)	**-14.565**	**83.135**	**145.446**	**209.166**
	± 4.300	± 4.300	± 0.100	± 0.100		**± 0.799**	**± 4.561**	**± 4.384**	**± 4.199**
	[2012GAM/GAJ]	[2012GAM/GAJ]	[2012GAM/GAJ]	[2012GAM/GAJ]					
$SnCl_2{\cdot}2H_2O$(cr)	-760.532	-918.260	211.750	166.400	$Sn^{2+} + 2\ Cl^- + 2\ H_2O$(l) $\rightleftarrows SnCl_2{\cdot}2H_2O$(cr)	**-0.684**	**3.902**	**-3.638**	**-24.830**
	± 1.489	± 1.420	± 1.500	± 0.500		**± 0.374**	**± 2.137**	**± 1.671**	**± 4.460**
	[2012GAM/GAJ]	[2012GAM/GAJ]	[2012GAM/GAJ]	[2012GAM/GAJ]					
$SnCl_3^-$	-433.588	-516.180	174.054	-142.256	$Sn^{2+} + 3\ Cl^- \rightleftarrows SnCl_3^-$	**2.143**	**-12.230**	**-6.155**	**20.585**
	± 1.966	± 3.347	± 8.368	± 33.472		**± 0.437**	**± 2.495**	**± 3.460**	**± 9.369**
	[2020JAE]	[2020JAE]	[2020JAE]	[2020JAE]					
$SnCl_4$(g)	-439.609	-478.500	366.900	98.400	$Sn^{2+} + 4\ Cl^- \rightleftarrows SnCl_4$(g) + 2 e^-	**-19.803**	**113.039**	**198.605**	**287.375**
	± 3.500	± 3.500	± 0.100	± 0.100		**± 0.671**	**± 3.831**	**± 3.616**	**± 4.239**
	[2012GAM/GAJ]	[2012GAM/GAJ]	[2012GAM/GAJ]	[2012GAM/GAJ]					
$SnCl_4$(l)		-517.000							
		± 2.000							
		[2012GAM/GAJ]							
$SnCl_4^{2-}$	-564.254	-696.092	185.770	-280.746	$Sn^{2+} + 4\ Cl^- \rightleftarrows SnCl_4^{2-}$	**2.033**	**-11.606**	**-18.987**	**-24.435**
	± 2.929	± 4.602	± 12.552	± 12.552		**± 0.581**	**± 3.318**	**± 4.691**	**± 13.248**
	[2020JAE]	[2020JAE]	[2020JAE]	[2020JAE]					
SnOHCl(aq)	-384.008	-445.178	125.520	-52.886	$Sn^{2+} + Cl^- + H_2O$(l) $\rightleftarrows$ SnOHCl(aq) + H^+	**-2.094**	**11.954**	**16.527**	**15.598**
	± 2.092	± 25.104	± 83.680			**± 0.452**	**± 2.582**	**± 25.118**	**± 83.785**
	[2020JAE]	[2020JAE]	[2020JAE]	[2020JAE]					
$Sn_{21}Cl_{16}(OH)_{14}O_6$(cr)	**-7615.742**				21 Sn^{2+} + 16 Cl^- + 20 H_2O(l)	34.020	-194.188		
	± 37.081				$\rightleftarrows Sn_{21}Cl_{16}(OH)_{14}O_6$(cr) + 26 H^+	± 3.360	± 19.179		
						[2012GAM/GAJ]	[2012GAM/GAJ]		
$SnBr^+$	-139.118	-151.586	96.274	4.184	$Sn^{2+} + Br^- \rightleftarrows SnBr^+$	**1.329**	**-7.586**	**-21.297**	**30.167**
	± 1.841	± 2.929	± 8.368	± 125.520		**± 0.418**	**± 2.385**	**± 3.050**	**± 9.358**
	[2020JAE]	[2020JAE]	[2020JAE]	[2020JAE]					
$SnBr_2$(aq)	-246.814	-292.838	201.250	-46.024	$Sn^{2+} + 2\ Br^- \rightleftarrows SnBr_2$(aq)	**1.969**	**-11.238**	**-41.045**	**52.300**
	± 1.966	± 11.297	± 37.656	± 209.200		**± 0.438**	**± 2.500**	**± 11.332**	**± 37.890**
	[2020JAE]	[2020JAE]	[2020JAE]	[2020JAE]					
$SnBr_2$(cr)	-237.876	-252.900	153.000	78.970	$Sn^{2+} + 2\ Br^- \rightleftarrows SnBr_2$(cr)	**0.403**	**-2.300**	**-1.107**	**4.050**
	± 2.304	± 2.300	± 0.300	± 0.160		**± 0.486**	**± 2.773**	**± 2.466**	**± 4.216**
	[2012GAM/GAJ]	[2012GAM/GAJ]	[2012GAM/GAJ]	[2012GAM/GAJ]					

Table A10 Selected thermodynamic data for tin (Sn) in JAEA-TDB-RN in 2020 (4/5)

Species / compound	$\Delta_f G^0_m$ (kJ.mol^{-1})	$\Delta_f H^0_m$ (kJ.mol^{-1})	S^0_m (J.K^{-1}.mol^{-1})	$C^0_{p,m}$ (J.K^{-1}.mol^{-1})	Reaction	$\log_{10} K°$	$\Delta_r G^0_m$ (kJ.mol^{-1})	$\Delta_r H^0_m$ (kJ.mol^{-1})	$\Delta_r S^0_m$ (J.K^{-1}.mol^{-1})
$SnBr_2$(g)	-155.751	-118.300	329.000	56.400	$Sn^{2+} + 2\ Br^- \rightleftarrows SnBr_2$(g)	**-13.985**	**79.825**	**133.493**	**180.050**
	± 4.301	± 4.300	± 0.100	± 0.100		**± 0.801**	**± 4.569**	**± 4.391**	**± 4.206**
	[2012GAM/GAJ]	[2012GAM/GAJ]	[2012GAM/GAJ]	[2012GAM/GAJ]					
$SnBr_3^-$	-350.619	-433.044	297.064	-209.200	$Sn^{2+} + 3\ Br^- \rightleftarrows SnBr_3^-$	**-14.745**	**84.166**	**106.800**	**76.042**
	± 2.092	± 16.736	± 54.392	± 292.880		**± 0.601**	**± 3.428**	**± 3.172**	**± 4.275**
	[2020JAE]	[2020JAE]	[2020JAE]	[2020JAE]					
$SnBr_4$(cr)	-359.497	-388.000	260.000	136.000	$Sn^{2+} + 4\ Br^- \rightleftarrows SnBr_4$(cr) + 2 e^-	**-14.745**	**84.166**	**106.800**	**76.042**
	± 3.006	± 3.000	± 0.260	± 0.500		**± 0.601**	**± 3.428**	**± 3.172**	**± 4.275**
	[2012GAM/GAJ]	[2012GAM/GAJ]	[2012GAM/GAJ]	[2012GAM/GAJ]					
$SnBr_4$(g)	-341.373	-324.200	413.200	103.300	$Sn^{2+} + 4\ Br^- \rightleftarrows SnBr_4$(g) + 2 e^-	**-17.920**	**102.290**	**170.600**	**229.242**
	± 4.504	± 4.500	± 0.100	± 0.200		**± 0.840**	**± 4.796**	**± 4.617**	**± 4.268**
	[2012GAM/GAJ]	[2012GAM/GAJ]	[2012GAM/GAJ]	[2012GAM/GAJ]					
$SnIn_2$(cr)	-153.143	-153.000	168.800	78.450					
	± 2.917	± 2.900	± 1.000	± 0.160					
	[2012GAM/GAJ]	[2012GAM/GAJ]	[2012GAM/GAJ]	[2012GAM/GAJ]					
$SnIn_2$(g)	-60.390	-8.100	342.700	56.700	$SnIn_2$(cr) ⇄ $SnIn_2$(g)			144.900	
	± 3.102	± 3.100	± 0.100	± 0.100				± 2.500	
	[2012GAM/GAJ]	[2012GAM/GAJ]	[2012GAM/GAJ]	[2012GAM/GAJ]				[2012GAM/GAJ]	
$SnIn_4$(cr)	-207.476	-207.700	282.710	131.960					
	± 2.623	± 2.600	± 1.000	± 0.260					
	[2012GAM/GAJ]	[2012GAM/GAJ]	[2012GAM/GAJ]	[2012GAM/GAJ]					
$SnIn_4$(g)	-168.166	-118.900	448.700	105.500	$SnIn_4$(cr) ⇄ $SnIn_4$(g)			88.600	
	± 4.005	± 4.000	± 0.200	± 0.200				± 2.600	
	[2012GAM/GAJ]	[2012GAM/GAJ]	[2012GAM/GAJ]	[2012GAM/GAJ]				[2012GAM/GAJ]	
SnS(herzenbergite)	-106.064	-107.947	76.986	49.258	SnS(herzenbergite) + $H^+ \rightleftarrows Sn^{2+} + HS^-$	**-15.862**	**90.542**	**83.052**	**-25.522**
	± 2.092	± 2.092	± 0.837			**± 0.458**	**± 2.612**		
	[2020JAE]	[2020JAE]	[2020JAE]	[2020JAE]					
Sn_2S_3(cr)	-253.588	-264.000	163.600	118.500	Sn_2S_3(cr) + 3 H^+ + 2 $e^- \rightleftarrows$ 2 Sn^{2+} + 3 HS^-	**-41.084**	**234.509**	**198.102**	**-123.153**
	± 21.076	± 21.000	± 6.000	± 1.600		**± 3.736**	**± 21.327**		
	[2012GAM/GAJ]	[2012GAM/GAJ]	[2012GAM/GAJ]	[2012GAM/GAJ]					
SnS_2(berndtite)	-145.185	-153.553	87.446	70.124	SnS_2(berndtite) + 2 H^+ + 2 $e^- \rightleftarrows Sn^{2+}$ + 2 HS^-	**-24.812**	**141.628**	**112.550**	**-98.462**
	± 4.184	± 4.184	± 0.167	± 0.628		**± 0.793**	**± 4.525**		
	[2020JAE]	[2020JAE]	[2020JAE]	[2020JAE]					
$Cu_2Sn_4S_9$(cr)	-165.599	-141.600	640.000		$Cu_2Sn_4S_9$(cr) + 9 H^+ + 6 $e^- \rightleftarrows$ 4 Sn^{2+} + 2 Cu^{2+} + 9 HS^-	**-51.595**	**294.508**	**92.856**	**-679.325**
	± 8.278	± 6.300	± 18.000			**± 1.913**	**± 10.917**		
	[2012GAM/GAJ]	[2012GAM/GAJ]	[2012GAM/GAJ]						
Cu_2SnS_3(cr)	-169.486	-150.000	279.000		Cu_2SnS_3(cr) + 3 $H^+ \rightleftarrows Sn^{2+}$ + 2 Cu^{2+} + 3 HS^-	**-54.145**	**309.064**	**224.266**	**-285.276**
	± 5.509	± 5.500	± 1.000			**± 1.027**	**± 5.862**		
	[2012GAM/GAJ]	[2012GAM/GAJ]	[2012GAM/GAJ]						
Cu_4SnS_4(cr)	-251.212	-220.800	414.000	230.000	Cu_4SnS_4(cr) + 4 $H^+ \rightleftarrows Sn^{2+}$ + 4 Cu^{2+} + 4 HS^- + 2 e^-	**-93.539**	**533.925**	**410.335**	**-415.536**
	± 11.132	± 9.400	± 20.000	± 0.200		**± 1.995**	**± 11.388**		
	[2012GAM/GAJ]	[2012GAM/GAJ]	[2012GAM/GAJ]	[2012GAM/GAJ]					

Table A10 Selected thermodynamic data for tin (Sn) in JAEA-TDB-RN in 2020 (5/5)

Species / compound	$\Delta_f G^0_m$ (kJ.mol^{-1})	$\Delta_f H^0_m$ (kJ.mol^{-1})	S^0_m (J.K^{-1}.mol^{-1})	$C^0_{p,m}$ (J.K^{-1}.mol^{-1})	Reaction	$\log_{10} K°$	$\Delta_r G^0_m$ (kJ.mol^{-1})	$\Delta_r H^0_m$ (kJ.mol^{-1})	$\Delta_r S^0_m$ (J.K^{-1}.mol^{-1})
Cu_8SnS_6(cr)				365.000 ± 29.000 [2012GAM/GAJ]					
$SnSO_4$(aq)	-791.529 ± 2.092 [2020JAE]	-919.016 ± 4.602 [2020JAE]	66.024 ± 13.389 [2020JAE]	-148.532 ± 83.680 [2020JAE]	$Sn^{2+} + SO_4^{2-} \rightleftarrows SnSO_4$(aq)	**3.430 ± 0.459**	**-19.581 ± 2.619**	**-0.628 ± 4.697**	**63.932 ± 14.036**
$Sn_3(OH)_2OSO_4$(cr)	-1566.191 ± 2.337 [2012GAM/GAJ]				$Sn_3(OH)_2OSO_4$(cr) + 4 $H^+ \rightleftarrows$ 3 $Sn^{2+} + SO_4^{2-}$ + 3 H_2O(l)	**-4.856 ± 0.896**	**27.717 ± 5.117**		
$SnSCN^+$	**56.834 ± 9.395**				$Sn^{2+} + SCN^- \rightleftarrows SnSCN^+$	1.500 ± 0.700 [2012GAM/GAJ]	-8.562 ± 3.996 [2012GAM/GAJ]		
$SnNO_3^+$	-145.645 ± 3.347 [2020JAE]	-213.342 ± 7.113 [2020JAE]	162.339 ± 20.920 [2020JAE]	108.784 ± 104.600 [2020JAE]	$Sn^{2+} + NO_3^- \rightleftarrows SnNO_3^+$	**1.268 ± 0.779**	**-7.238 ± 4.447**	**2.343 ± 7.174**	**32.133 ± 21.351**
$Sn(NO_3)_2$(aq)	-257.274 ± 5.858 [2020JAE]	-408.317 ± 9.205 [2020JAE]	351.498 ± 23.849 [2020JAE]	317.984 ± 292.880 [2020JAE]	Sn^{2+} + 2 $NO_3^- \rightleftarrows Sn(NO_3)_2$(aq)	**1.393 ± 1.377**	**-7.950 ± 7.861**	**14.267 ± 9.281**	**74.350 ± 24.271**
$Ag_6Sn_4P_{12}Ge_6$(cr)	-76.485 ± 8.063 [2012GAM/GAJ]	-147.000 ± 7.000 [2012GAM/GAJ]	903.130 ± 13.000 [2012GAM/GAJ]	628.820 ± 9.400 [2012GAM/GAJ]					
Sn_4As_3(cr)			327.000 ± 1.600 [2012GAM/GAJ]	180.500 ± 0.900 [2012GAM/GAJ]					
SnAs(cr)	-10.013 ± 3.209 [2012GAM/GAJ]	-9.500 ± 3.200 [2012GAM/GAJ]	88.000 ± 0.500 [2012GAM/GAJ]	51.200 ± 0.260 [2012GAM/GAJ]	SnAs(cr) + 4 H_2O(l) $\rightleftarrows$ $Sn^{2+} + AsO_4^{3-}$ + 8 H^+ + 7 e^-	**-49.561 ± 0.940**	**282.894 ± 5.366**	**255.927 ± 5.207**	**-89.852 ± 4.271**

[2012GAM/GAJ] Gamsjäger et al.[A20)]
[2020JAE] Japan Atomic Energy Agency [A1)].

Table A11 Selected thermodynamic data for antimony (Sb) in JAEA-TDB-RN in 2020 (1/2)

Values indicated by **boldface** are calculated and selected in the present report.

Species / compound	$\Delta_f G^0_m$ (kJ.mol^{-1})	$\Delta_f H^0_m$ (kJ.mol^{-1})	S^0_m (J.K^{-1}.mol^{-1})	$C^0_{p,m}$ (J.K^{-1}.mol^{-1})	Reaction	$\log_{10} K°$	$\Delta_r G^0_m$ (kJ.mol^{-1})	$\Delta_r H^0_m$ (kJ.mol^{-1})	$\Delta_r S^0_m$ (J.K^{-1}.mol^{-1})
Sb(cr)	0.000	0.000	45.520 ± 0.210 [2003GUI/FAN]	25.260 ± 0.200 [2003GUI/FAN]					
$Sb(OH)_3$(aq)	**-643.108**				Sb(cr) + 3 H_2O(l) ⇄ $Sb(OH)_3$(aq) + 3 H^+ + 3 e^-	-11.990	**68.439**		
Sb^{3+}	**72.606**				$Sb(OH)_3$(aq) + 3 H^+ ⇄ Sb^{3+} + 3 H_2O(l)	[1999LOT/OCH] -0.730	**4.167**		
Sb_2O_3(valentinite)	**-624.443**				2 $Sb(OH)_3$(aq) ⇄ Sb_2O_3(valentinite) + 3 H_2O(l)	[1999LOT/OCH] 8.720	**-49.774**		
Sb_2O_5(am)	**-841.946**				2 $Sb(OH)_5$(aq) ⇄ Sb_2O_5(am) + 5 H_2O(l)	[1999LOT/OCH] 7.400	**-42.240**		
$SbOH^{2+}$	**-173.481**				$Sb(OH)_3$(aq) + 2 H^+ ⇄ $SbOH^{2+}$ + 2 H_2O(l)	[1999LOT/OCH] 0.830	**-4.738**		
$Sb(OH)_2^+$	**-413.346**				$Sb(OH)_3$(aq) + H^+ ⇄ $Sb(OH)_2^+$ + H_2O(l)	[1999LOT/OCH] 1.300	**-7.420**		
$Sb(OH)_4^-$	**-1523.742**				$Sb(OH)_3$(aq) + H_2O(l) ⇄ $Sb(OH)_4^-$ + H^+	[1999LOT/OCH] -11.930	**68.097**		
$Sb(OH)_5$(aq)	**-992.810**				$Sb(OH)_3$(aq) + 2 H_2O(l) ⇄ $Sb(OH)_5$(aq) + 2 H^+ + 2 e^-	[1999LOT/OCH] -21.840	**124.664**		
$Sb(OH)_6^-$	**-1214.467**				$Sb(OH)_5$(aq) + H_2O(l) ⇄ $Sb(OH)_6^-$ + H^+	[1999LOT/OCH] -2.720	**15.526**		
$Sb_2(OH)_6$(aq)	**-1286.673**				2 $Sb(OH)_3$(aq) ⇄ $Sb_2(OH)_6$(aq)	[1999LOT/OCH] 0.080	**-0.457**		
$Sb_{12}(OH)_{64}^{4-}$	**-12978.551**				12 $Sb(OH)_5$(aq) + 4 H_2O(l) ⇄ $Sb_{12}(OH)_{64}^{4-}$ + 4 H^+	[1999LOT/OCH] 20.340	**-116.102**		
$Sb_{12}(OH)_{65}^{5-}$	**-13195.070**				12 $Sb(OH)_5$(aq) + 5 H_2O(l) ⇄ $Sb_{12}(OH)_{65}^{5-}$ + 5 H^+	[1999LOT/OCH] 16.720	**-95.438**		
						[1999LOT/OCH]			

Table A11 Selected thermodynamic data for antimony (Sb) in JAEA-TDB-RN in 2020 (2/2)

Species / compound	$\Delta_f G^0_m$ (kJ.mol^{-1})	$\Delta_f H^0_m$ (kJ.mol^{-1})	S^0_m (J.K^{-1}.mol^{-1})	$C^0_{p,m}$ (J.K^{-1}.mol^{-1})	Reaction	$\log_{10} K°$	$\Delta_r G^0_m$ (kJ.mol^{-1})	$\Delta_r H^0_m$ (kJ.mol^{-1})	$\Delta_r S^0_m$ (J.K^{-1}.mol^{-1})
$Sb_{12}(OH)_{66}^{6-}$	**-13404.683**				12 $Sb(OH)_5$(aq) + 6 H_2O(l) ⇄ $Sb_{12}(OH)_{66}^{6-}$ + 6 H^+	11.890 [1999LOT/OCH]	**-67.869**		
$Sb_{12}(OH)_{67}^{7-}$	**-13608.645**				12 $Sb(OH)_5$(aq) + 7 H_2O(l) ⇄ $Sb_{12}(OH)_{67}^{7-}$ + 7 H^+	6.070 [1999LOT/OCH]	**-34.648**		
SbF^{2+}	**-961.847**				$Sb(OH)_3$(aq) + 3 H^+ + F^- ⇄ SbF^{2+} + 3 H_2O(l)	6.480 [1999LOT/OCH]	**-36.988**		
SbF_2^+	**-1278.816**				$Sb(OH)_3$(aq) + 3 H^+ + 2 F^- ⇄ SbF_2^+ + 3 H2O(l)	12.650 [1999LOT/OCH]	**-72.207**		
SbF_3(aq)	**-1593.160**				$Sb(OH)_3$(aq) + 3 H^+ + 3 F^- ⇄ SbF_3(aq) + 3 H_2O(l)	18.360 [1999LOT/OCH]	**-104.800**		
$SbCl^{2+}$	**-790.266**				$Sb(OH)_3$(aq) + 3 H^+ + Cl^- ⇄ $SbCl^{2+}$ + 3 H_2O(l)	2.780 [1999LOT/OCH]	**-15.868**		
$SbCl_2^+$	**-924.353**				$Sb(OH)_3$(aq) + 3 H^+ + 2 Cl^- ⇄ $SbCl_2^+$ + 3 H_2O(l)	3.270 [1999LOT/OCH]	**-18.665**		
Sb_2S_3(stibnite)	**602.447**				2 $Sb(OH)_3$(aq) + 3 SO_4^{2-} + 30 H^+ + 24 e^- ⇄ Sb_2S_3(stibnite) + 18 H_2O(l)	156.219 [1999LOT/OCH]	**-891.705**		
$Sb_2S_4^{2-}$	**585.089**				2 $Sb(OH)_3$(aq) + 2 H^+ + 4 HS^- ⇄ $Sb_2S_4^{2-}$ + 6 H_2O(l)	42.530 [1999LOT/OCH]	**-242.763**		
$HSb_2S_4^-$	**530.007**				2 $Sb(OH)_3$(aq) + 3 H^+ + 4 HS^- ⇄ $HSb_2S_4^-$ + 6 H_2O(l)	52.180 [1999LOT/OCH]	**-297.846**		
$H_2Sb_2S_4$(aq)	**502.494**				2 $Sb(OH)_3$(aq) + 4 H^+ + 4 HS^- ⇄ $H_2Sb_2S_4$(aq) + 6 H_2O(l)	57.000 [1999LOT/OCH]	**-325.358**		

[1999LOT/OCH] Lothenbach et al.[A18)]
[2003GUI/FAN] Guillaumont et al.[A15)]

Table A12 Selected thermodynamic data for samarium (Sm) in JAEA-TDB-RN in 2020 (1/2)

Values indicated by **boldface** are calculated and selected in the present report.

Species / compound	$\Delta_f G^0_m$ (kJ.mol^{-1})	$\Delta_f H^0_m$ (kJ.mol^{-1})	S^0_m (J.K^{-1}.mol^{-1})	$C^0_{p,m}$ (J.K^{-1}.mol^{-1})	Reaction	$\log_{10} K°$	$\Delta_r G^0_m$ (kJ.mol^{-1})	$\Delta_r H^0_m$ (kJ.mol^{-1})	$\Delta_r S^0_m$ (J.K^{-1}.mol^{-1})
Sm(cr)	0.000	0.000	69.580	29.540					
Sm^{3+}	[1982WAG/EVA] -666.600	[1982WAG/EVA] -691.600	[1982WAG/EVA] -211.700	[1982WAG/EVA] -21.000	Sm(cr) ⇄ Sm^{3+} + 3 e^-	**116.783**	**-666.600**	**-691.600**	**-85.262**
$SmOH^{2+}$	[1982WAG/EVA] **-862.685**	[1982WAG/EVA]	[1982WAG/EVA]	[1982WAG/EVA]	Sm^{3+} + H_2O(l) ⇄ $SmOH^{2+}$ + H^+	-7.200 ± 0.500 [2010KIT/FUJ2]	**41.098 ± 2.854**		
$Sm(OH)_2^+$	**-1054.774**				Sm^{3+} + 2 H_2O(l) ⇄ $Sm(OH)_2^+$ + 2 H^+	-15.100 ± 0.700 [2010KIT/FUJ2]	**86.191 ± 3.996**		
$Sm(OH)_3$(am)	**-1281.682**				Sm^{3+} + 3 H_2O(l) ⇄ $Sm(OH)_3$(am) + 3 H^+	-16.900 ± 0.800 [2010KIT/FUJ2]	**96.466 ± 4.566**		
$Sm(OH)_3$(cr)	**-1289.102**				Sm^{3+} + 3 H_2O(l) ⇄ $Sm(OH)_3$(cr) + 3 H^+	-15.600 ± 0.600 [2010KIT/FUJ2]	**89.045 ± 3.425**		
$Sm(OH)_3$(aq)	**-1228.597**				Sm^{3+} + 3 H_2O(l) ⇄ $Sm(OH)_3$(aq) + 3 H^+	-26.200 ± 0.500 [2010KIT/FUJ2]	**149.551 ± 2.854**		
SmF^{2+}	**-967.758**				Sm^{3+} + F^- ⇄ SmF^{2+}	3.400 ± 0.400 [2010KIT/FUJ2]	**-19.407 ± 2.283**		
SmF_2^+	**-1263.208**				Sm^{3+} + 2 F^- ⇄ SmF_2^+	5.800 ± 0.200 [2010KIT/FUJ2]	**-33.107 ± 1.142**		
$SmCl^{2+}$	**-799.260**				Sm^{3+} + Cl^- ⇄ $SmCl^{2+}$	0.240 ± 0.030 [2010KIT/FUJ2]	**-1.370 ± 0.171**		
$SmCl_2^+$	**-924.956**				Sm^{3+} + 2 Cl^- ⇄ $SmCl_2^+$	-0.740 ± 0.050 [2010KIT/FUJ2]	**4.224 ± 0.285**		
$SmSO_4^+$	**-1429.896**				Sm^{3+} + SO_4^{2-} ⇄ $SmSO_4^+$	3.300 ± 0.150 [2010KIT/FUJ2]	**-18.837 ± 0.856**		
$Sm(SO_4)_2^-$	**-2176.638**				Sm^{3+} + 2 SO_4^{2-} ⇄ $Sm(SO_4)_2^-$	3.700 ± 0.150 [2010KIT/FUJ2]	**-21.120 ± 0.856**		
SmN_3^{2+}	**-327.932**				Sm^{3+} + N_3^- ⇄ SmN_3^{2+}	1.670 ± 0.100 [2010KIT/FUJ2]	**-9.532 ± 0.571**		

Table A12 Selected thermodynamic data for samarium (Sm) in JAEA-TDB-RN in 2020 (2/2)

Species / compound	$\Delta_f G^0_m$ (kJ.mol^{-1})	$\Delta_f H^0_m$ (kJ.mol^{-1})	S^0_m (J.K^{-1}.mol^{-1})	$C^0_{p,m}$ (J.K^{-1}.mol^{-1})	Reaction	$\log_{10} K°$	$\Delta_r G^0_m$ (kJ.mol^{-1})	$\Delta_r H^0_m$ (kJ.mol^{-1})	$\Delta_r S^0_m$ (J.K^{-1}.mol^{-1})
$SmNO_2^{2+}$	**-710.804**				$Sm^{3+} + NO_2^- \rightleftarrows SmNO_2^{2+}$	2.100	**-11.987**		
						± 0.200	**± 1.142**		
						[2010KIT/FUJ2]			
$SmNO_3^{2+}$	**-785.110**				$Sm^{3+} + NO_3^- \rightleftarrows SmNO_3^{2+}$	1.330	**-7.592**		
						± 0.200	**± 1.142**		
						[2010KIT/FUJ2]			
$SmPO_4$(am,hydr)	**-1826.906**				$Sm^{3+} + PO_4^{3-} \rightleftarrows SmPO_4$(am,hydr)	24.790	**-141.502**		
						± 0.600	**± 3.425**		
						[2010KIT/FUJ2]			
$SmH_2PO_4^{2+}$	**-1814.189**				$Sm^{3+} + 2\ H^+ + PO_4^{3-} \rightleftarrows SmH_2PO_4^{2+}$	22.562	**-128.785**		
						± 0.501	**± 2.860**		
						[2010KIT/FUJ2]			
$SmCO_3^+$	**-1240.247**				$Sm^{3+} + CO_3^{2-} \rightleftarrows SmCO_3^+$	8.000	**-45.664**		
						± 0.400	**± 2.283**		
						[2010KIT/FUJ2]			
$Sm(CO_3)_2^-$	**-1796.200**				$Sm^{3+} + 2\ CO_3^{2-} \rightleftarrows Sm(CO_3)_2^-$	12.900	**-73.634**		
						± 0.600	**± 3.425**		
						[2010KIT/FUJ2]			
$Sm(CO_3)_3^{3-}$	**-2336.170**				$Sm^{3+} + 3\ CO_3^{2-} \rightleftarrows Sm(CO_3)_3^{3-}$	15.000	**-85.621**		
						± 1.000	**± 5.708**		
						[2010KIT/FUJ2]			
$Sm_2(CO_3)_3$(am)	**-2726.501**				$2\ Sm^{3+} + 3\ CO_3^{2-} \rightleftarrows Sm_2(CO_3)_3$(am)	33.400	**-190.649**		
						± 1.100	**± 6.279**		
						[2010KIT/FUJ2]			
$SmHCO_3^{2+}$	**-1271.236**				$Sm^{3+} + H^+ + CO_3^{2-} \rightleftarrows SmHCO_3^{2+}$	13.429	**-76.653**		
						± 0.301	**± 1.718**		
						[2010KIT/FUJ2]			
$SmCO_3OH$(am)	**-1396.382**				$Sm^{3+} + CO_3^{2-} + H_2O(l) \rightleftarrows SmCO_3OH$(am) $+ H^+$	6.199	**-35.384**		
						± 1.000	**± 5.708**		
						[2010KIT/FUJ2]			
$SmCO_3OH•0.5H_2O$(cr)	**-1502.415**				$Sm^{3+} + CO_3^{2-} + 1.5\ H_2O(l) \rightleftarrows SmCO_3OH•0.5H_2O$(cr) $+ H^+$	8.399	**-47.942**		
						± 0.500	**± 2.854**		
						[2010KIT/FUJ2]			
$SmSiO(OH)_3^{2+}$	**-1964.783**				$Sm^{3+} + H_4SiO_4(aq) \rightleftarrows SmSiO(OH)_3^{2+} + H^+$	-1.680	**9.590**		
						± 0.180	**± 1.027**		
						[2010KIT/FUJ2]			
$SmSCN^{2+}$	**-581.136**				$Sm^{3+} + SCN^- \rightleftarrows SmSCN^{2+}$	1.300	**-7.420**		
						± 0.300	**± 1.712**		
						[2010KIT/FUJ2]			
$NaSm(CO_3)_2•5H_2O$(cr)	**-3050.491**				$Sm^{3+} + 2\ CO_3^{2-} + 5\ H_2O(l) + Na^+ \rightleftarrows NaSm(CO_3)_2•5H_2O$(cr)	21.000	**-119.869**		
						± 0.500	**± 2.854**		
						[2010KIT/FUJ2]			

[1982WAG/EVA] Wagman et al. [A5)]
[2010KIT/FUJ2] Kitamura et al.[A21)]

Table A13 Selected thermodynamic data for bismuth (Bi) in JAEA-TDB-RN in 2020 (1/3)

Values indicated by **boldface** are calculated and selected in the present report.

Species / compound	$\Delta_f G^0_m$ (kJ.mol^{-1})	$\Delta_f H^0_m$ (kJ.mol^{-1})	S^0_m (J.K^{-1}.mol^{-1})	$C^0_{p,m}$ (J.K^{-1}.mol^{-1})	Reaction	$\log_{10} K°$	$\Delta_r G^0_m$ (kJ.mol^{-1})	$\Delta_r H^0_m$ (kJ.mol^{-1})	$\Delta_r S^0_m$ (J.K^{-1}.mol^{-1})
Bi(cr)	0.000		56.740 ± 0.420 [2003GUI/FAN]	25.410 ± 0.200 [2003GUI/FAN]					
Bi^{3+}	**95.553**				$Bi(cr) \rightleftarrows Bi^{3+} + 3\ e^-$	-16.740	**95.553**		
α-Bi_2O_3(cr)	**-160.824**				$Bi^{3+} + 1.5\ H_2O(l) \rightleftarrows 0.5\ \alpha\text{-}Bi_2O_3(cr) + 3\ H^+$	[1999LOT/OCH] -31.501 ± 0.927	**179.809 ± 5.291**		
$BiOH^{2+}$	**-136.379**				$Bi^{3+} + H_2O(l) \rightleftarrows BiOH^{2+} + H^+$	[2010RAI/YUI] -0.920	**5.251**		
$Bi(OH)_2^+$	**-364.200**				$Bi^{3+} + 2\ H_2O(l) \rightleftarrows Bi(OH)_2^+ + 2\ H^+$	[1999LOT/OCH] -2.560 ± 1.000	**14.613 ± 5.708**		
$Bi(OH)_3$(am)	**-436.186**				$Bi^{3+} + 3\ H_2O(l) \rightleftarrows Bi(OH)_3(am) + 3\ H^+$	[2010RAI/YUI] -31.501 ± 0.927	**179.809 ± 5.291**		
$Bi(OH)_3$(aq)	**-564.965**				$Bi^{3+} + 3\ H_2O(l) \rightleftarrows Bi(OH)_3(aq) + 3\ H^+$	[2010RAI/YUI] -8.940 ± 0.500	**51.030 ± 2.854**		
$Bi(OH)_4^-$	**-729.542**				$Bi^{3+} + 4\ H_2O(l) \rightleftarrows Bi(OH)_4^- + 4\ H^+$	[2010RAI/YUI] -21.660 ± 0.870	**123.636 ± 4.966**		
$Bi_6(OH)_{12}^{6+}$	**-2280.524**				$6\ Bi^{3+} + 12\ H_2O(l) \rightleftarrows Bi_6(OH)_{12}^{6+} + 12\ H^+$	[2010RAI/YUI] 1.340	**-7.649**		
$Bi_9(OH)_{20}^{7+}$	**-3875.915**				$9\ Bi^{3+} + 20\ H_2O(l) \rightleftarrows Bi_9(OH)_{20}^{7+} + 20\ H^+$	[1999LOT/OCH] -1.360	**7.763**		
$Bi_9(OH)_{21}^{6+}$	**-4102.310**				$9\ Bi^{3+} + 21\ H_2O(l) \rightleftarrows Bi_9(OH)_{21}^{6+} + 21\ H^+$	[1999LOT/OCH] -3.250	**18.551**		
$Bi_9(OH)_{22}^{5+}$	**-4330.302**				$9\ Bi^{3+} + 22\ H_2O(l) \rightleftarrows Bi_9(OH)_{22}^{5+} + 22\ H^+$	[1999LOT/OCH] -4.860	**27.741**		
$Bi_3(OH)_4^{5+}$	**-657.506**				$3\ Bi^{3+} + 4\ H_2O(l) \rightleftarrows Bi_3(OH)_4^{5+} + 4\ H^+$	[1999LOT/OCH] -0.800	**4.566**		

Table A13 Selected thermodynamic data for bismuth (Bi) in JAEA-TDB-RN in 2020 (2/3)

Species / compound	$\Delta_f G^0_m$ (kJ.mol^{-1})	$\Delta_f H^0_m$ (kJ.mol^{-1})	S^0_m (J.K^{-1}.mol^{-1})	$C^0_{p,m}$ (J.K^{-1}.mol^{-1})	Reaction	$\log_{10} K°$	$\Delta_r G^0_m$ (kJ.mol^{-1})	$\Delta_r H^0_m$ (kJ.mol^{-1})	$\Delta_r S^0_m$ (J.K^{-1}.mol^{-1})
$BiCl^{2+}$	**-56.343**				$Bi^{3+} + Cl^- \rightleftarrows BiCl^{2+}$	3.610 ± 0.180 [2010RAI/YUI]	**-20.606 ± 1.027**		
$BiCl_2^+$	**-198.764**				$Bi^{3+} + 2\ Cl^- \rightleftarrows BiCl_2^+$	5.560 ± 0.240 [2010RAI/YUI]	**-31.737 ± 1.370**		
$BiCl_3$(aq)	**-338.159**				$Bi^{3+} + 3\ Cl^- \rightleftarrows BiCl_3$(aq)	6.980 ± 0.370 [2010RAI/YUI]	**-39.842 ± 2.112**		
$BiCl_4^-$	**-475.499**				$Bi^{3+} + 4\ Cl^- \rightleftarrows BiCl_4^-$	8.040 ± 0.200 [2010RAI/YUI]	**-45.893 ± 1.142**		
$BiCl_5^{2-}$	**-602.907**				$Bi^{3+} + 5\ Cl^- \rightleftarrows BiCl_5^{2-}$	7.360 ± 0.370 [2010RAI/YUI]	**-42.011 ± 2.112**		
BiOCl(s)	**-321.267**				$Bi^{3+} + H_2O$ (l)+ $Cl^- \rightleftarrows$ BiOCl(s) + $2\ H^+$	8.470 [1999LOT/OCH]	**-48.347**		
$BiPO_4$(aq)	**≥-1047.972**				$Bi^{3+} + PO_4^{3-} \rightleftarrows BiPO_4$(aq)	≤ 21.850 [2010RAI/YUI]	**≥-124.721**		
$BiNO_3^{2+}$	**-26.610**				$Bi^{3+} + NO_3^- \rightleftarrows BiNO_3^{2+}$	1.970 [1999LOT/OCH]	**-11.245**		
$Bi(NO_3)_2^+$	**-143.122**				$Bi^{3+} + 2\ NO_3^- \rightleftarrows Bi(NO_3)_2^+$	2.950 [1999LOT/OCH]	**-16.839**		
$Bi(NO_3)_3$(aq)	**-257.864**				$Bi^{3+} + 3\ NO_3^- \rightleftarrows Bi(NO_3)_3$(aq)	3.620 [1999LOT/OCH]	**-20.663**		
$Bi(NO_3)_4^-$	**-365.757**				$Bi^{3+} + 4\ NO_3^- \rightleftarrows Bi(NO_3)_4^-$	3.090 [1999LOT/OCH]	**-17.638**		
$BiONO_3$(s)	**-268.245**				Bi^{3+}+ H_2O(l) + $NO_3^- \rightleftarrows BiONO_3$(s) + $2\ H^+$	2.750 [1999LOT/OCH]	**-15.697**		
$BiClNO_3^+$	**-176.108**				$Bi^{3+} + Cl^- + NO_3^- \rightleftarrows BiClNO_3^+$	5.160 [1999LOT/OCH]	**-29.453**		
$BiCl(NO_3)_2$(aq)	**-287.711**				$Bi^{3+} + Cl^- + 2\ NO_3^- \rightleftarrows BiCl(NO_3)_2$(aq)	5.280 [1999LOT/OCH]	**-30.138**		

Table A13 Selected thermodynamic data for bismuth (Bi) in JAEA-TDB-RN in 2020 (3/3)

Species / compound	$\Delta_f G^0_m$ (kJ.mol^{-1})	$\Delta_f H^0_m$ (kJ.mol^{-1})	S^0_m (J.K^{-1}.mol^{-1})	$C^0_{p,m}$ (J.K^{-1}.mol^{-1})	Reaction	$\log_{10} K°$	$\Delta_r G^0_m$ (kJ.mol^{-1})	$\Delta_r H^0_m$ (kJ.mol^{-1})	$\Delta_r S^0_m$ (J.K^{-1}.mol^{-1})
$BiCl_2NO_3$(aq)	**-317.102**				$Bi^{3+} + 2\ Cl^- + NO_3^- \rightleftarrows BiCl_2NO_3$(aq)	6.860	**-39.157**		
						[1999LOT/OCH]			
$BiCl_2(NO_3)_2^-$	**-421.684**				$Bi^{3+} + 2\ Cl^- + 2\ NO_3^- \rightleftarrows BiCl_2(NO_3)_2^-$	5.750	**-32.821**		
						[1999LOT/OCH]			
$BiCl_3NO_3^-$	**-455.412**				$Bi^{3+} + 3\ Cl^- + NO_3^- \rightleftarrows BiCl_3NO_3^-$	8.090	**-46.178**		
						[1999LOT/OCH]			
$BiPO_4$(cr)	**-1096.490**				$Bi^{3+} + PO_4^{3-} \rightleftarrows BiPO_4$(cr)	30.350	**-173.239**		
						± 0.540	**± 3.082**		
						[2010RAI/YUI]			
$(BiO)_2CO_3$(cr)	**-892.695**				$2\ Bi^{3+} + 2\ H_2O$(l) $+ CO_3^{2-} \rightleftarrows (BiO)_2CO_3$(cr) $+ 4\ H^+$	3.941	**-22.495**		
						[1999LOT/OCH]			
$(BiO)_4(OH)_2CO_3$(cr)	**-1618.412**				$4\ Bi^{3+} + 6\ H_2O$(l) $+ CO_3^{2-} \rightleftarrows (BiO)_4(OH)_2CO_3$(cr) $+ 10\ H^+$	-1.649	**9.413**		
						[1999LOT/OCH]			

[1999LOT/OCH] Lothenbach et al. [A18)]
[2003GUI/FAN] Guillaumont et al. [A15)]
[2010RAI/YUI] Rai et al. [A22)]

Table A14 Selected thermodynamic data for polonium (Po) in JAEA-TDB-RN in 2020

Values indicated by **boldface** are calculated and selected in the present report.

Species / compound	$\Delta_f G^0_m$ (kJ.mol^{-1})	$\Delta_f H^0_m$ (kJ.mol^{-1})	S^0_m (J.K^{-1}.mol^{-1})	$C^0_{p,m}$ (J.K^{-1}.mol^{-1})	Reaction	$\log_{10} K°$	$\Delta_r G^0_m$ (kJ.mol^{-1})	$\Delta_r H^0_m$ (kJ.mol^{-1})	$\Delta_r S^0_m$ (J.K^{-1}.mol^{-1})
$Po(OH)_4$(s)					$Po(OH)_4(s) + 4\ H^+ \rightleftarrows Po^{4+} + 4\ H_2O(l)$	19.520	**-111.421**		
						[1982WAG/EVA]			

[1982WAG/EVA] Calculated using $\Delta_f G^0_m$ values by Wagman et al. [A5)]

Table A15 Selected thermodynamic data for radium (Ra) in JAEA-TDB-RN in 2020

Values indicated by **boldface** are calculated and selected in the present report.

Species / compound	$\Delta_f G^0_m$ (kJ.mol^{-1})	$\Delta_f H^0_m$ (kJ.mol^{-1})	S^0_m (J.K^{-1}.mol^{-1})	$C^0_{p,m}$ (J.K^{-1}.mol^{-1})	Reaction	$\log_{10} K°$	$\Delta_r G^0_m$ (kJ.mol^{-1})	$\Delta_r H^0_m$ (kJ.mol^{-1})	$\Delta_r S^0_m$ (J.K^{-1}.mol^{-1})
Ra(cr)	0.000	0.000	71.000						
			[1982WAG/EVA]						
Ra^{2+}	-555.581	-531.275	21.844		Ra(cr) ⇄ Ra^{2+} + 2 e^-	**97.333**	**-555.581**	**-531.275**	**81.523**
	± 1.778	± 1.793	± 0.786			**± 0.311**	**± 1.778**	**± 1.793**	
	[2021KIT/YOS]	[2021KIT/YOS]	[2021KIT/YOS]						
RaO(s)	-505.811	-534.553	77.176		Ra^{2+} + H_2O ⇄ RaO(s) + 2 H^+	**-50.272**	**286.953**	**282.560**	**-14.591**
	± 2.121	± 2.125	± 0.425			**± 0.485**	**± 2.770**	**± 2.783**	**± 0.897**
	[2021KIT/YOS]	[2021KIT/YOS]	[2021KIT/YOS]						
$RaOH^+$	-715.389	-727.240	133.826		Ra^{2+} + H_2O ⇄ $RaOH^+$ + H^+	**-13.555**	**77.375**	**89.873**	**42.059**
	± 2.257					**± 0.504**	**± 2.875**		
	[2021KIT/YOS]	[2021KIT/YOS]	[2021KIT/YOS]						
$Ra(OH)_2$(s)	-852.055	-940.376	110.602		Ra^{2+} + 2 H_2O ⇄ $Ra(OH)_2$(s) + 2 H^+	**-31.165**	**177.892**	**162.576**	**-51.088**
	± 7.838	± 8.316	± 9.325			**± 1.408**	**± 8.039**	**± 8.510**	**± 9.359**
	[2021KIT/YOS]	[2021KIT/YOS]	[2021KIT/YOS]						
RaF^+	-835.560	-855.049	41.691		Ra^{2+} + F^- ⇄ RaF^+	**-0.310**	**1.772**	**11.574**	**33.027**
	± 2.244					**± 0.515**	**± 2.940**		
	[2021KIT/YOS]	[2021KIT/YOS]	[2021KIT/YOS]						
$RaCl^+$	-683.703	-691.442	91.243		Ra^{2+} + Cl^- ⇄ $RaCl^+$	**-0.555**	**3.169**	**6.913**	**12.664**
	[2021KIT/YOS]	[2021KIT/YOS]	[2021KIT/YOS]						
$RaCl_2$(s)	-816.419	-866.295	126.793		Ra^{2+} + 2 Cl^- ⇄ $RaCl_2$(s)	**-0.305**	**1.742**	**-0.861**	**-8.521**
	± 2.806	± 2.807	± 0.271			**± 0.583**	**± 3.328**	**± 3.336**	**± 0.896**
	[2021KIT/YOS]	[2021KIT/YOS]	[2021KIT/YOS]						
$RaSO_4$(aq)	-1314.584	-1436.884	103.160		Ra^{2+} + SO_4^{2-} ⇄ $RaSO_4$(aq)	**2.548**	**-14.543**	**3.992**	**62.488**
	± 1.275	± 5.195	± 16.890			**± 0.392**	**± 2.236**	**± 5.512**	**± 16.916**
	[2021KIT/YOS]	[2021KIT/YOS]	[2021KIT/YOS]						
$RaSO_4$(cr)	-1366.507	-1478.556	137.547		Ra^{2+} + SO_4^{2-} ⇄ $RaSO_4$(cr)	**11.644**	**-66.467**	**-37.679**	**96.875**
	± 8.885	± 8.932	± 3.092			**± 1.589**	**± 9.072**	**± 9.120**	**± 3.230**
	[2021KIT/YOS]	[2021KIT/YOS]	[2021KIT/YOS]						
$RaCO_3$(aq)	-1098.439	-1193.183	66.695		Ra^{2+} + CO_3^{2-} ⇄ $RaCO_3$(aq)	**2.606**	**-14.874**	**13.327**	**94.850**
	[2021KIT/YOS]	[2021KIT/YOS]	[2021KIT/YOS]						
$RaCO_3$(cr)	-1130.720	-1210.790	115.913		Ra^{2+} + CO_3^{2-} ⇄ $RaCO_3$(cr)	**8.261**	**-47.155**	**-4.280**	**144.068**
	± 2.238	± 2.494	± 3.693			**± 0.503**	**± 2.873**	**± 3.105**	**± 3.992**
	[2021KIT/YOS]	[2021KIT/YOS]	[2021KIT/YOS]						

[1982WAG/EVA] Wagman et al. [A5)]

[2021KIT/YOS] Kitamura and Yoshida [A23)].

All the selected data have been re-calculated by the author due to give thermodynamic data to three decimal places.

Table A16 Selected thermodynamic data for actinium (Ac) in JAEA-TDB-RN in 2020 (1/2)

Values indicated by **boldface** are calculated and selected in the present report.

Species / compound	$\Delta_f G^0_m$ (kJ.mol^{-1})	$\Delta_f H^0_m$ (kJ.mol^{-1})	S^0_m (J.K^{-1}.mol^{-1})	$C^0_{p,m}$ (J.K^{-1}.mol^{-1})	Reaction	$\log_{10} K°$	$\Delta_r G^0_m$ (kJ.mol^{-1})	$\Delta_r H^0_m$ (kJ.mol^{-1})	$\Delta_r S^0_m$ (J.K^{-1}.mol^{-1})
Ac^{3+}	–640.152 ± 25.104 [1976FUG/OET]	–652.704 ± 25.104 [1976FUG/OET]	-179.912 ± 16.736 [1976FUG/OET]						
$AcOH^{2+}$	**-836.237 ± 25.420**				$Ac^{3+} + H_2O(l) \rightleftarrows AcOH^{2+} + H^+$	-7.200 ± 0.700 [2010KIT/FUJ2]	41.098 ± 3.996		
$Ac(OH)_2^+$	**-1028.326 ± 25.625**				$Ac^{3+} + 2\ H_2O(l) \rightleftarrows Ac\ OH)_2^+ + 2\ H^+$	-15.100 ± 0.900 [2010KIT/FUJ2]	86.191 ± 5.137		
$Ac(OH)_3(am)$	**-1255.234 ± 37.162**				$Ac^{3+} + 3\ H_2O(l) \rightleftarrows Ac(OH)_3(am) + 3\ H^+$	-16.900 ± 4.800 [2010KIT/FUJ2]	96.466 ± 27.399		
$Ac(OH)_3(aq)$	**-1202.149 ± 25.422**				$Ac^{3+} + 3\ H_2O(l) \rightleftarrows Ac(OH)_3(aq) + 3\ H^+$	-26.200 ± 0.700 [2010KIT/FUJ2]	149.551 ± 3.996		
AcF^{2+}	**-941.310 ± 25.345**				$Ac^{3+} + F^- \rightleftarrows AcF^{2+}$	3.400 ± 0.600 [2010KIT/FUJ2]	-19.407 ± 3.425		
AcF_2^+	**-1236.760 ± 25.243**				$Ac^{3+} + 2\ F^- \rightleftarrows AcF_2^+$	5.800 ± 0.400 [2010KIT/FUJ2]	-33.107 ± 2.283		
$AcCl^{2+}$	**-772.812 ± 25.139**				$Ac^{3+} + Cl^- \rightleftarrows AcCl^{2+}$	0.240 ± 0.230 [2010KIT/FUJ2]	-1.370 ± 1.313		
$AcCl_2^+$	**-898.508 ± 25.145**				$Ac^{3+} + 2\ Cl^- \rightleftarrows AcCl_2^+$	-0.740 ± 0.250 [2010KIT/FUJ2]	4.224 ± 1.427		
$AcSO_4^+$	**-1403.448 ± 25.188**				$Ac^{3+} + SO_4^{2-} \rightleftarrows AcSO_4^+$	3.300 ± 0.350 [2010KIT/FUJ2]	-18.837 ± 1.998		
$Ac(SO_4)_2^-$	**-2150.190 ± 25.200**				$Ac^{3+} + 2\ SO_4^{2-} \rightleftarrows Ac(SO_4)_2^-$	3.700 ± 0.350 [2010KIT/FUJ2]	-21.120 ± 1.998		
AcN_3^{2+}	**-301.484 ± 25.190**				$Ac^{3+} + N_3^- \rightleftarrows AcN_3^{2+}$	1.670 ± 0.100 [2010KIT/FUJ2]	-9.532 ± 0.571		
$AcNO_2^{2+}$	**-684.356 ± 26.560**				$Ac^{3+} + NO_2^- \rightleftarrows AcNO_2^{2+}$	2.100 ± 0.400 [2010KIT/FUJ2]	-11.987 ± 2.283		

Table A16 Selected thermodynamic data for actinium (Ac) in JAEA-TDB-RN in 2020 (2/2)

Species / compound	$\Delta_f G^0_m$ (kJ.mol^{-1})	$\Delta_f H^0_m$ (kJ.mol^{-1})	S^0_m (J.K^{-1}.mol^{-1})	$C^0_{p,m}$ (J.K^{-1}.mol^{-1})	Reaction	$\log_{10} K°$	$\Delta_r G^0_m$ (kJ.mol^{-1})	$\Delta_r H^0_m$ (kJ.mol^{-1})	$\Delta_r S^0_m$ (J.K^{-1}.mol^{-1})
$AcNO_3^{2+}$	**-758.662**				$Ac^{3+} + NO_3^- \rightleftarrows AcNO_3^{2+}$	1.330	-7.592		
	± 25.332					± 0.400	± 2.283		
						[2010KIT/FUJ2]			
$AcPO_4$(am,hydr)	**-1800.458**				$Ac^{3+} + PO_4^{3-} \rightleftarrows AcPO_4$(am,hydr)	24.790	-141.502		
	± 37.278					± 4.600	± 26.257		
						[2010KIT/FUJ2]			
$AcH_2PO_4^{2+}$	**-1787.741**				$Ac^{3+} + 2\ H^+ + PO_4^{3-} \rightleftarrows AcH_2PO_4^{2+}$	22.562	-128.785		
	± 26.763					± 0.701	± 4.001		
						[2010KIT/FUJ2]			
$AcCO_3^+$	**-1213.799**				$Ac^{3+} + CO_3^{2-} \rightleftarrows AcCO_3^+$	8.000	-45.664		
	± 25.338					± 0.600	± 3.425		
						[2010KIT/FUJ2]			
$Ac(CO_3)_2^-$	**-1769.752**				$Ac^{3+} + 2\ CO_3^{2-} \rightleftarrows Ac(CO_3)_2^-$	12.900	-73.634		
	± 25.523					± 0.800	± 4.566		
						[2010KIT/FUJ2]			
$Ac(CO_3)_3^{3-}$	**-2309.722**				$Ac^{3+} + 3\ CO_3^{2-} \rightleftarrows Ac(CO_3)_3^{3-}$	15.000	-85.621		
	± 26.037					± 1.200	± 6.850		
						[2010KIT/FUJ2]			
$Ac_2(CO_3)_3$(am)	**-3054.902**				$2\ Ac^{3+} + 3\ CO_3^{2-} \rightleftarrows Ac_2(CO_3)_3$(am)	33.400	-190.649		
	± 58.044					± 5.100	± 29.111		
						[2010KIT/FUJ2]			
$AcHCO_3^{2+}$	**-1244.788**				$Ac^{3+} + H^+ + CO_3^{2-} \rightleftarrows AcHCO_3^{2+}$	13.429	-76.653		
	± 25.267					± 0.500	± 2.854		
						[2010KIT/FUJ2]			
$AcCO_3OH$(am)	**-1440.702**				$Ac^{3+} + CO_3^{2-} + H_2O(l) \rightleftarrows AcCO_3OH(am) + H^+$	6.199	-35.384		
	± 38.011					± 5.000	± 28.540		
						[2010KIT/FUJ2]			
$AcSiO(OH)_3^{2+}$	**-1938.335**				$Ac^{3+} + H_4SiO_4(aq) \rightleftarrows AcSiO(OH)_3^{2+} + H^+$	-1.680	9.590		
	± 25.263					± 0.380	± 2.169		
						[2010KIT/FUJ2]			
$AcSCN^{2+}$	**-554.688**				$Ac^{3+} + SCN^- \rightleftarrows AcSCN^{2+}$	1.300	-7.420		
	± 26.615					± 0.500	± 2.854		
						[2010KIT/FUJ2]			

[1976FUG/OET] Fuger and Oetting [A24)] with conversion using 1 cal = 4.184 J by the author.
[2010KIT/FUJ2] Kitamura et al. [A21)]

Table A17 Selected thermodynamic data for thorium (Th) in JAEA-TDB-RN in 2020 (1/9)

Values indicated by **boldface** are calculated and selected in the present report.

Species / compound	$\Delta_f G^0_m$ (kJ.mol^{-1})	$\Delta_f H^0_m$ (kJ.mol^{-1})	S^0_m (J.K^{-1}.mol^{-1})	$C^0_{p,m}$ (J.K^{-1}.mol^{-1})	Reaction	$\log_{10} K°$	$\Delta_r G^0_m$ (kJ.mol^{-1})	$\Delta_r H^0_m$ (kJ.mol^{-1})	$\Delta_r S^0_m$ (J.K^{-1}.mol^{-1})
Th(cr)	0.000	0.000	52.640	26.230					
			± 0.500	± 0.050					
	[2008RAN/FUG]	[2008RAN/FUG]	[2008RAN/FUG]	[2008RAN/FUG]					
Th(g)	560.995	602.000	190.170	20.790	Th(g) ⇄ Th^{4+} + 4 e^-	**221.753**	**-1265.778**	**-1370.700**	**-351.912**
	± 6.002	± 6.000	± 0.010	± 0.005		**± 1.403**	**± 8.006**	**± 6.426**	**± 16.000**
	[2008RAN/FUG]	[2008RAN/FUG]	[2008RAN/FUG]	[2008RAN/FUG]					
Th^{4+}	-704.783	-768.700	-423.100	-224.000	Th(cr) ⇄ Th^{4+} + 4 e^-	**123.472**	**-704.783**	**-768.700**	**-214.382**
	± 5.298	± 2.300	± 16.000	± 15.000		**± 0.928**	**± 5.298**	**± 2.300**	**± 16.008**
	[2008RAN/FUG]	[2008RAN/FUG]	[2008RAN/FUG]	[2008RAN/FUG]					
ThO(g)	-51.299	-26.000	240.070	31.270	ThO(g) + 2 H^+ ⇄ Th^{4+} + H_2O(l) + 2 e^-	**156.037**	**-890.667**	**-1028.538**	**-462.568**
	± 6.002	± 6.000	± 0.050	± 0.100		**± 1.403**	**± 8.006**	**± 6.427**	**± 16.000**
	[2008RAN/FUG]	[2008RAN/FUG]	[2008RAN/FUG]	[2008RAN/FUG]					
ThO_2(cr)	-1168.988	-1226.400	65.230	61.740	ThO_2(cr) + 4 H^+ ⇄ Th^{4+} + 2 H_2O(l)	**1.780**	**-10.160**	**-113.977**	**-348.484**
	± 3.504	± 3.500	± 0.200	± 0.150		**± 1.113**	**± 6.355**	**± 4.193**	**± 16.002**
	[2008RAN/FUG]	[2008RAN/FUG]	[2008RAN/FUG]	[2008RAN/FUG]					
ThO_2(g)	-462.128	-455.000	281.700	46.840	ThO_2(g) + 4 H^+ ⇄ Th^{4+} + 2 H_2O(l)	**125.616**	**-717.020**	**-885.377**	**-564.954**
	± 15.430	± 15.403	± 3.000	± 0.500		**± 2.858**	**± 16.315**	**± 15.575**	**± 16.280**
	[2008RAN/FUG]	[2008RAN/FUG]	[2008RAN/FUG]	[2008RAN/FUG]					
ThO_2(am,hyd,fresh)	**-1126.173**				Th^{4+} + 4 OH^- ⇄ ThO_2(am,hyd,fresh) + 2 H_2O(l)	46.700	-266.566		
	± 7.389					± 0.900	± 5.137		
						[2008RAN/FUG]	[2008RAN/FUG]		
ThO_2(am,hyd,aged)	**-1130.740**				Th^{4+} + 4 OH^- ⇄ ThO_2(am,hyd,aged) + 2 H_2O(l)	47.500	-271.132		
	± 7.389					± 0.900	± 5.137		
						[2008RAN/FUG]	[2008RAN/FUG]		
ThH(g)			233.500	29.600					
			± 5.000	± 4.000					
			[2008RAN/FUG]	[2008RAN/FUG]					
ThH_2(cr)	-105.468	-145.000	50.730	36.710	ThH_2(cr) ⇄ Th^{4+} + 2 H^+ + 6 e^-	**104.995**	**-599.315**	**-623.700**	**-81.793**
	± 2.006	± 2.000	± 0.100	± 0.070		**± 0.992**	**± 5.665**	**± 3.048**	**± 16.001**
	[2008RAN/FUG]	[2008RAN/FUG]	[2008RAN/FUG]	[2008RAN/FUG]					
ThD_2(cr)			55.720	47.670					
			± 0.560	± 0.470					
			[2008RAN/FUG]	[2008RAN/FUG]					
ThT_2(cr)			60.460	54.300					
			± 0.600	± 0.540					
			[2008RAN/FUG]	[2008RAN/FUG]					
$ThH_{3.75}$(cr)	-142.877	-215.400	54.420	51.320	$ThH_{3.75}$(cr) ⇄ Th^{4+} + 3.75 H^+ + 7.75 e^-	**98.441**	**-561.906**	**-553.300**	**28.861**
	± 8.001	± 8.000	± 0.110	± 0.100		**± 1.681**	**± 9.596**	**± 8.324**	**± 16.001**
	[2008RAN/FUG]	[2008RAN/FUG]	[2008RAN/FUG]	[2008RAN/FUG]					

Table A17 Selected thermodynamic data for thorium (Th) in JAEA-TDB-RN in 2020 (2/9)

Species / compound	$\Delta_f G^0_m$ (kJ.mol^{-1})	$\Delta_f H^0_m$ (kJ.mol^{-1})	S^0_m (J.K^{-1}.mol^{-1})	$C^0_{p,m}$ (J.K^{-1}.mol^{-1})	Reaction	$\log_{10} K°$	$\Delta_r G^0_m$ (kJ.mol^{-1})	$\Delta_r H^0_m$ (kJ.mol^{-1})	$\Delta_r S^0_m$ (J.K^{-1}.mol^{-1})
$ThD_{3.75}$(cr)			63.970 ± 0.640 [2008RAN/FUG]	69.710 ± 0.700 [2008RAN/FUG]					
$ThT_{3.75}$(cr)			72.650 ± 0.730 [2008RAN/FUG]	81.490 ± 0.810 [2008RAN/FUG]					
$ThOH^{3+}$	**-927.695 ± 6.019**	**-1010.338 ± 6.708**	**-252.792 ± 28.180**		$Th^{4+} + H_2O(l) \rightleftarrows ThOH^{3+} + H^+$	-2.500 ± 0.500 [2008RAN/FUG]	14.270 ± 2.854 [2008RAN/FUG]	44.200 ± 6.300 [2008RAN/FUG]	100.385 ± 23.197 [2008RAN/FUG]
$Th(OH)_2^{2+}$	**-1143.758 ± 6.021**	**-1254.677 ± 41.464**	**-114.513 ± 140.103**		$Th^{4+} + 2\ H_2O(l) \rightleftarrows Th(OH)_2^{2+} + 2\ H^+$	-6.200 ± 0.500 [2008RAN/FUG]	35.390 ± 2.854 [2008RAN/FUG]	85.700 ± 41.400 [2008RAN/FUG]	168.741 ± 139.186 [2008RAN/FUG]
$Th(OH)_4$(aq)	**-1554.193 ± 6.648**	-2050.760 ± 7.325 [2008RAN/FUG]			$Th^{4+} + 4\ H_2O(l) \rightleftarrows Th(OH)_4(aq) + 4\ H^+$	-17.400 ± 0.700 [2008RAN/FUG]	99.320 ± 3.996 [2008RAN/FUG]		
$Th_2(OH)_2^{6+}$	**-1850.254 ± 10.975**	**-2050.777 ± 7.328**	**-623.770 ± 38.485**		$2\ Th^{4+} + 2\ H_2O(l) \rightleftarrows Th_2(OH)_2^{6+} + 2\ H^+$	-5.900 ± 0.500 [2008RAN/FUG]	33.677 ± 2.854 [2008RAN/FUG]	58.300 ± 5.700 [2008RAN/FUG]	82.584 ± 21.380 [2008RAN/FUG]
$Th_2(OH)_3^{5+}$	**-2082.299 ± 10.662**	-5118.440 ± 23.204 [2008RAN/FUG]			$2\ Th^{4+} + 3\ H_2O(l) \rightleftarrows Th_2(OH)_3^{5+} + 3\ H^+$	-6.800 ± 0.200 [2008RAN/FUG]	38.815 ± 1.142 [2008RAN/FUG]		
$Th_4(OH)_8^{8+}$	**-4600.149 ± 21.330**	**-5118.507 ± 23.217**	**-708.545 ± 96.223**		$4\ Th^{4+} + 8\ H_2O(l) \rightleftarrows Th_4(OH)_8^{8+} + 8\ H^+$	-20.400 ± 0.400 [2008RAN/FUG]	116.444 ± 2.283 [2008RAN/FUG]	243.000 ± 21.300 [2008RAN/FUG]	424.471 ± 71.850 [2008RAN/FUG]
$Th_4(OH)_{12}^{4+}$	**-5513.489 ± 21.257**				$4\ Th^{4+} + 12\ H_2O(l) \rightleftarrows Th_4(OH)_{12}^{4+} + 12\ H^+$	-26.600 ± 0.200 [2008RAN/FUG]	151.834 ± 1.142 [2008RAN/FUG]		
$Th_6(OH)_{14}^{10+}$	**-7339.198 ± 32.548**				$6\ Th^{4+} + 14\ H_2O(l) \rightleftarrows Th_6(OH)_{14}^{10+} + 14\ H^+$	-36.800 ± 1.200 [2008RAN/FUG]	210.056 ± 6.850 [2008RAN/FUG]		
$Th_6(OH)_{15}^{9+}$	**-7576.381 ± 32.955**	**-8426.975 ± 26.017**	**-608.507 ± 124.447**		$6\ Th^{4+} + 15\ H_2O(l) \rightleftarrows Th_6(OH)_{15}^{9+} + 15\ H^+$	-36.800 ± 1.500 [2008RAN/FUG]	210.056 ± 8.562 [2008RAN/FUG]	472.800 ± 22.000 [2008RAN/FUG]	881.248 ± 79.180 [2008RAN/FUG]
ThF(g)	-0.788 ± 15.422 [2008RAN/FUG]	30.000 ± 15.000 [2008RAN/FUG]	257.300 ± 12.000 [2008RAN/FUG]	34.700 ± 6.000 [2008RAN/FUG]	$ThF(g) \rightleftarrows Th^{4+} + F^- + 3\ e^-$	**172.694 ± 2.859**	**-985.746 ± 16.320**	**-1134.048 ± 15.190**	**-497.561 ± 20.007**
ThF^{3+}	**-1037.164 ± 5.408**	**-1104.448 ± 3.121**	**-267.807 ± 17.594**		$Th^{4+} + F^- \rightleftarrows ThF^{3+}$	8.870 ± 0.150 [2008RAN/FUG]	-50.630 ± 0.856 [2008RAN/FUG]	-0.400 ± 2.000 [2008RAN/FUG]	168.473 ± 7.297 [2008RAN/FUG]
ThF_2(g)	-601.857 ± 20.222 [2008RAN/FUG]	-590.000 ± 20.000 [2008RAN/FUG]	295.200 ± 10.000 [2008RAN/FUG]	52.400 ± 5.000 [2008RAN/FUG]	$ThF_2(g) \rightleftarrows Th^{4+} + 2\ F^- + 2\ e^-$	**116.752 ± 3.670**	**-666.427 ± 20.947**	**-849.395 ± 20.176**	**-613.980 ± 18.899**

Table A17 Selected thermodynamic data for thorium (Th) in JAEA-TDB-RN in 2020 (3/9)

Species / compound	$\Delta_f G^0_m$ (kJ.mol^{-1})	$\Delta_f H^0_m$ (kJ.mol^{-1})	S^0_m (J.K^{-1}.mol^{-1})	$C^0_{p,m}$ (J.K^{-1}.mol^{-1})	Reaction	$\log_{10} K°$	$\Delta_r G^0_m$ (kJ.mol^{-1})	$\Delta_r H^0_m$ (kJ.mol^{-1})	$\Delta_r S^0_m$ (J.K^{-1}.mol^{-1})
ThF_2^{2+}	**-1357.501**	**-1442.695**	**-161.293**		$Th^{4+} + 2\ F^- \rightleftarrows ThF_2^{2+}$	15.630	-89.217	-3.300	288.166
	± 5.620	**± 2.691**	**± 16.684**			± 0.230	± 1.313	± 0.400	± 4.603
						[2008RAN/FUG]	[2008RAN/FUG]	[2008RAN/FUG]	[2008RAN/FUG]
ThF_3(g)	-1159.774	-1165.000	339.300	73.300	$ThF_3(g) \rightleftarrows Th^{4+} + 3\ F^- + e^-$	**68.370**	**-390.261**	**-609.743**	**-736.599**
	± 15.294	± 15.000	± 10.000	± 5.000		**± 2.857**	**± 16.310**	**± 15.308**	**± 18.938**
	[2008RAN/FUG]	[2008RAN/FUG]	[2008RAN/FUG]	[2008RAN/FUG]					
ThF_3^+	**-1668.020**				$Th^{4+} + 3\ F^- \rightleftarrows ThF_3^+$	20.670	-117.985		
	± 5.739					± 0.160	± 0.913		
						[2008RAN/FUG]	[2008RAN/FUG]		
ThF_4(cr)	**-2013.165**	-2100.000	**166.984**	110.710	$Th^{4+} + 4\ HF(aq) \rightleftarrows ThF_4(cr) + 4\ H^+$	19.110	-109.081		
		± 10.000		± 0.130		± 0.400	± 2.283		
		[2008RAN/FUG]		[2008RAN/FUG]		[2008RAN/FUG]	[2008RAN/FUG]		
					$ThF_4(cr) \rightleftarrows Th^{4+} + 4\ F^-$	**-31.776**	**181.380**	**-10.090**	**-642.802**
								± 10.605	
ThF_4(g)	-1719.328	-1750.700	353.000	93.400	$ThF_4(g) \rightleftarrows Th^{4+} + 4\ F^-$	**19.702**	**-112.457**	**-359.390**	**-828.818**
	± 10.217	± 10.198	± 2.000	± 2.000		**± 2.070**	**± 11.816**	**± 10.792**	**± 16.271**
	[2008RAN/FUG]	[2008RAN/FUG]	[2008RAN/FUG]	[2008RAN/FUG]					
ThF_4(aq)	**-1977.797**				$Th^{4+} + 4\ F^- \rightleftarrows ThF_4(aq)$	25.580	-146.012		
	± 6.025					± 0.180	± 1.027		
						[2008RAN/FUG]	[2008RAN/FUG]		
ThOF(g)	-566.186	-550.000	310.900	49.500	$ThOF(g) + 2\ H^+ \rightleftarrows Th^{4+} + F^- + H_2O(l) + e^-$	**115.194**	**-657.530**	**-839.886**	**-611.917**
	± 12.366	± 12.000	± 10.000	± 5.000		**± 2.360**	**± 13.470**	**± 12.237**	**± 18.876**
	[2008RAN/FUG]	[2008RAN/FUG]	[2008RAN/FUG]	[2008RAN/FUG]					
$ThOF_2$(cr)	-1589.171	-1663.800	107.700		$ThOF_2(cr) + 2\ H^+ \rightleftarrows Th^{4+} + 2\ F^- + H_2O(l)$	**-14.664**	**83.704**	**-61.434**	**-487.236**
	± 7.948	± 7.800	± 5.100			**± 1.690**	**± 9.646**	**± 8.242**	**± 16.829**
	[2008RAN/FUG]	[2008RAN/FUG]	[2008RAN/FUG]						
ThCl(g)	215.688	247.000	269.200	36.400	$ThCl(g) \rightleftarrows Th^{4+} + Cl^- + 3\ e^-$	**184.259**	**-1051.761**	**-1182.780**	**-439.547**
	± 20.318	± 20.000	± 12.000	± 6.000		**± 3.679**	**± 20.998**	**± 20.132**	**± 20.001**
	[2008RAN/FUG]	[2008RAN/FUG]	[2008RAN/FUG]	[2008RAN/FUG]					
$ThCl^{3+}$	**-996.237**				$Th^{4+} + Cl^- \rightleftarrows ThCl^{3+}$	1.700	-9.704		
	± 5.371					± 0.100	± 0.571		
						[2008RAN/FUG]	[2008RAN/FUG]		
$ThCl_2$(g)	-191.337	-179.000	317.100	55.300	$ThCl_2(g) \rightleftarrows Th^{4+} + 2\ Cl^- + 2\ e^-$	**135.953**	**-776.025**	**-923.859**	**-496.051**
	± 22.202	± 22.000	± 10.000	± 5.000		**± 3.999**	**± 22.826**	**± 22.121**	**± 18.871**
	[2008RAN/FUG]	[2008RAN/FUG]	[2008RAN/FUG]	[2008RAN/FUG]					
$ThCl_3$(g)	-563.764	-569.000	369.700	78.000	$ThCl_3(g) \rightleftarrows Th^{4+} + 3\ Cl^- + e^-$	**93.708**	**-534.888**	**-700.939**	**-557.255**
	± 25.178	± 25.000	± 10.000	± 5.000		**± 4.508**	**± 25.731**	**± 25.107**	**± 18.875**
	[2008RAN/FUG]	[2008RAN/FUG]	[2008RAN/FUG]	[2008RAN/FUG]					
β-$ThCl_4$	-1092.293	-1186.300	183.500	120.300	$\beta\text{-}ThCl_4 \rightleftarrows Th^{4+} + 4\ Cl^-$	**24.115**	**-137.649**	**-250.719**	**-379.660**
	± 1.984	± 1.300	± 5.000	± 6.000		**± 0.994**	**± 5.672**	**± 2.665**	**± 16.776**
	[2008RAN/FUG]	[2008RAN/FUG]	[2008RAN/FUG]	[2008RAN/FUG]					

Table A17 Selected thermodynamic data for thorium (Th) in JAEA-TDB-RN in 2020 (4/9)

Species / compound	$\Delta_f G^0_m$ (kJ.mol^{-1})	$\Delta_f H^0_m$ (kJ.mol^{-1})	S^0_m (J.K^{-1}.mol^{-1})	$C^0_{p,m}$ (J.K^{-1}.mol^{-1})	Reaction	$\log_{10} K°$	$\Delta_r G^0_m$ (kJ.mol^{-1})	$\Delta_r H^0_m$ (kJ.mol^{-1})	$\Delta_r S^0_m$ (J.K^{-1}.mol^{-1})
$ThCl_4 \cdot 2H_2O$(cr)		-1822.400 ± 12.000 [2008RAN/FUG]			$ThCl_4 \cdot 2H_2O(cr) \rightleftarrows Th^{4+} + 4\ Cl^- + 2\ H_2O(l)$			**-186.295 ± 12.225**	
$ThCl_4 \cdot 4H_2O$(cr)		-2456.200 ± 12.000 [2008RAN/FUG]			$ThCl_4 \cdot 4H_2O(cr) \rightleftarrows Th^{4+} + 4\ Cl^- + 4\ H_2O(l)$			**-124.172 ± 12.231**	
$ThCl_4 \cdot 7H_2O$(cr)		-3361.900 ± 12.000 [2008RAN/FUG]			$ThCl_4 \cdot 7H_2O(cr) \rightleftarrows Th^{4+} + 4\ Cl^- + 7\ H_2O(l)$			**-75.987 ± 12.245**	
$ThCl_4 \cdot 8H_2O$(cr)		-3661.300 ± 12.000 [2008RAN/FUG]			$ThCl_4 \cdot 8H_2O(cr) \rightleftarrows Th^{4+} + 4\ Cl^- + 8\ H_2O(l)$			**-62.425 ± 12.252**	
$ThCl_4$(g)	-922.956 ± 5.304 [2008RAN/FUG]	-951.400 ± 5.166 [2008RAN/FUG]	403.400 ± 4.000 [2008RAN/FUG]	101.400 ± 3.000 [2008RAN/FUG]	$ThCl_4(g) \rightleftarrows Th^{4+} + 4\ Cl^-$	**53.781 ± 1.315**	**-306.986 ± 7.507**	**-485.619 ± 5.666**	**-599.560 ± 16.506**
$ThOCl_2$(cr)	-1153.564 ± 2.276 [2008RAN/FUG]	-1231.500 ± 2.100 [2008RAN/FUG]	116.900 ± 2.900 [2008RAN/FUG]		$ThOCl_2(cr) + 2\ H^+ \rightleftarrows Th^{4+} + 2\ Cl^- + H_2O(l)$	**8.931 ± 1.011**	**-50.981 ± 5.771**	**-157.198 ± 3.121**	**-356.607 ± 16.264**
$ThClO_3^{3+}$	**-721.580 ± 5.415**				$Th^{4+} + ClO_3^- \rightleftarrows ThClO_3^{3+}$	1.550 ± 0.130 [2008RAN/FUG]	-8.847 ± 0.742 [2008RAN/FUG]		
ThBr(g)	319.575 ± 20.318 [2008RAN/FUG]	365.000 ± 20.000 [2008RAN/FUG]	281.100 ± 12.000 [2008RAN/FUG]	37.400 ± 6.000 [2008RAN/FUG]	$ThBr(g) \rightleftarrows Th^{4+} + Br^- + 3\ e^-$	**197.686 ± 3.679**	**-1128.402 ± 20.998**	**-1255.203 ± 20.132**	**-425.338 ± 20.001**
$ThBr^{3+}$	**-816.704 ± 5.352**				$Th^{4+} + Br^- \rightleftarrows ThBr^{3+}$	1.380 ± 0.130 [2008RAN/FUG]	-7.877 ± 0.742 [2008RAN/FUG]		
$ThBr_2$(g)	-0.027 ± 20.222 [2008RAN/FUG]	40.000 ± 20.000 [2008RAN/FUG]	339.100 ± 10.000 [2008RAN/FUG]	56.700 ± 5.000 [2008RAN/FUG]	$ThBr_2(g) \rightleftarrows Th^{4+} + 2\ Br^- + 2\ e^-$	**159.922 ± 3.663**	**-912.843 ± 20.907**	**-1051.707 ± 20.134**	**-465.835 ± 18.873**
$ThBr_3$(g)	-371.073 ± 15.295 [2008RAN/FUG]	-334.000 ± 15.000 [2008RAN/FUG]	405.300 ± 10.000 [2008RAN/FUG]	80.800 ± 5.000 [2008RAN/FUG]	$ThBr_3(g) \rightleftarrows Th^{4+} + 3\ Br^- + e^-$	**113.146 ± 2.837**	**-645.841 ± 16.194**	**-799.210 ± 15.182**	**-514.531 ± 18.878**
β-$ThBr_4$	-925.023 ± 2.505 [2008RAN/FUG]	-963.800 ± 2.000 [2008RAN/FUG]	227.000 ± 5.000 [2008RAN/FUG]	125.200 ± 6.000 [2008RAN/FUG]	$\beta\text{-}ThBr_4 \rightleftarrows Th^{4+} + 4\ Br^-$	**34.326 ± 1.033**	**-195.934 ± 5.898**	**-290.913 ± 3.107**	**-318.727 ± 16.784**
$ThBr_4 \cdot 7H_2O$(cr)		-3163.900 ± 12.000 [2008RAN/FUG]			$ThBr_4 \cdot 7H_2O(cr) \rightleftarrows Th^{4+} + 4\ Br^- + 7\ H_2O(l)$			**-91.682 ± 12.255**	
$ThBr_4 \cdot 10H_2O$(cr)		-4074.600 ± 12.000 [2008RAN/FUG]			$ThBr_4 \cdot 10H_2O(cr) \rightleftarrows Th^{4+} + 4\ Br^- + 10\ H_2O(l)$			**-38.497 ± 12.278**	

Table A17 Selected thermodynamic data for thorium (Th) in JAEA-TDB-RN in 2020 (5/9)

Species / compound	$\Delta_f G^0_m$ (kJ.mol^{-1})	$\Delta_f H^0_m$ (kJ.mol^{-1})	S^0_m (J.K^{-1}.mol^{-1})	$C^0_{p,m}$ (J.K^{-1}.mol^{-1})	Reaction	$\log_{10} K°$	$\Delta_r G^0_m$ (kJ.mol^{-1})	$\Delta_r H^0_m$ (kJ.mol^{-1})	$\Delta_r S^0_m$ (J.K^{-1}.mol^{-1})
$ThBr_4 \cdot 12H_2O(cr)$		-4677.800 ± 12.000 [2008RAN/FUG]			$ThBr_4 \cdot 12H_2O(cr) \rightleftarrows Th^{4+} + 4\ Br^- + 12\ H_2O(l)$			**-6.973** **± 12.298**	
$ThBr_4(g)$	-769.026 ± 5.593 [2008RAN/FUG]	-742.300 ± 5.385 [2008RAN/FUG]	446.700 ± 5.000 [2008RAN/FUG]	104.900 ± 3.000 [2008RAN/FUG]	$ThBr_4(g) \rightleftarrows Th^{4+} + 4\ Br^-$	**61.655** **± 1.355**	**-351.931** **± 7.733**	**-512.413** **± 5.887**	**-538.427** **± 16.784**
$ThOBr_2(cr)$		-1129.800 ± 5.400 [2008RAN/FUG]			$ThOBr_2(cr) + 2\ H^+ \rightleftarrows Th^{4+} + 2\ Br^- + H_2O(l)$			**-167.745** **± 5.878**	
$ThBrO_3^{3+}$	**-697.009** **± 5.394**				$Th^{4+} + BrO_3^- \rightleftarrows ThBrO_3^{3+}$	1.900 ± 0.100 [2008RAN/FUG]	-10.845 ± 0.571 [2008RAN/FUG]		
ThI(g)			288.600 ± 12.000 [2008RAN/FUG]	37.500 ± 6.000 [2008RAN/FUG]					
$ThI_2(g)$			355.600 ± 10.000 [2008RAN/FUG]	57.400 ± 5.000 [2008RAN/FUG]					
$ThI_3(g)$			430.000 ± 10.000 [2008RAN/FUG]	81.800 ± 5.000 [2008RAN/FUG]					
$ThI_4(cr)$	-659.487 ± 2.668 [2008RAN/FUG]	-669.600 ± 2.200 [2008RAN/FUG]	251.000 ± 5.000 [2008RAN/FUG]	137.100 ± 10.000 [2008RAN/FUG]	$ThI_4(cr) \rightleftarrows Th^{4+} + 4\ I^-$	**44.322** **± 1.193**	**-252.990** **± 6.811**	**-326.710** **± 4.619**	**-247.332** **± 16.784**
$ThI_4(g)$	-518.316 ± 5.753 [2008RAN/FUG]	-460.600 ± 5.463 [2008RAN/FUG]	478.500 ± 6.000 [2008RAN/FUG]	106.200 ± 4.000 [2008RAN/FUG]	$ThI_4(g) \rightleftarrows Th^{4+} + 4\ I^-$	**69.054** **± 1.490**	**-394.161** **± 8.507**	**-535.710** **± 6.807**	**-474.832** **± 17.108**
$ThOI_2(cr)$		-996.600 ± 2.300 [2008RAN/FUG]			$ThOI_2(cr) + 2\ H^+ \rightleftarrows Th^{4+} + 2\ I^- + H_2O(l)$			**-171.743** **± 3.659**	
$ThIO_3^{3+}$	**-856.445** **± 9.921**				$Th^{4+} + IO_3^- \rightleftarrows ThIO_3^{3+}$	4.140 ± 0.100 [2008RAN/FUG]	-23.631 ± 0.571 [2008RAN/FUG]		
$Th(IO_3)_2^{2+}$	**-1000.629** **± 17.568**				$Th^{4+} + 2\ IO_3^- \rightleftarrows Th(IO_3)_2^{2+}$	6.970 ± 0.120 [2008RAN/FUG]	-39.785 ± 0.685 [2008RAN/FUG]		
$Th(IO_3)_3^+$	**-1145.212** **± 25.665**				$Th^{4+} + 3\ IO_3^- \rightleftarrows Th(IO_3)_3^+$	9.870 ± 0.110 [2008RAN/FUG]	-56.338 ± 0.628 [2008RAN/FUG]		
ThS(cr)	-391.862 ± 6.205 [2008RAN/FUG]	-396.300 ± 6.200 [2008RAN/FUG]	69.810 ± 0.700 [2008RAN/FUG]	47.720 ± 0.500 [2008RAN/FUG]	$ThS(cr) + H^+ \rightleftarrows Th^{4+} + HS^- + 2\ e^-$	**52.725** **± 1.431**	**-300.955** **± 8.170**	**-388.508**	**-294.032**

Table A17 Selected thermodynamic data for thorium (Th) in JAEA-TDB-RN in 2020 (6/9)

Species / compound	$\Delta_f G^0_m$ (kJ.mol^{-1})	$\Delta_f H^0_m$ (kJ.mol^{-1})	S^0_m (J.K^{-1}.mol^{-1})	$C^0_{p,m}$ (J.K^{-1}.mol^{-1})	Reaction	$\log_{10} K°$	$\Delta_r G^0_m$ (kJ.mol^{-1})	$\Delta_r H^0_m$ (kJ.mol^{-1})	$\Delta_r S^0_m$ (J.K^{-1}.mol^{-1})
ThS_2(cr)			96.230 ± 1.700 [2008RAN/FUG]	70.290 ± 0.500 [2008RAN/FUG]					
Th_2S_3(cr)		-1079.000 ± 5.500 [2008RAN/FUG]							
ThOS(cr)			76.300 ± 1.500 [2008RAN/FUG]	67.250 ± 1.350 [2008RAN/FUG]					
$ThSO_4^{2+}$	**-1484.461 ± 5.623**	**-1657.382 ± 2.452**	**-215.980 ± 17.319**		$Th^{4+} + SO_4^{2-} \rightleftarrows ThSO_4^{2+}$	6.170 ± 0.320 [2008RAN/FUG]	-35.218 ± 1.827 [2008RAN/FUG]	20.920 ± 0.740 [2008RAN/FUG]	188.292 ± 6.610 [2008RAN/FUG]
$Th(SO_4)_2$(cr)	-4391.269 ± 5.404 [2008RAN/FUG]			173.500 ± 5.000 [2008RAN/FUG]					
$Th(SO_4)_2 \cdot 9H_2O$(cr)	**-4392.560 ± 5.480**				$Th^{4+} + 2\ SO_4^{2-} + 9\ H_2O(l) \rightleftarrows Th(SO_4)_2 \cdot 9H_2O$(cr)	11.250 ± 0.096 [2008RAN/FUG]	-64.215 ± 0.548 [2008RAN/FUG]		
$Th(SO_4)_2$(aq)	**-2249.012 ± 5.594**	**-2547.523 ± 2.675**	**-64.495 ± 17.229**		$Th^{4+} + 2\ SO_4^{2-} \rightleftarrows Th(SO_4)_2$(aq)	9.690 ± 0.270 [2008RAN/FUG]	-55.311 ± 1.541 [2008RAN/FUG]	40.380 ± 1.080 [2008RAN/FUG]	320.949 ± 6.312 [2008RAN/FUG]
$Th(SO_4)_3^{2-}$	**-2999.510 ± 5.492**				$Th^{4+} + 3\ SO_4^{2-} \rightleftarrows Th(SO_4)_3^{2-}$	10.748 ± 0.076 [2008RAN/FUG]	-61.350 ± 0.434 [2008RAN/FUG]		
ThOSe(cr)			93.500 ± 1.900 [2008RAN/FUG]	72.650 ± 1.500 [2008RAN/FUG]					
ThN(cr)	-353.638 ± 10.011 [2008RAN/FUG]	-381.200 ± 10.000 [2008RAN/FUG]	56.000 ± 1.500 [2008RAN/FUG]	45.000 ± 1.100 [2008RAN/FUG]	$ThN(cr) + 3\ H_2O(l) \rightleftarrows Th^{4+} + NO_3^- + 6\ H^+ + 9\ e^-$	**-43.708 ± 2.033**	**249.485 ± 11.605**	**263.116 ± 10.274**	**46.128 ± 16.095**
ThN_3^{3+}	**-381.927 ± 6.739**				$Th^{4+} + N_3^- \rightleftarrows ThN_3^{3+}$	4.440 ± 0.640 [2008RAN/FUG]	-25.344 ± 3.653 [2008RAN/FUG]		
$Th(N_3)_2^{2+}$	**-57.415 ± 7.577**				$Th^{4+} + 2\ N_3^- \rightleftarrows Th(N_3)_2^{2+}$	8.590 ± 0.640 [2008RAN/FUG]	-49.032 ± 3.653 [2008RAN/FUG]		
Th_3N_4(cr)	-1200.051 ± 15.659 [2008RAN/FUG]	-1306.800 ± 15.000 [2008RAN/FUG]	183.100 ± 15.000 [2008RAN/FUG]	147.700 ± 8.000 [2008RAN/FUG]	$Th_3N_4(cr) + 12\ H_2O(l) \rightleftarrows 3\ Th^{4+} + 4\ NO_3^- + 24\ H^+ + 32\ e^-$	**-260.724 ± 4.292**	**1488.222 ± 24.497**	**1603.165 ± 16.643**	**387.154 ± 50.413**
$Th(NO_3)_4 \cdot 4H_2O$(cr)		-2702.400 ± 3.800 [2008RAN/FUG]			$Th(NO_3)_4 \cdot 4H_2O(cr) \rightleftarrows Th^{4+} + 4\ NO_3^- + 4\ H_2O(l)$			**-37.249 ± 4.765**	

Table A17 Selected thermodynamic data for thorium (Th) in JAEA-TDB-RN in 2020 (7/9)

Species / compound	$\Delta_f G^0_m$ (kJ.mol^{-1})	$\Delta_f H^0_m$ (kJ.mol^{-1})	S^0_m (J.K^{-1}.mol^{-1})	$C^0_{p,m}$ (J.K^{-1}.mol^{-1})	Reaction	$\log_{10} K°$	$\Delta_r G^0_m$ (kJ.mol^{-1})	$\Delta_r H^0_m$ (kJ.mol^{-1})	$\Delta_r S^0_m$ (J.K^{-1}.mol^{-1})
$Th(NO_3)_4 \cdot 5H_2O$(cr)	-2322.651 ± 2.814 [2008RAN/FUG]	-3005.400 ± 2.800 [2008RAN/FUG]	543.100 ± 0.800 [2008RAN/FUG]	480.700 ± 0.800 [2008RAN/FUG]	$Th(NO_3)_4 \cdot 5H_2O$(cr) ⇄ Th^{4+} + 4 NO_3^- + 5 H_2O(l)	**2.053 ± 2.051**	**-11.716 ± 11.708**	**-20.087 ± 4.025**	**-28.817 ± 16.371**
$ThNO_3^{3+}$	**-823.121 ± 5.973**				Th^{4+} + NO_3^- ⇄ $ThNO_3^{3+}$	1.300 ± 0.200 [2008RAN/FUG]	-7.420 ± 1.142 [2008RAN/FUG]		
$Th(NO_3)_2^{2+}$	**-939.747 ± 7.648**				Th^{4+} + 2 NO_3^- ⇄ $Th(NO_3)_2^{2+}$	2.300 ± 0.400 [2008RAN/FUG]	-13.128 ± 2.283 [2008RAN/FUG]		
$Th_4(PO_4)_4P_2O_7$(cr)				569.000 ± 15.000 [2008RAN/FUG]					
$ThH_2PO_4^{3+}$	**-1867.126 ± 5.666**				Th^{4+} + H_3PO_4(aq) ⇄ $ThH_2PO_4^{3+}$ + H^+	3.450 ± 0.320 [2008RAN/FUG]	-19.693 ± 1.827 [2008RAN/FUG]		
$ThH_3PO_4^{4+}$	**-1858.222 ± 5.648**				Th^{4+} + H_3PO_4(aq) ⇄ $ThH_3PO_4^{4+}$	1.890 ± 0.310 [2008RAN/FUG]	-10.788 ± 1.769 [2008RAN/FUG]		
$Th(H_2PO_4)_2^{2+}$	**-3025.473 ± 5.849**				Th^{4+} + 2 H_3PO_4(aq) ⇄ $Th(H_2PO_4)_2^{2+}$ + 2 H^+	6.200 ± 0.320 [2008RAN/FUG]	-35.390 ± 1.827 [2008RAN/FUG]		
$Th(H_3PO_4)(H_2PO_4)^{3+}$	**-3021.021 ± 5.849**				Th^{4+} + 2 H_3PO_4(aq) ⇄ $Th(H_3PO_4)(H_2PO_4)^{3+}$ + H^+	5.420 ± 0.320 [2008RAN/FUG]	-30.937 ± 1.827 [2008RAN/FUG]		
ThAs(cr)			79.800 ± 0.500 [2008RAN/FUG]	50.500 ± 0.500 [2008RAN/FUG]					
Th_3As_4(cr)			274.600 ± 1.500 [2008RAN/FUG]	183.300 ± 1.500 [2008RAN/FUG]					
ThBi(cr)		-162.300 ± 4.200 [2008RAN/FUG]							
$ThBi_2$(cr)		-207.100 ± 6.300 [2008RAN/FUG]							
Th_3Bi_4(cr)		-597.500 ± 14.600 [2008RAN/FUG]							
Th_5Bi_3(cr)		-532.200 ± 16.700 [2008RAN/FUG]							

Table A17 Selected thermodynamic data for thorium (Th) in JAEA-TDB-RN in 2020 (8/9)

Species / compound	$\Delta_f G^0_m$ (kJ.mol^{-1})	$\Delta_f H^0_m$ (kJ.mol^{-1})	S^0_m (J.K^{-1}.mol^{-1})	$C^0_{p,m}$ (J.K^{-1}.mol^{-1})	Reaction	$\log_{10} K°$	$\Delta_r G^0_m$ (kJ.mol^{-1})	$\Delta_r H^0_m$ (kJ.mol^{-1})	$\Delta_r S^0_m$ (J.K^{-1}.mol^{-1})
Th_5Sn_3(cr)		-510.400 ± 32.000 [2008RAN/FUG]			Th_5Sn_3(cr) ⇄ 5 Th^{4+} + 3 Sn^{2+} + 26 e^-			**-3361.951** **± 34.205**	
$ThC_{0.97}$(cr)	-124.466 ± 6.308 [2008RAN/FUG]	-124.200 ± 6.300 [2008RAN/FUG]	59.100 ± 0.900 [2008RAN/FUG]	45.200 ± 0.400 [2008RAN/FUG]	$ThC_{0.97}$(cr) + 2.91 H_2O(l) ⇄ Th^{4+} + 0.97 CO_3^{2-} + 5.82 H^+ + 7.88 e^-	**70.472** **± 1.445**	**-402.259** **± 8.248**	**-467.688** **± 6.728**	**-219.300** **± 16.077**
$ThC_{1.94}$(s)	-126.705 ± 7.503 [2008RAN/FUG]	-124.700 ± 7.500 [2008RAN/FUG]	70.500 ± 0.400 [2008RAN/FUG]	56.800 ± 0.200 [2008RAN/FUG]	$ThC_{1.94}$(s) + 5.82 H_2O(l) ⇄ Th^{4+} + 1.94 CO_3^{2-} + 11.64 H^+ + 11.76 e^-	**38.886** **± 1.615**	**-221.963** **± 9.221**	**-290.377** **± 7.917**	**-229.158** **± 16.210**
$Th(CO_3)_5^{6-}$	**-3521.647** **± 6.795**				Th^{4+} + 5 CO_3^{2-} ⇄ $Th(CO_3)_5^{6-}$	31.000 ± 0.700 [2008RAN/FUG]	-176.948 ± 3.996 [2008RAN/FUG]		
$Th(CO_3)_2(OH)_2^{2-}$	**-2285.399** **± 6.048**				Th^{4+} + 2 CO_3^{2-} + 2 OH^- ⇄ $Th(CO_3)_2(OH)_2^{2-}$	36.800 ± 0.500 [2008RAN/FUG]	-210.055 ± 2.854 [2008RAN/FUG]		
$Th(CO_3)_4OH^{5-}$	**-3177.218** **± 6.131**				Th^{4+} + 4 CO_3^{2-} + OH^- ⇄ $Th(CO_3)_4OH^{5-}$	35.600 ± 0.500 [2008RAN/FUG]	-203.205 ± 2.854 [2008RAN/FUG]		
$ThCO_3(OH)_4^{2-}$	**-2092.560** **± 6.323**				Th^{4+} + CO_3^{2-} + 4 OH^- ⇄ $ThCO_3(OH)_4^{2-}$	40.400 ± 0.600 [2008RAN/FUG]	-230.604 ± 3.425 [2008RAN/FUG]		
$ThSCN^{3+}$	**-623.314** **± 10.307**				Th^{4+} + SCN^- ⇄ $ThSCN^{3+}$	2.000 ± 0.500 [2008RAN/FUG]	-11.416 ± 2.854 [2008RAN/FUG]		
$Th(SCN)_2^{2+}$	**-538.421** **± 18.139**				Th^{4+} + 2 SCN^- ⇄ $Th(SCN)_2^{2+}$	3.400 ± 0.800 [2008RAN/FUG]	-19.407 ± 4.566 [2008RAN/FUG]		
$ThSi_2$(cr)		-169.500 ± 9.600 [2008RAN/FUG]			$ThSi_2$(cr) + 4 H_2O(l) ⇄ Th^{4+} + $Si(OH)_4$(aq) + 4 H^+ + 8 e^-			**-2369.695** **± 12.042**	
$ThSiO_4$(huttonite)		-2110.800 ± 4.700 [2008RAN/FUG]			$ThSiO_4$(huttonite) + 4 H^+ ⇄ Th^{4+} + $Si(OH)_4$(aq)			**-114.824** **± 6.263**	
$ThSiO_4$(thorite)		-2117.500 ± 4.200 [2008RAN/FUG]			$ThSiO_4$(thorite) + 4 H^+ ⇄ Th^{4+} + $Si(OH)_4$(aq)			**-108.124** **± 5.897**	
$Na_6Th(CO_3)_5 \cdot 12H_2O$(cr)	**-8003.053** **± 7.286**				Th^{4+} + 5 CO_3^{2-} + 12 H_2O(l) + 6 Na^+ ⇄ $Na_6Th(CO_3)_5$•12H_2O(cr)	42.200 ± 0.800 [2008RAN/FUG]	-240.878 ± 4.566 [2008RAN/FUG]		
$ThTi_2O_6$(cr)		-3095.000 ± 4.300 [2008RAN/FUG]			$ThTi_2O_6$(cr) + 2 H_2O(l) + 4 H^+ ⇄ Th^{4+} + 2 $Ti(OH)_4$(aq)			**-142.955** **± 17.433**	

Table A17 Selected thermodynamic data for thorium (Th) in JAEA-TDB-RN in 2020 (9/9)

Species / compound	$\Delta_f G^0_m$ (kJ.mol^{-1})	$\Delta_f H^0_m$ (kJ.mol^{-1})	S^0_m (J.K^{-1}.mol^{-1})	$C^0_{p,m}$ (J.K^{-1}.mol^{-1})	Reaction	$\log_{10} K°$	$\Delta_r G^0_m$ (kJ.mol^{-1})	$\Delta_r H^0_m$ (kJ.mol^{-1})	$\Delta_r S^0_m$ (J.K^{-1}.mol^{-1})
$Th(OH)_3(H_3SiO_4)_3^{2-}$	**-5180.964**				$Th^{4+} + 3\ H_4SiO_4(aq) + 3\ H_2O(l)$	-27.800	**158.683**		
	± 8.597				$\rightleftarrows Th(OH)_3(H_3SiO_4)_3^{2-} + 6\ H^+$	± 0.700	**± 3.996**		
						[2008RAI/YUI]			
$Ca_4[Th(OH)_8]^{4+}$	**-4455.466**				$Th^{4+} + 8\ H_2O(l) + 4\ Ca^{2+} \rightleftarrows Ca_4[Th(OH)_8]^{4+} + 8\ H^+$	-62.708	**357.938**		
	± 8.105					± 0.908	**± 5.183**		
						[2008ALT/NEC]			

[2008RAN/FUG] Rand et al. [A25)]
[2008ALT/NEC] Altmaier et al. [A10)]
[2008RAI/YUI] Rai et al. [A26)]

Table A18 Selected thermodynamic data for protactinium (Pa) in JAEA-TDB-RN in 2020 (1/2)

Values indicated by **boldface** are calculated and selected in the present report.

Species / compound	$\Delta_f G^0_m$ (kJ.mol^{-1})	$\Delta_f H^0_m$ (kJ.mol^{-1})	S^0_m (J.K^{-1}.mol^{-1})	$C^0_{p,m}$ (J.K^{-1}.mol^{-1})	Reaction	$\log_{10} K°$	$\Delta_r G^0_m$ (kJ.mol^{-1})	$\Delta_r H^0_m$ (kJ.mol^{-1})	$\Delta_r S^0_m$ (J.K^{-1}.mol^{-1})
$PaOH^{3+}$					$Pa^{4+} + H_2O(l) \rightleftarrows PaOH^{3+} + H^+$	0.840	**-4.795**		
$Pa(OH)_2^{2+}$					$Pa^{4+} + 2\ H_2O(l) \rightleftarrows Pa(OH)_2^{2+} + 2\ H^+$	[1976BAE/MES] -0.020	**0.114**		
$Pa(OH)_3^{+}$					$Pa^{4+} + 3\ H_2O(l) \rightleftarrows Pa(OH)_3^{+} + 3\ H^+$	[1976BAE/MES] -1.500	**8.562**		
$PaOOH^{2+}$					$Pa^{4+} + 2\ H_2O(l) \rightleftarrows PaOOH^{2+} + e^- + 3\ H^+$	[1976BAE/MES] 1.860	**-10.617**		
$PaO(OH)_2^{+}$					$PaOOH^{2+} + H_2O(l) \rightleftarrows PaO(OH)_2^{+} + H^+$	[1976FUG/OET] -1.240 ± 0.020	**7.078** **± 0.114**		
$Pa(OH)_5(aq)$					$PaOOH^{2+} + 3\ H_2O(l) \rightleftarrows Pa(OH)_5(aq) + 2\ H^+$	[2002TRU/LEN] [2003TRU/LEN] -8.270 ± 0.151	**47.206** **± 0.862**		
$PaOOHCl^{+}$					$PaOOH^{2+} + Cl^- \rightleftarrows PaOOHCl^{+}$	[2002TRU/LEN] [2003TRU/LEN] 1.922 ± 0.020	**-10.971** **± 0.114**		
$PaOSO_4^{+}$					$PaOOH^{2+} + SO_4^{2-} + H^+ \rightleftarrows PaOSO_4^{+} + H_2O(l)$	[2010KIT/FUJ] 3.890 ± 0.180	**-22.204** **± 1.027**		
$PaO(SO_4)_2^{-}$					$PaOOH^{2+} + 2\ SO_4^{2-} + H^+ \rightleftarrows PaO(SO_4)_2^{-} + H_2O(l)$	[2007DIG/TRU] 7.000 ± 0.200	**-39.956** **± 1.142**		
$PaO(SO_4)_3^{3-}$					$PaOOH^{2+} + 3\ SO_4^{2-} + H^+ \rightleftarrows PaO(SO_4)_3^{3-} + H_2O(l)$	[2007DIG/TRU] 8.590 ± 0.230	**-49.032** **± 1.313**		
$PaO_2(cr)$					$PaO_2(cr) + 4\ H^+ \rightleftarrows Pa^{4+} + 2\ H_2O(l)$	[2007DIG/TRU] -0.600	**3.425**		
$PaCl_4(s)$					$PaCl_4(s) \rightleftarrows Pa^{4+} + 4\ Cl^-$	[1976BAE/MES] -24.010	**137.050**		
						[1998SHI/SHI]			

Table A18 Selected thermodynamic data for protactinium (Pa) in JAEA-TDB-RN in 2020 (2/2)

Species / compound	$\Delta_f G^0_m$ (kJ.mol^{-1})	$\Delta_f H^0_m$ (kJ.mol^{-1})	S^0_m (J.K^{-1}.mol^{-1})	$C^0_{p,m}$ (J.K^{-1}.mol^{-1})	Reaction	$\log_{10} K°$	$\Delta_r G^0_m$ (kJ.mol^{-1})	$\Delta_r H^0_m$ (kJ.mol^{-1})	$\Delta_r S^0_m$ (J.K^{-1}.mol^{-1})
Pa_2O_5(s)					$Pa_2O_5(s) + 4\ H^+ \rightleftarrows 2\ PaOOH^{2+} + H_2O(l)$	≤ 1.520	**≥ -8.676**		
						[2014KIT/DOI]			
$PaCl_5$(cr)					$PaCl_5(cr) + e^- \rightleftarrows Pa^{4+} + 5\ Cl^-$	-32.850	**187.509**		
						[1998SHI/SHI]			

[1976FUG/OET] Fuger and Oetting [A24].
[1976BAE/MES] Baes and Mesmer [A27].
[1998SHI/SHI] Shibutani and Shibutani [A28].
[2002TRU/LEN] Trubert et al. [A28]
[2003TRU/LEN] Trubert et al. [A29]
[2007DIG/TRU] Di Giandomenico et al. [A30]
[2010KIT/FUJ] Kitamura et al. [A13]
[2014KIT/DOI] Kitamura et al. [A32]

Table A19 Selected thermodynamic data for uranium (U) in JAEA-TDB-RN in 2020 (1/25)

Values indicated by **boldface** are calculated and selected in the present report.

Species / compound	$\Delta_f G^0_m$ (kJ.mol^{-1})	$\Delta_f H^0_m$ (kJ.mol^{-1})	S^0_m (J.K^{-1}.mol^{-1})	$C^0_{p,m}$ (J.K^{-1}.mol^{-1})	Reaction	$\log_{10} K°$	$\Delta_r G^0_m$ (kJ.mol^{-1})	$\Delta_r H^0_m$ (kJ.mol^{-1})	$\Delta_r S^0_m$ (J.K^{-1}.mol^{-1})
U(cr)	0.000	0.000	50.200	27.660					
			± 0.200	± 0.050					
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]					
U(g)	488.400	533.000	199.790	23.690					
	± 8.000	± 8.000	± 0.030	± 0.030					
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]					
U^{3+}	-476.473	-489.100	-188.172	-150.000	$U^{4+} + e^- \rightleftarrows U^{3+}$	-9.353	53.387	102.100	163.383
	± 1.810	± 3.712	± 13.853	± 50.000		± 0.070	± 0.400	± 1.700	± 5.857
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]		[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]
U^{4+}	**-529.775**	-591.200	-416.895	-220.000	$UO_2^{2+} + 4\ H^+ + 2\ e^- \rightleftarrows U^{4+} + 2\ H_2O(l)$	9.038	-51.589		
	± 1.774	± 3.300	± 12.553	± 50.000		± 0.041	± 0.234		
		[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]		[2003GUI/FAN]	[2003GUI/FAN]		
UO(g)	5.327	35.000	252.300	39.600	$UO(g) + 2\ H^+ \rightleftarrows U^{4+} + H_2O(l) + 2\ e^-$	**135.313**	**-772.370**	**-912.038**	**-468.593**
	± 10.018	± 10.000	± 2.000	± 2.000		**± 1.782**	**± 10.173**	**± 10.531**	**± 12.712**
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]					
UO_2(cr)	-1031.833	-1085.000	77.030	63.600	$UO_2(cr) + 4\ H^+ \rightleftarrows U^{4+} + 2\ H_2O(l)$	**-4.837**	**27.608**	**-77.877**	**-354.079**
	± 1.004	± 1.000	± 0.200	± 0.080		**± 0.357**	**± 2.040**	**± 10.531**	**± 12.556**
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]					
UO_2(am,hyd)	**-995.773**				$U^{4+} + 4\ OH^- \rightleftarrows UO_2(am,hyd) + 2\ H_2O(l)$	53.700	**-311.088**		
	± 5.986					± 1.000	**± 5.708**		
						[2010FUJ/KIT]			
UO_2(g)	-481.064	-477.800	266.300	59.500	$UO_2(g) + 4\ H^+ \rightleftarrows U^{4+} + 2\ H_2O(l)$	**91.653**	**-523.161**	**-685.077**	**-543.349**
	± 20.036	± 20.000	± 4.000	± 2.000		**± 3.524**	**± 20.115**	**± 20.272**	**± 13.176**
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]					
UO_2^+	**-961.022**	-1025.127	-25.000		$UO_2^{2+} + e^- \rightleftarrows UO_2^+$	1.484	-8.471	**-6.127**	**7.861**
	± 1.752	± 2.960	± 8.000			± 0.022	± 0.126	**± 3.318**	**± 8.544**
		[2003GUI/FAN]	[2003GUI/FAN]			[2003GUI/FAN]	[2003GUI/FAN]		
UO_2^{2+}	-952.551	-1019.000	-98.200	42.400					
	± 1.747	± 1.500	± 3.000	± 3.000					
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]					
β-$UO_{2.25}$	-1069.083	-1127.400	85.400		$\beta\text{-}UO_{2.25} + 4.5\ H^+ + 0.5\ e^- \rightleftarrows U^{4+} + 2.25\ H_2O(l)$	**-0.974**	**5.562**	**-106.936**	**-377.638**
	± 1.702	± 1.700	± 0.200			**± 0.431**	**± 2.462**	**± 3.720**	**± 12.556**
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]						
$UO_{2.25}$(cr)	-1069.125	-1128.000	83.530	73.340	$UO_{2.25}(cr) + 4.5\ H^+ + 0.5\ e^- \rightleftarrows U^{4+} + 2.25\ H_2O(l)$	**-0.982**	**5.604**	**-106.336**	**-375.768**
	± 1.702	± 1.700	± 0.170	± 0.150		**± 0.431**	**± 2.462**	**± 3.720**	**± 12.556**
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]					
α-$UO_{2.3333}$			82.17	71.420					
			± 0.500	± 0.140					
			[2003GUI/FAN]	[2003GUI/FAN]					

Table A19 Selected thermodynamic data for uranium (U) in JAEA-TDB-RN in 2020 (2/25)

Species / compound	$\Delta_f G^0_m$ (kJ.mol^{-1})	$\Delta_f H^0_m$ (kJ.mol^{-1})	S^0_m (J.K^{-1}.mol^{-1})	$C^0_{p,m}$ (J.K^{-1}.mol^{-1})	Reaction	$\log_{10} K°$	$\Delta_r G^0_m$ (kJ.mol^{-1})	$\Delta_r H^0_m$ (kJ.mol^{-1})	$\Delta_r S^0_m$ (J.K^{-1}.mol^{-1})
β-$UO_{2.3333}$	-1079.572 ± 2.002 [2003GUI/FAN]	-1141.000 ± 2.000 [2003GUI/FAN]	83.510 ± 0.200 [2003GUI/FAN]	71.840 ± 0.140 [2003GUI/FAN]	β-$UO_{2.3333}$ + 4.6666 H^+ + 0.6666 e^- ⇄ U^{4+} + 2.3333 H_2O(l)	**0.649 ± 0.469**	**-3.706 ± 2.679**	**-117.147 ± 3.866**	**-380.809 ± 12.556**
$UO_{2.6667}$(cr)	-1123.157 ± 0.804 [2003GUI/FAN]	-1191.600 ± 0.800 [2003GUI/FAN]	94.180 ± 0.170 [2003GUI/FAN]	79.310 ± 0.160 [2003GUI/FAN]	$UO_{2.6667}$(cr) + 1.3334 H^+ ⇄ UO_2^{2+} + 0.6667 H_2O(l) + 0.6666 e^-	**-2.186 ± 0.337**	**12.476 ± 1.924**	**-17.968 ± 1.701**	**-102.207 ± 3.005**
$UO_{2.86}$·0.5H_2O(cr)		-1367.000 ± 10.000 [2003GUI/FAN]			$UO_{2.86}$·0.5H_2O(cr) + 1.72 H^+ ⇄ UO_2^{2+} + 1.36 H_2O(l) + 0.28 e^-			**-40.740 ± 10.113**	
$UO_{2.86}$·1.5H_2O(cr)		-1666.000 ± 10.000 [2003GUI/FAN]			$UO_{2.86}$·1.5H_2O(cr) + 1.72 H^+ ⇄ UO_2^{2+} + 2.36 H_2O(l) + 0.28 e^-			**-27.578 ± 10.115**	
α-$UO_{2.95}$		-1211.280 ± 1.284 [2003GUI/FAN]			α-$UO_{2.95}$ + 1.9 H^+ ⇄ UO_2^{2+} + 0.95 H_2O(l) + 0.1 e^-			**-79.266 ± 1.977**	
α-UO_3	-1135.330 ± 1.482 [2003GUI/FAN]	-1212.410 ± 1.450 [2003GUI/FAN]	99.400 ± 1.000 [2003GUI/FAN]	81.840 ± 0.300 [2003GUI/FAN]	α-UO_3 + 2 H^+ ⇄ UO_2^{2+} + H_2O(l)	**9.531 ± 0.402**	**-54.404 ± 2.293**	**-92.428 ± 2.089**	**-127.677 ± 3.163**
β-UO_3	-1142.301 ± 1.307 [2003GUI/FAN]	-1220.300 ± 1.300 [2003GUI/FAN]	96.320 ± 0.400 [2003GUI/FAN]	81.340 ± 0.160 [2003GUI/FAN]	β-UO_3 + 2 H^+ ⇄ UO_2^{2+} + H_2O(l)	**8.310 ± 0.383**	**-47.433 ± 2.184**	**-84.538 ± 1.988**	**-124.597 ± 3.028**
γ-UO_3	-1145.739 ± 1.207 [2003GUI/FAN]	-1223.800 ± 1.200 [2003GUI/FAN]	96.110 ± 0.400 [2003GUI/FAN]	81.670 ± 0.160 [2003GUI/FAN]	γ-UO_3 + 2 H^+ ⇄ UO_2^{2+} + H_2O(l)	**7.707 ± 0.372**	**-43.995 ± 2.126**	**-81.038 ± 1.924**	**-124.387 ± 3.028**
δ-UO_3		-1213.730 ± 1.440 [2003GUI/FAN]			δ-UO_3 + 2 H^+ ⇄ UO_2^{2+} + H_2O(l)			**-91.108 ± 2.082**	
ε-UO_3		-1217.200 ± 1.300 [2003GUI/FAN]			ε-UO_3 + 2 H^+ ⇄ UO_2^{2+} + H_2O(l)			**-87.638 ± 1.988**	
UO_3(g)	-784.761 ± 15.012 [2003GUI/FAN]	-799.200 ± 15.000 [2003GUI/FAN]	309.500 ± 2.000 [2003GUI/FAN]	64.500 ± 2.000 [2003GUI/FAN]	UO_3(g) + 2 H^+ ⇄ UO_2^{2+} + H_2O(l)	**70.948 ± 2.648**	**-404.973 ± 15.114**	**-505.638 ± 15.075**	**-337.777 ± 3.607**
β-UH_3	-72.556 ± 0.148 [2003GUI/FAN]	-126.980 ± 0.130 [2003GUI/FAN]	63.680 ± 0.130 [2003GUI/FAN]	49.290 ± 0.080 [2003GUI/FAN]	β-UH_3 ⇄ U^{3+} + 3 H^+ + 6 e^-	**70.763 ± 0.318**	**-403.917 ± 1.816**	**-362.120 ± 3.714**	**140.185 ± 13.854**
UOH^{3+}	**-765.415 ± 2.501**	**-830.128 ± 9.541**	**-199.972 ± 12.907**		U^{4+} + H_2O(l) ⇄ UOH^{3+} + H^+	-0.285 ± 0.311 [2010FUJ/KIT]	**1.628 ± 1.774**	46.910 ± 10.096 [2003GUI/FAN]	147.000 ± 3.000 [2003GUI/FAN]
UO_2OH^+	**-1159.767 ± 2.222**	-1261.371 ± 15.072 [2003GUI/FAN]	17.000 ± 50.000 [2003GUI/FAN]		UO_2^{2+} + H_2O(l) ⇄ UO_2OH^+ + H^+	-5.250 ± 0.240 [2003GUI/FAN]	29.967 ± 1.370 [2003GUI/FAN]	**43.467 ± 15.147**	**45.277 ± 50.090**

Table A19 Selected thermodynamic data for uranium (U) in JAEA-TDB-RN in 2020 (3/25)

Species / compound	$\Delta_f G^0_m$ (kJ.mol^{-1})	$\Delta_f H^0_m$ (kJ.mol^{-1})	S^0_m (J.K^{-1}.mol^{-1})	$C^0_{p,m}$ (J.K^{-1}.mol^{-1})	Reaction	$\log_{10} K°$	$\Delta_r G^0_m$ (kJ.mol^{-1})	$\Delta_r H^0_m$ (kJ.mol^{-1})	$\Delta_r S^0_m$ (J.K^{-1}.mol^{-1})
$UO_3{\cdot}0.393H_2O$(cr)		-1347.800 ± 1.300 [2003GUI/FAN]			$UO_3{\cdot}0.393H_2O$(cr) + 2 H^+ ⇄ UO_2^{2+} + 1.393 H_2O(l)			**-69.373 ± 1.990**	
$UO_3{\cdot}0.648H_2O$(cr)		-1424.600 ± 1.300 [2003GUI/FAN]			$UO_3{\cdot}0.648H_2O$(cr) + 2 H^+ ⇄ UO_2^{2+} + 1.648 H_2O(l)			**-65.462 ± 1.992**	
α-$UO_3{\cdot}0.85H_2O$		-1491.900 ± 1.300 [2003GUI/FAN]			α-$UO_3{\cdot}0.85H_2O$ + 2 H^+ ⇄ UO_2^{2+} + 1.85 H_2O(l)			**-55.901 ± 1.994**	
α-$UO_3{\cdot}0.9H_2O$	-1374.560 ± 2.460 [2003GUI/FAN]	-1506.300 ± 1.300 [2003GUI/FAN]	126.000 ± 7.000 [2003GUI/FAN]	140.000 ± 30.000 [2003GUI/FAN]	α-$UO_3{\cdot}0.9H_2O$ + 2 H^+ ⇄ UO_2^{2+} + 1.9 H_2O(l)	**5.017 ± 0.530**	**-28.638 ± 3.023**	**-55.793 ± 1.995**	**-91.346 ± 7.617**
δ-$UO_3{\cdot}H_{0.83}$		-1285.400 ± 2.020 [2003GUI/FAN]			δ-$UO_3{\cdot}H_{0.83}$ + 1.17 H^+ ⇄ UO_2^{2+} + H_2O(l) + 0.83 e^-			**-19.438 ± 2.518**	
$U(OH)_2^{2+}$	**-994.120 ± 2.158**				U^{4+} + 2 H_2O(l) ⇄ $U(OH)_2^{2+}$ + 2 H^+	-1.770 ± 0.215 [2010FUJ/KIT]	**10.105 ± 1.226**		
$UO_2(OH)_2$(aq)	**-1357.563 ± 1.803**				UO_2^{2+} + 2 H_2O(l) ⇄ $UO_2(OH)_2$(aq) + 2 H^+	-12.150 ± 0.070 [2003GUI/FAN]	69.353 ± 0.400 [2003GUI/FAN]		
β-$UO_2(OH)_2$	-1398.683 ± 1.765 [2003GUI/FAN]	-1533.800 ± 1.300 [2003GUI/FAN]	138.000 ± 4.000 [2003GUI/FAN]	141.000 ± 15.000 [2003GUI/FAN]	UO_2^{2+} + 2 H_2O(l) ⇄ β-$UO_2(OH)_2$ + 2 H^+	**-4.946 ± 0.436**	**28.233 ± 2.491**	**56.877 ± 1.996**	**96.354 ± 5.003**
γ-$UO_2(OH)_2$		-1531.400 ± 1.300 [2003GUI/FAN]			UO_2^{2+} + 2 H_2O(l) ⇄ γ-$UO_2(OH)_2$ + 2 H^+			**59.277 ± 1.996**	
$U(OH)_3^+$	**-1212.094 ± 2.189**				U^{4+} + 3 H_2O(l) ⇄ $U(OH)_3^+$ + 3 H^+	-5.136 ± 0.221 [2010FUJ/KIT]	**29.314 ± 1.259**		
$U(OH)_4$(aq)	**-1417.053 ± 8.210**				U^{4+} + 4 H_2O(l) ⇄ $U(OH)_4$(aq) + 4 H^+	-10.781 ± 1.403 [2010FUJ/KIT]	**61.537 ± 8.008**		
$UO_2(OH)_3^-$	**-1548.511 ± 2.981**				UO_2^{2+} + 3 H_2O(l) ⇄ $UO_2(OH)_3^-$ + 3 H^+	-20.250 ± 0.420 [2003GUI/FAN]	115.588 ± 2.397 [2003GUI/FAN]		
$UO_3{\cdot}2H_2O$(cr)	-1636.506 ± 1.705 [2003GUI/FAN]	-1826.100 ± 1.700 [2003GUI/FAN]	188.540 ± 0.380 [2003GUI/FAN]	172.070 ± 0.340 [2003GUI/FAN]	UO_2^{2+} + 3 H_2O(l) ⇄ $UO_3{\cdot}2H_2O$(cr) + 2 H^+	**-4.834 ± 0.431**	**27.593 ± 2.460**	**50.415 ± 2.289**	**76.971 ± 3.034**
$UO_4{\cdot}2H_2O$(cr)		-1784.000 ± 4.200 [2003GUI/FAN]			UO_2^{2+} + 4 H_2O(l) ⇄ $UO_4{\cdot}2H_2O$(cr) + 4 H^+ + 2 e^-			**378.353 ± 4.479**	

Table A19 Selected thermodynamic data for uranium (U) in JAEA-TDB-RN in 2020 (4/25)

Species / compound	$\Delta_f G^0_m$ (kJ.mol^{-1})	$\Delta_f H^0_m$ (kJ.mol^{-1})	S^0_m (J.K^{-1}.mol^{-1})	$C^0_{p,m}$ (J.K^{-1}.mol^{-1})	Reaction	$\log_{10} K°$	$\Delta_r G^0_m$ (kJ.mol^{-1})	$\Delta_r H^0_m$ (kJ.mol^{-1})	$\Delta_r S^0_m$ (J.K^{-1}.mol^{-1})
$UO_4{\cdot}4H_2O$(cr)		-2384.700 ± 2.100 [2003GUI/FAN]			UO_2^{2+} + 6 H_2O(l) ⇄ $UO_4{\cdot}4H_2O$(cr) + 4 H^+ + 2 e^-			**349.330 ± 2.656**	
$(UO_2)_2OH^{3+}$	**-2126.873 ± 6.693**				2 UO_2^{2+} + H_2O(l) ⇄ $(UO_2)_2OH^{3+}$ + H^+	-2.700 ± 1.000 [2003GUI/FAN]	15.412 ± 5.708 [2003GUI/FAN]		
$(UO_2)_2(OH)_2^{2+}$	**-2347.388 ± 3.507**	-2572.065 ± 5.682 [2003GUI/FAN]	-38.000 ± 15.000 [2003GUI/FAN]		2 UO_2^{2+} + 2 H_2O(l) ⇄ $(UO_2)_2(OH)_2^{2+}$ + 2 H^+	-5.620 ± 0.040 [2003GUI/FAN]	32.079 ± 0.228 [2003GUI/FAN]	**37.612 ± 6.429**	**18.554 ± 16.156**
$(UO_2)_3(OH)_4^{2+}$	**-3738.457 ± 5.528**				3 UO_2^{2+} + 4 H_2O(l) ⇄ $(UO_2)_3(OH)_4^{2+}$ + 4 H^+	-11.900 ± 0.300 [2003GUI/FAN]	67.926 ± 1.712 [2003GUI/FAN]		
$(UO_2)_3(OH)_5^{+}$	**-3954.806 ± 5.309**	-4389.086 ± 10.394 [2003GUI/FAN]	83.000 ± 30.000 [2003GUI/FAN]		3 UO_2^{2+} + 5 H_2O(l) ⇄ $(UO_2)_3(OH)_5^{+}$ + 5 H^+	-15.550 ± 0.120 [2003GUI/FAN]	88.760 ± 0.685 [2003GUI/FAN]	**97.106 ± 11.338**	**27.985 ± 31.324**
$(UO_2)_3(OH)_7^{-}$	**-4334.132 ± 6.986**				3 UO_2^{2+} + 7 H_2O(l) ⇄ $(UO_2)_3(OH)_7^{-}$ + 7 H^+	-32.200 ± 0.800 [2003GUI/FAN]	183.799 ± 4.566 [2003GUI/FAN]		
$(UO_2)_4(OH)_7^{+}$	**-5345.472 ± 9.050**				4 UO_2^{2+} + 7 H_2O(l) ⇄ $(UO_2)_4(OH)_7^{+}$ + 7 H^+	-21.900 ± 1.000 [2003GUI/FAN]	125.010 ± 5.708 [2003GUI/FAN]		
UF(g)	-76.876 ± 20.020 [2003GUI/FAN]	-47.000 ± 20.000 [2003GUI/FAN]	251.800 ± 3.000 [2003GUI/FAN]	37.900 ± 3.000 [2003GUI/FAN]	UF(g) ⇄ U^{4+} + F^- + 3 e^-	**128.719 ± 3.523**	**-734.735 ± 20.109**	**-879.548 ± 20.281**	**-485.856 ± 12.918**
UF^{3+}	**-865.381 ± 3.469**	**-932.148 ± 3.404**	**-268.513 ± 16.001**		U^{4+} + F^- ⇄ UF^{3+}	9.420 ± 0.510 [2003GUI/FAN]	-53.770 ± 2.911 [2003GUI/FAN]	-5.600 ± 0.500 [2003GUI/FAN]	161.562 ± 9.907 [2003GUI/FAN]
UF_2(g)	-558.697 ± 25.177 [2003GUI/FAN]	-540.000 ± 25.000 [2003GUI/FAN]	315.700 ± 10.000 [2003GUI/FAN]	56.200 ± 5.000 [2003GUI/FAN]	UF_2(g) ⇄ U^{4+} + 2 F^- + 2 e^-	**93.669 ± 4.428**	**-534.664 ± 25.274**	**-721.895 ± 25.252**	**-628.275 ± 16.086**
UF_2^{2+}	**-1187.886 ± 4.619**	**-1265.395 ± 3.611**	**-137.954 ± 18.643**		U^{4+} + 2 F^- ⇄ UF_2^{2+}	16.560 ± 0.710 [2003GUI/FAN]	-94.525 ± 4.053 [2003GUI/FAN]	-3.500 ± 0.600 [2003GUI/FAN]	305.300 ± 13.741 [2003GUI/FAN]
UF_3(cr)	-1432.531 ± 4.702 [2003GUI/FAN]	-1501.400 ± 4.700 [2003GUI/FAN]	123.400 ± 0.400 [2003GUI/FAN]	95.100 ± 0.400 [2003GUI/FAN]	UF_3(cr) ⇄ U^{3+} + 3 F^-	**-19.412 ± 0.950**	**110.806 ± 5.424**	**6.257 ± 6.317**	**-351.111 ± 13.955**
UF_3(g)	-1062.947 ± 20.221 [2003GUI/FAN]	-1065.000 ± 20.000 [2003GUI/FAN]	347.500 ± 10.000 [2003GUI/FAN]	76.200 ± 5.000 [2003GUI/FAN]	UF_3(g) ⇄ U^{3+} + 3 F^-	**45.336 ± 3.574**	**-258.778 ± 20.401**	**-430.143 ± 20.440**	**-575.211 ± 17.163**
UF_4(aq)	**-1807.212 ± 6.349**	**-1941.020 ± 8.589**	**6.387 ± 21.244**		U^{4+} + 4 F^- ⇄ UF_4(aq)	26.340 ± 0.960 [2003GUI/FAN]	-150.350 ± 5.480 [2003GUI/FAN]	-8.430 ± 7.464 [2003GUI/FAN]	476.000 ± 17.000 [2003GUI/FAN]

Table A19 Selected thermodynamic data for uranium (U) in JAEA-TDB-RN in 2020 (5/25)

Species / compound	$\Delta_f G^0_m$ (kJ.mol^{-1})	$\Delta_f H^0_m$ (kJ.mol^{-1})	S^0_m (J.K^{-1}.mol^{-1})	$C^0_{p,m}$ (J.K^{-1}.mol^{-1})	Reaction	$\log_{10} K°$	$\Delta_r G^0_m$ (kJ.mol^{-1})	$\Delta_r H^0_m$ (kJ.mol^{-1})	$\Delta_r S^0_m$ (J.K^{-1}.mol^{-1})
UF_4(cr)	-1823.538	-1914.200	151.700	116.000	UF_4(cr) ⇄ U^{4+} + 4 F^-	**-29.200**	**166.676**	**-18.390**	**-621.313**
	± 4.201	± 4.200	± 0.200	± 0.100		**± 0.926**	**± 5.285**	**± 5.975**	**± 12.742**
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]					
UF_4(g)	-1576.851	-1605.200	360.700	95.100	UF_4(g) ⇄ U^{4+} + 4 F^-	**14.017**	**-80.011**	**-327.390**	**-830.313**
	± 6.698	± 6.530	± 5.000	± 3.000		**± 1.301**	**± 7.426**	**± 7.791**	**± 13.686**
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]					
UF_4·2.5H_2O(cr)	-2440.282	-2671.475	263.500	263.700	UF_4·2.5H_2O(cr) ⇄ U^{4+} + 4 F^- + 2.5 H_2O(l)	**-33.368**	**190.463**	**24.289**	**-558.306**
	± 6.188	± 4.277	± 15.000	± 15.000		**± 1.222**	**± 6.974**	**± 6.035**	**± 19.681**
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]					
α-UF_5	-1968.688	-2075.300	199.600	132.200	α-UF_5 + 2 H_2O(l) ⇄ UO_2^+ + 5 F^- + 4 H^+	**-12.838**	**73.279**	**-54.888**	**-430.344**
	± 6.995	± 5.900	± 12.600	± 4.200		**± 1.393**	**± 7.953**	**± 7.404**	**± 15.172**
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]					
β-UF_5	-1970.595	-2083.200	179.500	132.200	β-UF_5 + 2 H_2O(l) ⇄ UO_2^+ + 5 F^- + 4 H^+	**-13.172**	**75.186**	**-46.988**	**-410.244**
	± 5.635	± 4.200	± 12.600	± 12.000		**± 1.189**	**± 6.787**	**± 6.136**	**± 15.172**
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]					
UF_5(g)	-1862.083	-1913.000	386.400	110.600	UF_5(g) + 2 H_2O(l) ⇄ UO_2^+ + 5 F^- + 4 H^+	**5.838**	**-33.326**	**-217.188**	**-617.144**
	± 15.294	± 15.000	± 10.000	± 5.000		**± 2.760**	**± 15.755**	**± 15.653**	**± 13.093**
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]					
UF_5^-	**-2096.897**				U^{4+} + 5 F^- ⇄ UF_5^-	27.730	-158.284		
	± 5.671					± 0.740	± 4.224		
						[2003GUI/FAN]	[2003GUI/FAN]		
UF_6(cr)	-2069.205	-2197.700	227.600	166.800	UF_6(cr) + 2 H_2O(l) ⇄ UO_2^{2+} + 6 F^- + 4 H^+	**17.429**	**-99.484**	**-261.709**	**-544.724**
	± 1.842	± 1.800	± 1.300	± 0.200		**± 0.833**	**± 4.756**	**± 4.655**	**± 4.623**
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]					
UF_6(g)	-2064.440	-2148.600	376.300	129.400	UF_6(g) + 2 H_2O(l) ⇄ UO_2^{2+} + 6 F^- + 4 H^+	**18.264**	**-104.249**	**-310.809**	**-693.424**
	± 1.893	± 1.868	± 1.000	± 0.500		**± 0.837**	**± 4.776**	**± 4.682**	**± 4.547**
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]					
UF_6^{2-}	**-2390.463**				U^{4+} + 6 F^- ⇄ UF_6^{2-}	29.800	-170.100		
	± 5.934					± 0.700	± 3.996		
						[2003GUI/FAN]	[2003GUI/FAN]		
U_2F_9(cr)	-3812.000	-4015.923	329.000	251.000	U_2F_9(cr) + e^- ⇄ 2 U^{4+} + 9 F^-	**-37.933**	**216.525**	**-184.605**	**-1346.746**
	± 17.000	± 18.016	± 20.000	± 16.700		**± 3.220**	**± 18.378**	**± 20.111**	**± 32.470**
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]					
U_2F_{10}(g)		-3993.200			U_2F_{10}(g) + 4 H_2O(l) ⇄ 2 UO_2^+ + 10 F^- + 8 H^+			**-239.377**	
		± 30.366						**± 31.306**	
		[2003GUI/FAN]							
U_4F_{17}(cr)	-7464.000	-7849.655	631.000	485.300	U_4F_{17}(cr) + e^- ⇄ 4 U^{4+} + 17 F^-	**-97.196**	**554.800**	**-216.054**	**-2587.973**
	± 30.000	± 32.284	± 40.000	± 33.000		**± 5.756**	**± 32.854**	**± 36.688**	**± 64.859**
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]					
UOF_2(cr)	-1434.127	-1504.600	119.200		UOF_2(cr) + 2 H^+ ⇄ U^{4+} + 2 F^- + H_2O(l)	**-18.147**	**103.583**	**-43.134**	**-492.531**
	± 6.424	± 6.300	± 4.200			**± 1.191**	**± 6.796**	**± 7.238**	**± 13.282**
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]						

Table A19 Selected thermodynamic data for uranium (U) in JAEA-TDB-RN in 2020 (6/25)

Species / compound	$\Delta_f G^0_m$ (kJ.mol^{-1})	$\Delta_f H^0_m$ (kJ.mol^{-1})	S^0_m (J.K^{-1}.mol^{-1})	$C^0_{p,m}$ (J.K^{-1}.mol^{-1})	Reaction	$\log_{10} K°$	$\Delta_r G^0_m$ (kJ.mol^{-1})	$\Delta_r H^0_m$ (kJ.mol^{-1})	$\Delta_r S^0_m$ (J.K^{-1}.mol^{-1})
UOF_4(cr)	-1816.264	-1924.600	195.000		$UOF_4(cr) + H_2O(l) \rightleftarrows UO_2^{2+} + 4\ F^- + 2\ H^+$	**4.574**	**-26.107**	**-149.952**	**-415.841**
	± 4.269	± 4.000	± 5.000			**± 0.935**	**± 5.334**	**± 5.043**	**± 6.224**
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]						
UOF_4(g)	-1704.814	-1763.000	363.200	108.100	$UOF_4(g) + H_2O(l) \rightleftarrows UO_2^{2+} + 4\ F^- + 2\ H^+$	**24.099**	**-137.557**	**-311.552**	**-584.041**
	± 20.142	± 20.000	± 8.000	± 5.000		**± 3.573**	**± 20.394**	**± 20.234**	**± 8.817**
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]					
UO_2F^+	**-1263.755**	**-1352.648**	**-6.891**		$UO_2^{2+} + F^- \rightleftarrows UO_2F^+$	5.160	-29.453	1.700	104.489
	± 1.902	**± 1.645**	**± 3.269**			± 0.060	± 0.342	± 0.080	± 1.180
						[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]
UO_2F_2(aq)	**-1566.454**	**-1687.595**	**51.534**		$UO_2^{2+} + 2\ F^- \rightleftarrows UO_2F_2(aq)$	8.830	-50.402	2.100	176.093
	± 2.248	**± 2.020**	**± 3.597**			± 0.080	± 0.457	± 0.190	± 1.659
						[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]
UO_2F_2(cr)	-1557.322	-1653.500	135.560	103.220	$UO_2F_2(cr) \rightleftarrows UO_2^{2+} + 2\ F^-$	**-7.230**	**41.270**	**-36.195**	**-260.119**
	± 1.307	± 1.300	± 0.420	± 0.420		**± 0.448**	**± 2.560**	**± 2.394**	**± 3.219**
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]					
UO_2F_2(g)	-1318.081	-1352.500	342.700	86.400	$UO_2F_2(g) \rightleftarrows UO_2^{2+} + 2\ F^-$	**34.683**	**-197.971**	**-337.195**	**-467.259**
	± 10.242	± 10.084	± 0.600	± 3.000		**± 1.835**	**± 10.476**	**± 10.282**	**± 3.247**
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]					
$UO_2F_3^-$	**-1860.021**	**-2022.693**	**78.822**		$UO_2^{2+} + 3\ F^- \rightleftarrows UO_2F_3^-$	10.900	-62.218	2.350	216.561
	± 2.722	**± 2.526**	**± 4.051**			± 0.100	± 0.571	± 0.310	± 2.179
						[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]
$UO_2F_4^{2-}$	**-2147.136**	**-2360.100**	**76.730**		$UO_2^{2+} + 4\ F^- \rightleftarrows UO_2F_4^{2-}$	11.840	-67.583	0.290	227.648
	± 3.258	**± 3.105**	**± 4.545**			± 0.110	± 0.628	± 0.470	± 2.631
						[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]
$U_2O_3F_6$(cr)	-3372.730	-3579.200	324.000		$U_2O_3F_6(cr) + H_2O(l) \rightleftarrows 2\ UO_2^{2+} + 6\ F^- + 2\ H^+$	**-2.507**	**14.307**	**-185.047**	**-669.401**
	± 14.801	± 13.546	± 20.000			**± 2.756**	**± 15.730**	**± 14.444**	**± 21.134**
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]						
$U_3O_5F_8$(cr)	-4890.135	-5192.950	459.000	304.100	$U_3O_5F_8(cr) + H_2O(l) \rightleftarrows 3\ UO_2^{2+} + 8\ F^- + 2\ H^+$	**-2.744**	**15.660**	**-260.992**	**-928.960**
	± 9.771	± 3.929	± 30.000	± 4.143		**± 2.157**	**± 12.314**	**± 8.024**	**± 31.622**
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]					
H_3OUF_6(cr)		-2641.400			$H_3OUF_6(cr) + H_2O(l) \rightleftarrows UO_2^+ + 6\ F^- + 5\ H^+$			**-1135.101**	
		± 3.157						**± 7.820**	
		[2003GUI/FAN]							
UOFOH(cr)	-1336.930	-1426.700	121.000		$UOFOH(cr) \rightleftarrows UO_2^{2+} + F^- + H^+ + 2\ e^-$	**-17.980**	**102.628**	**72.352**	**-101.701**
	± 12.948	± 12.600	± 10.000			**± 2.292**	**± 13.082**	**± 12.707**	**± 10.455**
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]						
$UOFOH·0.5H_2O$(cr)	-1458.117	-1576.100	143.000		$UOFOH·0.5H_2O(cr) \rightleftarrows UO_2^{2+} + F^- + H^+ + 0.5\ H_2O(l) + 2\ e^-$	**-18.434**	**105.224**	**78.833**	**-88.739**
	± 6.970	± 6.300	± 10.000			**± 1.264**	**± 7.217**	**± 6.511**	**± 10.455**
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]						
$UOF_2·H_2O$(cr)	-1674.474	-1802.000	161.100		$UOF_2·H_2O(cr) + 2\ H^+ \rightleftarrows U^{4+} + 2\ F^- + 2\ H_2O(l)$	**-18.701**	**106.748**	**-31.572**	**-464.508**
	± 4.143	± 3.300	± 8.400			**± 0.824**	**± 4.702**	**± 4.860**	**± 15.144**
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]						

Table A19 Selected thermodynamic data for uranium (U) in JAEA-TDB-RN in 2020 (7/25)

Species / compound	$\Delta_f G^0_m$ (kJ.mol^{-1})	$\Delta_f H^0_m$ (kJ.mol^{-1})	S^0_m (J.K^{-1}.mol^{-1})	$C^0_{p,m}$ (J.K^{-1}.mol^{-1})	Reaction	$\log_{10} K°$	$\Delta_r G^0_m$ (kJ.mol^{-1})	$\Delta_r H^0_m$ (kJ.mol^{-1})	$\Delta_r S^0_m$ (J.K^{-1}.mol^{-1})
$UO_2FOH·H_2O$(cr)	-1721.700	-1894.500	178.345		$UO_2FOH·H_2O(cr) + H^+ \rightleftarrows UO_2^{2+} + F^- + 2\ H_2O(l)$	**-2.283**	**13.033**	**-31.524**	**-149.879**
	± 7.500	± 8.400	± 37.770			**± 1.355**	**± 7.732**	**± 8.562**	**± 37.893**
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]						
$UO_2FOH·2H_2O$(cr)	-1961.032	-2190.010	223.180		$UO_2FOH·2H_2O(cr) + H^+ \rightleftarrows UO_2^{2+} + F^- + 3\ H_2O(l)$	**-2.660**	**15.183**	**-21.853**	**-124.791**
	± 8.408	± 9.392	± 38.244			**± 1.510**	**± 8.619**	**± 9.540**	**± 38.366**
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]						
$UO_2F_2·3H_2O$(cr)	-2269.658	-2534.390	270.000		$UO_2F_2·3H_2O(cr) \rightleftarrows UO_2^{2+} + 2\ F^- + 3\ H_2O(l)$	**-7.368**	**42.058**	**-12.820**	**-184.790**
	± 6.939	± 4.398	± 18.000			**± 1.276**	**± 7.286**	**± 4.846**	**± 18.282**
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]						
UCl(g)	155.945	187.000	265.900	43.200	$UCl(g) \rightleftarrows U^{4+} + Cl^- + 3\ e^-$	**143.148**	**-817.095**	**-945.280**	**-430.042**
	± 20.020	± 20.000	± 3.000	± 3.000		**± 3.521**	**± 20.098**	**± 20.271**	**± 12.908**
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]					
UCl^{3+}	**-670.968**	**-777.280**	**-390.957**		$U^{4+} + Cl^- \rightleftarrows UCl^{3+}$	1.720	-9.818	-19.000	-30.797
	± 1.917	**± 9.586**	**± 32.788**			± 0.130	± 0.742	± 9.000	± 30.289
						[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]
UCl_2(g)	-174.624	-155.000	339.100	59.900	$UCl_2(g) \rightleftarrows U^{4+} + 2\ Cl^- + 2\ e^-$	**108.236**	**-617.815**	**-770.359**	**-511.846**
	± 20.221	± 20.000	± 10.000	± 5.000		**± 3.556**	**± 20.299**	**± 20.271**	**± 16.053**
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]					
UCl_3(cr)	-796.103	-863.700	158.100	102.520	$UCl_3(cr) \rightleftarrows U^{4+} + 3\ Cl^- + e^-$	**13.006**	**-74.239**	**-126.639**	**-176.067**
	± 2.006	± 2.000	± 0.500	± 0.500		**± 0.476**	**± 2.719**	**± 4.225**	**± 13.871**
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]					
UCl_3(g)	-521.652	-523.000	380.300	82.400	$UCl_3(g) \rightleftarrows U^{4+} + 3\ Cl^- + e^-$	**61.088**	**-348.690**	**-467.339**	**-398.267**
	± 20.221	± 20.000	± 10.000	± 5.000		**± 3.557**	**± 20.304**	**± 20.343**	**± 17.093**
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]					
UCl_4(cr)	-929.605	-1018.800	197.200	121.800	$UCl_4(cr) \rightleftarrows U^{4+} + 4\ Cl^-$	**21.971**	**-125.414**	**-240.719**	**-387.155**
	± 2.512	± 2.500	± 0.800	± 0.400		**± 0.542**	**± 3.096**	**± 4.155**	**± 12.596**
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]					
UCl_4(g)	-789.442	-815.400	409.300	103.500	$UCl_4(g) \rightleftarrows U^{4+} + 4\ Cl^-$	**46.527**	**-265.577**	**-444.119**	**-599.255**
	± 4.947	± 4.717	± 5.000	± 3.000		**± 0.923**	**± 5.268**	**± 5.767**	**± 13.529**
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]					
UCl_5(cr)	-930.115	-1039.000	242.700	150.600	$UCl_5(cr) + 2\ H_2O(l) \rightleftarrows UO_2^+ + 5\ Cl^- + 4\ H^+$	**37.314**	**-212.989**	**-249.849**	**-123.871**
	± 3.908	± 3.000	± 8.400	± 8.400		**± 0.756**	**± 4.317**	**± 4.242**	**± 11.631**
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]					
UCl_5(g)	-849.552	-900.000	438.700	123.600	$UCl_5(g) + 2\ H_2O(l) \rightleftarrows UO_2^+ + 5\ Cl^- + 4\ H^+$	**51.428**	**-293.552**	**-388.849**	**-319.871**
	± 15.074	± 15.000	± 10.000	± 5.000		**± 2.660**	**± 15.185**	**± 15.297**	**± 12.835**
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]					
UCl_6(cr)	-937.120	-1066.500	285.500	175.000	$UCl_6(cr) + 2\ H_2O(l) \rightleftarrows UO_2^{2+} + 6\ Cl^- + 4\ H^+$	**57.604**	**-328.804**	**-383.301**	**-183.136**
	± 3.043	± 3.000	± 1.700	± 4.200		**± 0.625**	**± 3.566**	**± 3.402**	**± 3.595**
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]					
UCl_6(g)	-901.588	-985.500	438.000	147.200	$UCl_6(g) + 2\ H_2O(l) \rightleftarrows UO_2^{2+} + 6\ Cl^- + 4\ H^+$	**63.829**	**-364.336**	**-464.301**	**-335.636**
	± 5.218	± 5.000	± 5.000	± 3.000		**± 0.970**	**± 5.539**	**± 5.251**	**± 5.919**
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]					

Table A19 Selected thermodynamic data for uranium (U) in JAEA-TDB-RN in 2020 (8/25)

Species / compound	$\Delta_f G^0_m$ (kJ.mol^{-1})	$\Delta_f H^0_m$ (kJ.mol^{-1})	S^0_m (J.K^{-1}.mol^{-1})	$C^0_{p,m}$ (J.K^{-1}.mol^{-1})	Reaction	$\log_{10} K°$	$\Delta_r G^0_m$ (kJ.mol^{-1})	$\Delta_r H^0_m$ (kJ.mol^{-1})	$\Delta_r S^0_m$ (J.K^{-1}.mol^{-1})
U_2Cl_{10}(g)		-1965.300 ± 10.208 [2003GUI/FAN]			$U_2Cl_{10}(g) + 4\ H_2O(l) \rightleftarrows 2\ UO_2^+ + 10\ Cl^- + 8\ H^+$			**-612.397 ± 11.840**	
UOCl(cr)	-785.654 ± 4.890 [2003GUI/FAN]	-833.900 ± 4.200 [2003GUI/FAN]	102.500 ± 8.400 [2003GUI/FAN]	71.000 ± 5.000 [2003GUI/FAN]	$UOCl(cr) + 2\ H^+ \rightleftarrows U^{3+} + Cl^- + H_2O(l)$	**10.387 ± 0.914**	**-59.291 ± 5.216**	**-108.118 ± 5.607**	**-164.014 ± 16.202**
$UOCl_2$(cr)	-998.478 ± 2.701 [2003GUI/FAN]	-1069.300 ± 2.700 [2003GUI/FAN]	138.320 ± 0.210 [2003GUI/FAN]	95.060 ± 0.420 [2003GUI/FAN]	$UOCl_2(cr) + 2\ H^+ \rightleftarrows U^{4+} + 2\ Cl^- + H_2O(l)$	**5.456 ± 0.567**	**-31.144 ± 3.234**	**-141.898 ± 4.269**	**-371.822 ± 12.559**
$UOCl_3$(cr)	-1045.576 ± 8.383 [2003GUI/FAN]	-1140.000 ± 8.000 [2003GUI/FAN]	170.700 ± 8.400 [2003GUI/FAN]	117.200 ± 4.200 [2003GUI/FAN]	$UOCl_3(cr) + H_2O(l) \rightleftarrows UO_2^+ + 3\ F^- + 2\ H^+$	**12.637 ± 1.501**	**-72.132 ± 8.570**	**-100.528 ± 8.535**	**-95.418 ± 11.611**
UO_2Cl(cr)	-1095.253 ± 8.383 [2003GUI/FAN]	-1171.100 ± 8.000 [2003GUI/FAN]	112.500 ± 8.400 [2003GUI/FAN]	88.000 ± 5.000 [2003GUI/FAN]	$UO_2Cl(cr) \rightleftarrows UO_2^+ + Cl^-$	**-0.515 ± 1.500**	**2.942 ± 8.565**	**-21.107 ± 8.530**	**-80.765 ± 11.611**
UO_2Cl^+	**-1084.811 ± 1.754**	-1178.080 ± 2.502 [2003GUI/FAN]	**-11.378 ± 7.360**		$UO_2^{2+} + Cl^- \rightleftarrows UO_2Cl^+$	0.170 ± 0.020 [2003GUI/FAN]	-0.970 ± 0.114 [2003GUI/FAN]	8.000 ± 2.000 [2003GUI/FAN]	30.087 ± 6.719 [2003GUI/FAN]
UO_2Cl_2(aq)	**-1208.851 ± 2.882**	**-1338.159 ± 6.187**	44.251 ± 21.744 [2003GUI/FAN]		$UO_2^{2+} + 2\ Cl^- \rightleftarrows UO_2Cl_2(aq)$	-1.100 ± 0.400 [2003GUI/FAN]	6.279 ± 2.283 [2003GUI/FAN]	15.000 ± 6.000 [2003GUI/FAN]	29.251 ± 21.532 [2003GUI/FAN]
UO_2Cl_2(cr)	-1145.838 ± 1.303 [2003GUI/FAN]	-1243.600 ± 1.300 [2003GUI/FAN]	150.540 ± 0.210 [2003GUI/FAN]	107.860 ± 0.170 [2003GUI/FAN]	$UO_2Cl_2(cr) \rightleftarrows UO_2^{2+} + 2\ Cl^-$	**12.139 ± 0.383**	**-69.292 ± 2.189**	**-109.559 ± 1.993**	**-135.270 ± 3.026**
UO_2Cl_2(g)	-938.984 ± 15.106 [2003GUI/FAN]	-970.300 ± 15.000 [2003GUI/FAN]	373.400 ± 6.000 [2003GUI/FAN]	92.600 ± 3.000 [2003GUI/FAN]	$UO_2Cl_2(g) \rightleftarrows UO_2^{2+} + 2\ Cl^-$	**48.378 ± 2.664**	**-276.146 ± 15.208**	**-382.859 ± 15.076**	**-358.130 ± 6.717**
$U_2O_2Cl_5$(cr)	-2037.306 ± 4.891 [2003GUI/FAN]	-2197.400 ± 4.200 [2003GUI/FAN]	326.300 ± 8.400 [2003GUI/FAN]	219.400 ± 5.000 [2003GUI/FAN]	$U_2O_2Cl_5(cr) + 2\ H_2O(l) \rightleftarrows 2\ UO_2^{2+} + 5\ Cl^- + 4\ H^+ + 3\ e^-$	**8.738 ± 1.057**	**-49.879 ± 6.035**	**-104.322 ± 5.184**	**-182.853 ± 10.358**
$(UO_2)_2Cl_3$(cr)	-2234.755 ± 2.931 [2003GUI/FAN]	-2404.500 ± 1.700 [2003GUI/FAN]	276.000 ± 8.000 [2003GUI/FAN]	203.600 ± 5.000 [2003GUI/FAN]	$(UO_2)_2Cl_3(cr) + e^- \rightleftarrows 2\ UO_2^{2+} + 3\ Cl^- + e^-$	**11.250 ± 0.801**	**-64.216 ± 4.571**	**-134.739 ± 3.458**	**-236.855 ± 10.013**
$UO_2ClO_3^+$	**-963.355 ± 1.978**	**-1126.914 ± 1.744**	**60.631 ± 9.046**		$UO_2^{2+} + ClO_3^- \rightleftarrows UO_2ClO_3^+$	0.500 ± 0.070 [2003GUI/FAN]	-2.854 ± 0.400 [2003GUI/FAN]	-3.900 ± 0.300 [2003GUI/FAN]	-3.508 ± 1.676 [2003GUI/FAN]
$U_5O_{12}Cl$(cr)	-5517.951 ± 12.412 [2003GUI/FAN]	-5854.400 ± 8.600 [2003GUI/FAN]	465.000 ± 30.000 [2003GUI/FAN]		$U_5O_{12}Cl(cr) + 4\ H^+ \rightleftarrows 5\ UO_2^{2+} + Cl^- + 2\ H_2O(l) + 5\ e^-$	**-26.198 ± 2.659**	**149.541 ± 15.179**	**20.644 ± 11.413**	**-432.722 ± 33.542**
$UO_2Cl_2 \cdot H_2O$(cr)	-1405.003 ± 3.269 [2003GUI/FAN]	-1559.800 ± 2.100 [2003GUI/FAN]	192.500 ± 8.400 [2003GUI/FAN]		$UO_2Cl_2 \cdot H_2O(cr) \rightleftarrows UO_2^{2+} + 2\ Cl^- + H_2O(l)$	**8.288 ± 0.651**	**-47.310 ± 3.713**	**-79.198 ± 2.589**	**-107.307 ± 8.926**

Table A19 Selected thermodynamic data for uranium (U) in JAEA-TDB-RN in 2020 (9/25)

Species / compound	$\Delta_f G^0_m$ (kJ.mol^{-1})	$\Delta_f H^0_m$ (kJ.mol^{-1})	S^0_m (J.K^{-1}.mol^{-1})	$C^0_{p,m}$ (J.K^{-1}.mol^{-1})	Reaction	$\log_{10} K°$	$\Delta_r G^0_m$ (kJ.mol^{-1})	$\Delta_r H^0_m$ (kJ.mol^{-1})	$\Delta_r S^0_m$ (J.K^{-1}.mol^{-1})
$UO_2ClOH·2H_2O$(cr)	-1782.219	-2010.400	236.000		$UO_2ClOH·2H_2O(cr) + H^+ \rightleftarrows UO_2^{2+} + Cl^- + 3\ H_2O(l)$	**2.307**	**-13.170**	**-33.195**	**-67.696**
	± 4.507	± 1.700	± 14.000			**± 0.849**	**± 4.844**	**± 2.290**	**± 14.321**
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]						
$UO_2Cl_2·3H_2O$(cr)	-1894.616	-2164.800	272.000		$UO_2Cl_2·3H_2O(cr) \rightleftarrows UO_2^{2+} + 2\ Cl^- + 3\ H_2O(l)$	**5.617**	**-32.062**	**-45.874**	**-46.961**
	± 3.028	± 1.700	± 8.400			**± 0.616**	**± 3.515**	**± 2.296**	**± 8.929**
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]						
UCl_3F(cr)	-1146.573	-1243.000	162.800	118.800	$UCl_3F(cr) \rightleftarrows U^{4+} + 3\ Cl^- + F^-$	**10.320**	**-58.907**	**-184.787**	**-422.669**
	± 5.155	± 5.000	± 4.200	± 4.200		**± 0.963**	**± 5.498**	**± 6.034**	**± 13.258**
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]					
UCl_2F_2(cr)	-1375.967	-1466.000	174.100	119.700	$UCl_2F_2(cr) \rightleftarrows U^{4+} + 2\ Cl^- + 2\ F^-$	**-3.508**	**20.026**	**-130.055**	**-503.884**
	± 5.592	± 5.000	± 8.400	± 4.200		**± 1.054**	**± 6.018**	**± 6.141**	**± 15.147**
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]					
$UClF_3$(cr)	-1606.360	-1690.000	185.400	120.900	$UClF_3(cr) \rightleftarrows U^{4+} + Cl^- + 3\ F^-$	**-17.512**	**99.959**	**-74.322**	**-585.099**
	± 5.155	± 5.000	± 4.200	± 4.200		**± 1.018**	**± 5.808**	**± 6.319**	**± 13.338**
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]					
UBr(g)	199.623	245.000	278.500	44.500	$UBr(g) \rightleftarrows U^{4+} + Br^- + 3\ e^-$	**146.027**	**-833.527**	**-957.703**	**-416.533**
	± 15.027	± 15.000	± 3.000	± 3.000		**± 2.651**	**± 15.131**	**± 15.359**	**± 12.908**
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]					
UBr^{3+}	**-642.238**				$U^{4+} + Br^- \rightleftarrows UBr^{3+}$	1.460	-8.334		
	± 2.109					± 0.200	± 1.142		
						[2003GUI/FAN]	[2003GUI/FAN]		
UBr_2(g)	-86.896	-40.000	359.700	61.400	$UBr_2(g) \rightleftarrows U^{4+} + 2\ Br^- + 2\ e^-$	**114.059**	**-651.051**	**-794.207**	**-480.230**
	± 15.294	± 15.000	± 10.000	± 5.000		**± 2.698**	**± 15.399**	**± 15.362**	**± 16.055**
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]					
UBr_3(cr)	-673.198	-698.700	192.980	105.830	$UBr_3(cr) \rightleftarrows U^{3+} + 3\ Br^-$	**20.218**	**-115.406**	**-154.910**	**-132.622**
	± 4.205	± 4.200	± 0.500	± 0.500		**± 0.807**	**± 4.605**	**± 5.623**	**± 13.876**
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]					
UBr_3(g)	-408.115	-371.000	403.000	85.200	$UBr_3(g) \rightleftarrows U^{3+} + 3\ Br^-$	**66.658**	**-380.489**	**-482.610**	**-342.642**
	± 20.494	± 20.000	± 15.000	± 5.000		**± 3.605**	**± 20.580**	**± 20.347**	**± 20.428**
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]					
UBr_4(cr)	-767.479	-802.100	238.500	128.000	$UBr_4(cr) \rightleftarrows U^{4+} + 4\ Br^-$	**31.281**	**-178.555**	**-275.113**	**-324.022**
	± 3.544	± 2.500	± 8.400	± 4.200		**± 0.703**	**± 4.015**	**± 4.184**	**± 15.127**
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]					
UBr_4(g)	-634.604	-605.600	451.900	106.900	$UBr_4(g) \rightleftarrows U^{4+} + 4\ Br^-$	**54.560**	**-311.430**	**-471.613**	**-537.422**
	± 4.951	± 4.717	± 5.000	± 3.000		**± 0.928**	**± 5.299**	**± 5.788**	**± 13.538**
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]					
UBr_5(cr)	-769.308	-810.400	292.900	160.700	$UBr_5(cr) + 2\ H_2O(l) \rightleftarrows UO_2^+ + 5\ Br^- + 4\ H^+$	**41.619**	**-237.565**	**-250.567**	**-43.530**
	± 9.205	± 8.400	± 12.600	± 8.000		**± 1.648**	**± 9.410**	**± 8.941**	**± 14.963**
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]					
UBr_5(g)	-668.212	-647.945	498.700	129.000	$UBr_5(g) + 2\ H_2O(l) \rightleftarrows UO_2^+ + 5\ Br^- + 4\ H^+$	**59.331**	**-338.661**	**-413.022**	**-249.330**
	± 15.295	± 15.000	± 10.000	± 5.000		**± 2.701**	**± 15.419**	**± 15.309**	**± 12.850**
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]					

Table A19 Selected thermodynamic data for uranium (U) in JAEA-TDB-RN in 2020 (10/25)

Species / compound	$\Delta_f G^0_m$ (kJ.mol^{-1})	$\Delta_f H^0_m$ (kJ.mol^{-1})	S^0_m (J.K^{-1}.mol^{-1})	$C^0_{p,m}$ (J.K^{-1}.mol^{-1})	Reaction	$\log_{10} K°$	$\Delta_r G^0_m$ (kJ.mol^{-1})	$\Delta_r H^0_m$ (kJ.mol^{-1})	$\Delta_r S^0_m$ (J.K^{-1}.mol^{-1})
$UOBr_2$(cr)	-929.648	-973.600	157.570	98.000	$UOBr_2(cr) + 2\ H^+ \rightleftarrows U^{4+} + 2\ Br^- + H_2O(l)$	**7.968**	**-45.482**	**-146.445**	**-338.856**
	± 8.401	± 8.400	± 0.290	± 0.400		**± 1.505**	**± 8.592**	**± 9.031**	**± 12.564**
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]					
$UOBr_3$(cr)	-901.498	-954.000	205.000	120.900	$UOBr_3(cr) + H_2O(l) \rightleftarrows UO_2^+ + 3\ Br^- + 2\ H^+$	**23.558**	**-134.471**	**-149.799**	**-51.393**
	± 21.334	± 21.000	± 12.600	± 4.200		**± 3.751**	**± 21.412**	**± 21.213**	**± 14.939**
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]					
UO_2Br^+	**-1057.851**				$UO_2^{2+} + Br^- \rightleftarrows UO_2Br^+$	0.220	-1.256		
	± 1.759					± 0.020	± 0.114		
						[2003GUI/FAN]	[2003GUI/FAN]		
UO_2Br_2(cr)	-1066.422	-1137.400	169.500	116.000	$UO_2Br_2(cr) \rightleftarrows UO_2^{2+} + 2\ Br^-$	**16.506**	**-94.216**	**-124.607**	**-102.014**
	± 1.808	± 1.300	± 4.200	± 8.000		**± 0.444**	**± 2.536**	**± 2.008**	**± 5.178**
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]					
$UO_2BrO_3^+$	**-937.528**	**-1085.970**	**75.909**		$UO_2^{2+} + BrO_3^- \rightleftarrows UO_2BrO_3^+$	0.630	-3.596	0.100	12.397
	± 1.990	**± 1.744**	**± 3.614**			± 0.080	± 0.457	± 0.300	± 1.833
						[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]
$UO_2Br_2 \cdot H_2O$(cr)	-1328.644	-1455.900	214.000		$UO_2Br_2 \cdot H_2O(cr) \rightleftarrows UO_2^{2+} + 2\ Br^- + H_2O(l)$	**12.119**	**-69.177**	**-91.945**	**-76.591**
	± 2.515	± 1.400	± 7.000			**± 0.540**	**± 3.082**	**± 2.076**	**± 7.628**
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]						
$UO_2BrOH \cdot 2H_2O$(cr)	-1744.162	-1958.200	248.000		$UO_2BrOH \cdot 2H_2O(cr) + H^+ \rightleftarrows UO_2^{2+} + Br^- + 3\ H_2O(l)$	**4.201**	**-23.980**	**-39.818**	**-53.588**
	± 4.372	± 1.300	± 14.000			**± 0.827**	**± 4.721**	**± 2.015**	**± 14.322**
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]						
$UO_2Br_2 \cdot 3H_2O$(cr)	-1818.486	-2058.000	304.000		$UO_2Br_2 \cdot 3H_2O(cr) \rightleftarrows UO_2^{2+} + 2\ Br^- + 3\ H_2O(l)$	**9.408**	**-53.700**	**-61.522**	**-26.745**
	± 5.573	± 1.500	± 18.000			**± 1.026**	**± 5.858**	**± 2.165**	**± 18.255**
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]						
UBr_2Cl(cr)	-714.389	-750.600	192.500		$UBr_2Cl(cr) \rightleftarrows U^{3+} + 2\ Br^- + Cl^-$	**17.775**	**-101.461**	**-148.586**	**-158.251**
	± 9.765	± 8.400	± 16.700			**± 1.741**	**± 9.937**	**± 9.189**	**± 21.703**
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]						
UBr_3Cl(cr)	-807.114	-852.300	238.500		$UBr_3Cl(cr) \rightleftarrows U^{4+} + 3\ Br^- + Cl^-$	**29.111**	**-166.166**	**-270.490**	**-350.130**
	± 9.766	± 8.400	± 16.700			**± 1.741**	**± 9.937**	**± 9.037**	**± 20.902**
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]						
$UBrCl_2$(cr)	-760.315	-812.100	175.700		$UBrCl_2(cr) \rightleftarrows U^{3+} + Br^- + 2\ Cl^-$	**14.503**	**-82.781**	**-132.663**	**-167.559**
	± 9.765	± 8.400	± 16.700			**± 1.740**	**± 9.935**	**± 9.187**	**± 21.701**
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]						
UBr_2Cl_2(cr)	-850.896	-907.900	234.300		$UBr_2Cl_2(cr) \rightleftarrows U^{4+} + 2\ Br^- + 2\ Cl^-$	**26.214**	**-149.631**	**-260.466**	**-372.039**
	± 9.765	± 8.400	± 16.700			**± 1.740**	**± 9.931**	**± 9.032**	**± 20.899**
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]						
$UBrCl_3$(cr)	-893.500	-967.300	213.400		$UBrCl_3(cr) \rightleftarrows U^{4+} + Br^- + 3\ Cl^-$	**23.523**	**-134.273**	**-246.642**	**-377.247**
	± 9.202	± 8.400	± 12.600			**± 1.643**	**± 9.376**	**± 9.030**	**± 17.794**
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]						
UI(g)	288.861	342.000	286.500	44.800	$UI(g) \rightleftarrows U^{4+} + I^- + 3\ e^-$	**152.529**	**-870.644**	**-990.102**	**-400.685**
	± 25.045	± 25.000	± 5.000	± 5.000		**± 4.401**	**± 25.121**	**± 25.231**	**± 13.514**
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]					

Table A19 Selected thermodynamic data for uranium (U) in JAEA-TDB-RN in 2020 (11/25)

Species / compound	$\Delta_f G^0_m$ (kJ.mol^{-1})	$\Delta_f H^0_m$ (kJ.mol^{-1})	S^0_m (J.K^{-1}.mol^{-1})	$C^0_{p,m}$ (J.K^{-1}.mol^{-1})	Reaction	$\log_{10} K°$	$\Delta_r G^0_m$ (kJ.mol^{-1})	$\Delta_r H^0_m$ (kJ.mol^{-1})	$\Delta_r S^0_m$ (J.K^{-1}.mol^{-1})
UI^{3+}	**-588.918**				$U^{4+} + I^- \rightleftarrows UI^{3+}$	1.250	-7.135		
	± 2.597					± 0.300	± 1.712		
						[2003GUI/FAN]	[2003GUI/FAN]		
$UI_2(g)$	40.341	103.000	376.500	61.900	$UI_2(g) \rightleftarrows U^{4+} + 2\ I^- + 2\ e^-$	**118.087**	**-674.048**	**-808.005**	**-449.332**
	± 25.177	± 25.000	± 10.000	± 5.000		**± 4.431**	**± 25.294**	**± 25.272**	**± 16.055**
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]					
$UI_3(cr)$	-466.122	-466.900	221.800	112.100	$UI_3(cr) \rightleftarrows U^{4+} + 3\ I^- + e^-$	**29.103**	**-166.121**	**-192.907**	**-89.896**
	± 4.892	± 4.200	± 8.400	± 6.000		**± 1.014**	**± 5.789**	**± 6.142**	**± 16.213**
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]					
$UI_3(g)$	-198.654	-137.000	431.200	86.000	$UI_3(g) \rightleftarrows U^{4+} + 3\ I^- + e^-$	**75.961**	**-433.589**	**-522.807**	**-299.296**
	± 25.178	± 25.000	± 10.000	± 5.000		**± 4.444**	**± 25.367**	**± 25.398**	**± 17.097**
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]					
$UI_4(cr)$	-512.671	-518.300	263.600	126.400	$UI_4(cr) \rightleftarrows U^{4+} + 4\ I^-$	**39.398**	**-224.883**	**-300.510**	**-253.727**
	± 3.761	± 2.800	± 8.400	± 4.200		**± 0.935**	**± 5.335**	**± 5.471**	**± 15.127**
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]					
$UI_4(g)$	-369.585	-305.000	499.100	108.800	$UI_4(g) \rightleftarrows U^{4+} + 4\ I^-$	**64.465**	**-367.969**	**-513.810**	**-489.227**
	± 6.210	± 5.731	± 8.000	± 4.000		**± 1.274**	**± 7.272**	**± 7.412**	**± 14.909**
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]					
$UO_2IO_3^+$	**-1091.997**	**-1230.534**	**91.366**		$UO_2^{2+} + IO_3^- \rightleftarrows UO_2IO_3^+$	2.000	-11.416	9.800	71.159
	± 8.549	**± 8.549**	**± 9.396**			± 0.020	± 0.114	± 0.900	± 3.043
						[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]
$UO_2(IO_3)_2(aq)$	**-1229.104**				$UO_2^{2+} + 2\ IO_3^- \rightleftarrows UO_2(IO_3)_2(aq)$	3.590	-20.492		
	± 16.849					± 0.150	± 0.856		
						[2003GUI/FAN]	[2003GUI/FAN]		
$UO_2(IO_3)_2(cr)$	**-1253.591**	**-1464.658**	279.000		$UO_2^{2+} + 2\ IO_3^- \rightleftarrows UO_2(IO_3)_2(cr)$	7.880	-44.979	**-2.991**	**140.386**
	± 16.837	**± 17.049**	± 9.000			± 0.100	± 0.571	**± 23.938**	**± 19.238**
			[2003GUI/FAN]			[2003GUI/FAN]	[2003GUI/FAN]		
$UClI_3(cr)$	-615.789	-643.800	242.000		$UClI_3(cr) \rightleftarrows U^{4+} + Cl^- + 3\ I^-$	**35.236**	**-201.131**	**-285.187**	**-282.084**
	± 11.350	± 10.000	± 18.000			**± 2.060**	**± 11.758**	**± 10.826**	**± 21.954**
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]						
$UCl_2I_2(cr)$	-723.356	-768.800	237.000		$UCl_2I_2(cr) \rightleftarrows U^{4+} + 2\ Cl^- + 2\ I^-$	**30.296**	**-172.930**	**-270.364**	**-327.041**
	± 11.350	± 10.000	± 18.000			**± 2.034**	**± 11.609**	**± 10.664**	**± 21.951**
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]						
$UCl_3I(cr)$	-829.877	-898.300	213.400		$UCl_3I(cr) \rightleftarrows U^{4+} + 3\ Cl^- + I^-$	**25.539**	**-145.776**	**-251.041**	**-353.398**
	± 8.766	± 8.400	± 8.400			**± 1.574**	**± 8.986**	**± 9.068**	**± 15.114**
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]						
$UBrI_3(cr)$		-589.600			$UBrI_3(cr) \rightleftarrows U^{4+} + Br^- + 3\ I^-$			**-293.811**	
		± 10.000						**± 10.827**	
		[2003GUI/FAN]							
$UBr_2I_2(cr)$		-660.400			$UBr_2I_2(cr) \rightleftarrows U^{4+} + 2\ Br^- + 2\ I^-$			**-287.612**	
		± 10.000						**± 10.667**	
		[2003GUI/FAN]							

Table A19 Selected thermodynamic data for uranium (U) in JAEA-TDB-RN in 2020 (12/25)

Species / compound	$\Delta_f G^0_m$ (kJ.mol^{-1})	$\Delta_f H^0_m$ (kJ.mol^{-1})	S^0_m (J.K^{-1}.mol^{-1})	$C^0_{p,m}$ (J.K^{-1}.mol^{-1})	Reaction	$\log_{10} K°$	$\Delta_r G^0_m$ (kJ.mol^{-1})	$\Delta_r H^0_m$ (kJ.mol^{-1})	$\Delta_r S^0_m$ (J.K^{-1}.mol^{-1})
UBr_3I(cr)		-727.600 ± 8.400 [2003GUI/FAN]			$UBr_3I(cr) \rightleftarrows U^{4+} + 3\ Br^- + I^-$			**-285.012 ± 9.075**	
US(cr)	-320.929 ± 12.600 [2003GUI/FAN]	-322.200 ± 12.600 [2003GUI/FAN]	77.990 ± 0.210 [2003GUI/FAN]	50.540 ± 0.080 [2003GUI/FAN]	$US(cr) + H^+ \rightleftarrows U^{4+} + HS^- + 2\ e^-$	**34.507 ± 2.230**	**-196.965 ± 12.730**	**-285.108**	**-296.007**
$US_{1.90}$(cr)	-509.470 ± 20.900 [2003GUI/FAN]	-509.900 ± 20.900 [2003GUI/FAN]	109.660 ± 0.210 [2003GUI/FAN]	73.970 ± 0.130 [2003GUI/FAN]	$US_{1.90}(cr) + 1.9\ H^+ \rightleftarrows U^{4+} + 1.9\ HS^- + 0.2\ e^-$	**-0.411 ± 3.677**	**2.346 ± 20.989**	**-111.906**	**-383.909**
US_2(cr)	-519.241 ± 8.001 [2003GUI/FAN]	-520.400 ± 8.000 [2003GUI/FAN]	110.420 ± 0.210 [2003GUI/FAN]	74.640 ± 0.130 [2003GUI/FAN]	$US_2(cr) + 2\ H^+ \rightleftarrows U^{4+} + 2\ HS^-$	**-2.332 ± 1.443**	**13.313 ± 8.236**	**-103.017**	**-390.917**
US_3(cr)	-537.253 ± 12.600 [2003GUI/FAN]	-539.600 ± 12.600 [2003GUI/FAN]	138.490 ± 0.210 [2003GUI/FAN]	95.600 ± 0.250 [2003GUI/FAN]	$US_3(cr) + 2\ H_2O(l) \rightleftarrows UO_2^{2+} + 3\ HS^- + H^+$	**-16.637 ± 2.240**	**94.966 ± 12.784**	**43.951**	**-171.938**
U_2S_3(cr)	-879.787 ± 67.002 [2003GUI/FAN]	-879.000 ± 67.000 [2003GUI/FAN]	199.200 ± 1.700 [2003GUI/FAN]	133.700 ± 0.800 [2003GUI/FAN]	$U_2S_3(cr) + 3\ H^+ \rightleftarrows 2\ U^{3+} + 3\ HS^-$	**6.528 ± 11.757**	**-37.260 ± 67.111**	**-147.525**	**-370.946**
U_2S_5(cr)			243.000 ± 25.000 [2003GUI/FAN]						
U_3S_5(cr)	-1425.076 ± 100.278 [2003GUI/FAN]	-1431.000 ± 100.000 [2003GUI/FAN]	291.000 ± 25.000 [2003GUI/FAN]		$U_3S_5(cr) + 5\ H^+ \rightleftarrows 3\ U^{4+} + 5\ HS^- + 2\ e^-$	**18.338 ± 17.596**	**-104.673 ± 100.439**	**-423.142**	**-1070.010**
USO_4^{2+}	**-1311.878 ± 2.122**	**-1492.802 ± 4.284**	**-245.262 ± 15.908**		$U^{4+} + SO_4^{2-} \rightleftarrows USO_4^{2+}$	6.580 ± 0.190 [2003GUI/FAN]	-37.559 ± 1.085 [2003GUI/FAN]	8.000 ± 2.700 [2003GUI/FAN]	152.805 ± 9.759 [2003GUI/FAN]
UO_2SO_3(aq)	**-1476.823 ± 9.209**				$UO_2^{2+} + SO_3^{2-} \rightleftarrows UO_2SO_3$(aq)	6.600 ± 0.600 [2003GUI/FAN]	-37.673 ± 3.425 [2003GUI/FAN]		
UO_2SO_3(cr)	-1530.370 ± 12.727 [2003GUI/FAN]	-1661.000 ± 12.600 [2003GUI/FAN]	157.000 ± 6.000 [2003GUI/FAN]		$UO_2SO_3(cr) \rightleftarrows UO_2^{2+} + SO_3^{2-}$	**-15.981 ± 2.686**	**91.220 ± 15.331**	**6.450 ± 15.200**	**-284.488 ± 83.948**
$UO_2S_2O_3$(aq)	**-1491.116 ± 8.718**				$UO_2^{2+} + S_2O_3^{2-} \rightleftarrows UO_2S_2O_3$(aq)	2.800 ± 0.300 [2003GUI/FAN]	-15.983 ± 1.712 [2003GUI/FAN]		
UO_2SO_4(aq)	**-1714.990 ± 1.810**	**-1909.102 ± 2.233**	**46.338 ± 6.180**		$UO_2^{2+} + SO_4^{2-} \rightleftarrows UO_2SO_4$(aq)	3.150 ± 0.020 [2003GUI/FAN]	-17.980 ± 0.114 [2003GUI/FAN]	19.500 ± 1.600 [2003GUI/FAN]	125.710 ± 5.380 [2003GUI/FAN]
UO_2SO_4(cr)	**-1311.878 ± 2.122**	**-1492.802 ± 4.284**	**-245.262 ± 15.908**	145.000 ± 3.000 [2003GUI/FAN]	$UO_2SO_4(cr) \rightleftarrows UO_2^{2+} + SO_4^{2-}$	**1.968 ± 0.561**	**-11.235 ± 3.201**	**-83.462 ± 1.769**	**-242.572 ± 8.934**

Table A19 Selected thermodynamic data for uranium (U) in JAEA-TDB-RN in 2020 (13/25)

Species / compound	$\Delta_f G^0_m$ (kJ.mol^{-1})	$\Delta_f H^0_m$ (kJ.mol^{-1})	S^0_m (J.K^{-1}.mol^{-1})	$C^0_{p,m}$ (J.K^{-1}.mol^{-1})	Reaction	$\log_{10} K°$	$\Delta_r G^0_m$ (kJ.mol^{-1})	$\Delta_r H^0_m$ (kJ.mol^{-1})	$\Delta_r S^0_m$ (J.K^{-1}.mol^{-1})
$U(SO_3)_2$(cr)	-1712.826	-1883.000	159.000		$U(SO_3)_2$(cr) ⇄ U^{4+} + 2 SO_3^{2-}	**-36.749**	**209.768**	**20.701**	**-634.471**
	± 21.171	± 21.000	± 9.000			**± 4.738**	**± 27.045**	**± 27.055**	**± 168.071**
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]						
$U(SO_4)_2$(aq)	**-2078.770**	**-2377.703**	**-68.350**		U^{4+} + 2 SO_4^{2-} ⇄ $U(SO_4)_2$(aq)	10.510	-59.992	32.700	310.889
	± 2.295	**± 4.408**	**± 16.169**			± 0.200	± 1.142	± 2.800	± 10.142
						[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]
$U(SO_4)_2$(cr)	-2084.521	-2309.600	180.000		$U(SO_4)_2$(cr) ⇄ U^{4+} + 2 SO_4^{2-}	**-11.518**	**65.743**	**-100.803**	**-559.239**
	± 14.070	± 12.600	± 21.000			**± 2.489**	**± 14.210**	**± 13.052**	**± 24.486**
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]						
$UO_2(SO_4)_2^{2-}$	**-2465.100**	**-2803.103**	**136.352**		UO_2^{2+} + 2 SO_4^{2-} ⇄ $UO_2(SO_4)_2^{2-}$	4.140	-23.631	35.100	196.896
	± 2.015	**± 1.988**	**± 4.802**			± 0.070	± 0.400	± 1.000	± 3.612
						[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]
$UO_2(SO_4)_3^{4-}$	**-3203.166**				UO_2^{2+} + 3 SO_4^{2-} ⇄ $UO_2(SO_4)_3^{4-}$	3.020	-17.238		
	± 3.109					± 0.380	± 2.169		
						[2003GUI/FAN]	[2003GUI/FAN]		
$U(OH)_2SO_4$(cr)	**-1766.834**				U^{4+} + SO_4^{2-} + 2 OH^- ⇄ $U(OH)_2SO_4$(cr)	31.170	-177.920		
	± 3.391					± 0.500	± 2.854		
						[2003GUI/FAN]	[2003GUI/FAN]		
$UO_2SO_4·2.5H_2O$(cr)	**-2299.037**	-2607.000	246.053		UO_2^{2+} + SO_4^{2-} + 2.5 H_2O(l) ⇄ $UO_2SO_4·2.5H_2O$(cr)	1.589	-9.070	**36.197**	**150.617**
	± 1.827	± 0.900	± 6.762			± 0.019	± 0.110	**± 1.818**	**± 7.418**
		[2003GUI/FAN]	[2003GUI/FAN]			[2003GUI/FAN]	[2003GUI/FAN]		
$UO_2SO_4·3H_2O$(cr)	-2416.561	-2751.500	274.087		$UO_2SO_4·3H_2O$(cr) ⇄ UO_2^{2+} + SO_4^{2-} + 3 H_2O(l)	**-1.402**	**8.003**	**-34.617**	**-143.690**
	± 1.811	± 4.600	± 16.582			**± 0.451**	**± 2.576**	**± 4.867**	**± 16.861**
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]						
$UO_2SO_4·3.5H_2O$(cr)	-2535.595	-2901.600	286.520		UO_2^{2+} + SO_4^{2-} + 3.5 H_2O(l) ⇄ $UO_2SO_4·3.5H_2O$(cr)	1.585	-9.050	**27.436**	**121.161**
	± 1.806	± 0.800	± 6.628			± 0.019	± 0.110	**± 1.789**	**± 7.299**
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]			[2003GUI/FAN]	[2003GUI/FAN]		
$U(SO_4)_2·4H_2O$(cr)	-3033.310	-3483.200	359.000		$U(SO_4)_2·4H_2O$(cr) ⇄ U^{4+} + 2 SO_4^{2-} + 4 H_2O(l)	**-11.528**	**65.801**	**-70.557**	**-458.547**
	± 11.433	± 6.300	± 32.000			**± 2.034**	**± 11.612**	**± 7.173**	**± 34.390**
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]						
$U(SO_4)_2·8H_2O$(cr)	-3987.898	-4662.600	538.000		$U(SO_4)_2·8H_2O$(cr) ⇄ U^{4+} + 2 SO_4^{2-} + 8 H_2O(l)	**-12.554**	**71.659**	**-34.510**	**-357.855**
	± 16.735	± 6.300	± 52.000			**± 2.956**	**± 16.872**	**± 7.210**	**± 53.507**
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]						
USe(cr)	See Table A4								
α-USe_2	-427.072	-427.000	134.980	79.160	α-USe_2 + 2 H^+ ⇄ U^{4+} + 2 HSe^-	**2.776**	**-15.846**		
	± 42.000	± 42.000	± 0.250	± 0.170		**± 7.399**	**± 42.231**		
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]					
β-USe_2	-427.972	-427.000	138.000		β-USe_2 + 2 H^+ ⇄ U^{4+} + 2 HSe^-	**77.595**	**-442.918**		
	± 42.179	± 42.000	± 13.000			**± 0.773**	**± 4.415**		
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]						
USe_3(cr)	-451.997	-452.000	177.000		USe_3(cr) + 2 H_2O(l) ⇄ UO_2^{2+} + 3 HSe^- + H^+	**-18.259**	**104.224**		
	± 42.305	± 42.000	± 17.000			**± 7.494**	**± 42.774**		
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]						

Table A19 Selected thermodynamic data for uranium (U) in JAEA-TDB-RN in 2020 (14/25)

Species / compound	$\Delta_f G^0_m$ (kJ.mol^{-1})	$\Delta_f H^0_m$ (kJ.mol^{-1})	S^0_m (J.K^{-1}.mol^{-1})	$C^0_{p,m}$ (J.K^{-1}.mol^{-1})	Reaction	$\log_{10} K°$	$\Delta_r G^0_m$ (kJ.mol^{-1})	$\Delta_r H^0_m$ (kJ.mol^{-1})	$\Delta_r S^0_m$ (J.K^{-1}.mol^{-1})
U_2Se_3(cr)	-721.194 ± 75.002 [2003GUI/FAN]	-711.000 ± 75.000 [2003GUI/FAN]	261.400 ± 1.700 [2003GUI/FAN]		U_2Se_3(cr) + 3 H^+ ⇄ 2 U^{3+} + 3 HSe^-	**17.754 ± 13.198**	**-101.339 ± 75.334**		
U_3Se_4(cr)	See Table A4								
U_3Se_5(cr)	-1130.611 ± 113.567 [2003GUI/FAN]	-1130.000 ± 113.000 [2003GUI/FAN]	364.000 ± 38.000 [2003GUI/FAN]		U_3Se_5(cr) + 5 H^+ ⇄ 3 U^{4+} + 5 HSe^- + 2 e^-	**42.329 ± 19.996**	**-241.614 ± 114.140**		
UO_2SeO_3(cr)	See Table A4								
UO_2SeO_4(cr)	See Table A4								
UOTe(cr)			111.700 ± 1.300 [2003GUI/FAN]	80.600 ± 0.800 [2003GUI/FAN]					
$UTeO_5$(cr)		-1603.100 ± 2.800 [2003GUI/FAN]							
UTe_3O_9(cr)		-2275.800 ± 8.000 [2003GUI/FAN]							
UN(cr)	-265.082 ± 3.001 [2003GUI/FAN]	-290.000 ± 3.000 [2003GUI/FAN]	62.430 ± 0.220 [2003GUI/FAN]	47.570 ± 0.400 [2003GUI/FAN]	UN(cr) + 3 H_2O(l) ⇄ U^{4+} + NO_3^- + 6 H^+ + 9 e^-	**-58.838 ± 0.754**	**335.852 ± 4.303**	**349.416 ± 4.490**	**45.903 ± 12.586**
β-$UN_{1.466}$		-362.200 ± 2.300 [2003GUI/FAN]			β-$UN_{1.466}$ + 4.398 H_2O(l) ⇄ U^{4+} + 1.466 NO_3^- + 8.796 H^+ + 11.33 e^-			**724.803 ± 4.095**	
α-$UN_{1.59}$	-338.202 ± 5.201 [2003GUI/FAN]	-379.200 ± 5.200 [2003GUI/FAN]	65.020 ± 0.300 [2003GUI/FAN]		α-$UN_{1.59}$ + 4.77 H_2O(l) ⇄ U^{4+} + 1.59 NO_3^- + 9.54 H^+ + 11.95 e^-	**-133.731 ± 1.192**	**763.344 ± 6.806**	**822.480 ± 6.215**	**198.996 ± 12.635**
α-$UN_{1.606}$		-381.400 ± 5.000 [2003GUI/FAN]			α-$UN_{1.606}$ + 4.818 H_2O(l) ⇄ U^{4+} + 1.606 NO_3^- + 9.636 H^+ + 12.03 e^-			**835.090 ± 6.049**	
α-$UN_{1.674}$		-390.800 ± 5.000 [2003GUI/FAN]			α-$UN_{1.674}$ + 5.022 H_2O(l) ⇄ U^{4+} + 1.674 NO_3^- + 10.044 H^+ + 12.37 e^-			**888.731 ± 6.054**	
α-$UN_{1.73}$	-353.753 ± 7.501 [2003GUI/FAN]	-398.500 ± 7.500 [2003GUI/FAN]	65.860 ± 0.300 [2003GUI/FAN]		α-$UN_{1.73}$ + 5.19 H_2O(l) ⇄ U^{4+} + 1.73 NO_3^- + 10.38 H^+ + 12.65 e^-	**-151.187 ± 1.552**	**862.983 ± 8.861**	**932.866 ± 8.244**	**235.098 ± 12.649**
$UO_2N_3^+$	**-619.078 ± 2.705**				UO_2^{2+} + N_3^- ⇄ $UO_2N_3^+$	2.580 ± 0.090 [2003GUI/FAN]	-14.727 ± 0.514 [2003GUI/FAN]		
$UO_2(N_3)_2$(aq)	-280.867 ± 4.558 [2003GUI/FAN]				UO_2^{2+} + 2 N_3^- ⇄ $UO_2(N_3)_2$(aq)	4.330 ± 0.230 [2003GUI/FAN]	-24.716 ± 1.313 [2003GUI/FAN]		

Table A19 Selected thermodynamic data for uranium (U) in JAEA-TDB-RN in 2020 (15/25)

Species / compound	$\Delta_f G^0_m$ (kJ.mol^{-1})	$\Delta_f H^0_m$ (kJ.mol^{-1})	S^0_m (J.K^{-1}.mol^{-1})	$C^0_{p,m}$ (J.K^{-1}.mol^{-1})	Reaction	$\log_{10} K°$	$\Delta_r G^0_m$ (kJ.mol^{-1})	$\Delta_r H^0_m$ (kJ.mol^{-1})	$\Delta_r S^0_m$ (J.K^{-1}.mol^{-1})
$UO_2(N_3)_3^-$	59.285 ± 6.374 [2003GUI/FAN]				$UO_2^{2+} + 3\ N_3^- \rightleftarrows UO_2(N_3)_3^-$	5.740 ± 0.220 [2003GUI/FAN]	-32.764 ± 1.256 [2003GUI/FAN]		
$UO_2(N_3)_4^{2-}$	412.166 ± 8.302 [2003GUI/FAN]				$UO_2^{2+} + 4\ N_3^- \rightleftarrows UO_2(N_3)_4^{2-}$	4.920 ± 0.240 [2003GUI/FAN]	-28.084 ± 1.370 [2003GUI/FAN]		
UNO_3^{3+}	**-649.169 ± 3.157**				$U^{4+} + NO_3^- \rightleftarrows UNO_3^{3+}$	1.470 ± 0.130 [2003GUI/FAN]	-8.391 ± 0.742 [2003GUI/FAN]		
$UO_2NO_3^+$	**-1065.181 ± 3.176**				$UO_2^{2+} + NO_3^- \rightleftarrows UO_2NO_3^+$	0.300 ± 0.150 [2003GUI/FAN]	-1.712 ± 0.856 [2003GUI/FAN]		
$U(NO_3)_2^{2+}$	**-764.824 ± 5.685**				$U^{4+} + 2\ NO_3^- \rightleftarrows U(NO_3)_2^{2+}$	2.300 ± 0.350 [2003GUI/FAN]	-13.128 ± 1.998 [2003GUI/FAN]		
$UO_2(NO_3)_2$(cr)	-1106.094 ± 5.675 [2003GUI/FAN]	-1351.000 ± 5.000 [2003GUI/FAN]	241.000 ± 9.000 [2003GUI/FAN]		$UO_2(NO_3)_2$(cr) $\rightleftarrows UO_2^{2+} + 2\ NO_3^-$	**11.964 ± 1.362**	**-68.293 ± 7.776**	**-81.798 ± 5.287**	**-45.316 ± 9.633**
$UO_2(NO_3)_2{\cdot}H_2O$(cr)	-1362.965 ± 10.524 [2003GUI/FAN]	-1664.000 ± 10.000 [2003GUI/FAN]	286.000 ± 11.000 [2003GUI/FAN]		$UO_2(NO_3)_2{\cdot}H_2O$(cr) $\rightleftarrows UO_2^{2+} + 2\ NO_3^- + H_2O$(l)	**8.515 ± 2.066**	**-48.604 ± 11.791**	**-54.636 ± 10.147**	**-20.393 ± 11.524**
$UO_2(NO_3)_2{\cdot}2H_2O$(cr)	-1620.500 ± 2.000 [2003GUI/FAN]	-1978.700 ± 1.700 [2003GUI/FAN]	327.520 ± 8.806 [2003GUI/FAN]	278.000 ± 4.000 [2003GUI/FAN]	$UO_2(NO_3)_2{\cdot}2H_2O$(cr) $\rightleftarrows UO_2^{2+} + 2\ NO_3^- + 2\ H_2O$(l)	**4.949 ± 0.996**	**-28.252 ± 5.683**	**-25.774 ± 2.426**	**8.010 ± 9.454**
$UO_2(NO_3)_2{\cdot}3H_2O$(cr)	-1864.694 ± 1.965 [2003GUI/FAN]	-2280.400 ± 1.700 [2003GUI/FAN]	367.900 ± 3.300 [2003GUI/FAN]	320.100 ± 1.700 [2003GUI/FAN]	$UO_2(NO_3)_2{\cdot}3H_2O$(cr) $\rightleftarrows UO_2^{2+} + 2\ NO_3^- + 3\ H_2O$(l)	**3.721 ± 0.994**	**-21.240 ± 5.676**	**-9.913 ± 2.437**	**37.553 ± 4.770**
$UO_2(NO_3)_2{\cdot}6H_2O$(cr)	-2584.213 ± 1.615 [2003GUI/FAN]	-3167.500 ± 1.500 [2003GUI/FAN]	505.600 ± 2.000 [2003GUI/FAN]	468.000 ± 2.500 [2003GUI/FAN]	$UO_2(NO_3)_2{\cdot}6H_2O$(cr) $\rightleftarrows UO_2^{2+} + 2\ NO_3^- + 6\ H_2O$(l)	**2.325 ± 0.979**	**-13.269 ± 5.589**	**19.672 ± 2.365**	**109.622 ± 4.007**
UP(cr)	-265.921 ± 11.101 [2003GUI/FAN]	-269.800 ± 11.100 [2003GUI/FAN]	78.280 ± 0.420 [2003GUI/FAN]	50.290 ± 0.500 [2003GUI/FAN]	UP(cr) + 4 H_2O(l) $\rightleftarrows U^{4+} + PO_4^{3-} + 8\ H^+ + 9\ e^-$	**58.516 ± 2.456**	**-334.013 ± 14.019**	**-455.422 ± 14.293**	**-408.564 ± 84.618**
UP_2(cr)	-294.555 ± 15.031 [2003GUI/FAN]	-304.000 ± 15.000 [2003GUI/FAN]	100.700 ± 3.200 [2003GUI/FAN]	78.800 ± 3.500 [2003GUI/FAN]	UP_2(cr) + 8 H_2O(l) $\rightleftarrows U^{4+} + 2\ PO_4^{3-} + 16\ H^+ + 14\ e^-$	**65.776 ± 3.956**	**-375.452 ± 22.578**	**-555.244 ± 22.731**	**-605.731 ± 167.862**
U_3P_4(cr)	-826.435 ± 26.014 [2003GUI/FAN]	-843.000 ± 26.000 [2003GUI/FAN]	259.400 ± 2.600 [2003GUI/FAN]	176.900 ± 3.600 [2003GUI/FAN]	U_3P_4(cr) + 16 H_2O(l) $\rightleftarrows 3\ U^{4+} + 4\ PO_4^{3-} + 32\ H^+ + 32\ e^-$	**182.802 ± 7.490**	**-1043.440 ± 42.752**	**-1466.688 ± 43.557**	**-1424.999 ± 336.845**
UPO_5(cr)	-1924.713 ± 4.990 [2003GUI/FAN]	-2064.000 ± 4.000 [2003GUI/FAN]	137.000 ± 10.000 [2003GUI/FAN]	124.000 ± 12.000 [2003GUI/FAN]	UPO_5(cr) + H_2O(l) $\rightleftarrows UO_2^+ + PO_4^{3-} + 2\ H^+$	**-31.897 ± 1.734**	**182.071 ± 9.900**	**47.336 ± 9.736**	**-453.675 ± 84.654**

Table A19 Selected thermodynamic data for uranium (U) in JAEA-TDB-RN in 2020 (16/25)

Species / compound	$\Delta_f G^0_m$ (kJ.mol^{-1})	$\Delta_f H^0_m$ (kJ.mol^{-1})	S^0_m (J.K^{-1}.mol^{-1})	$C^0_{p,m}$ (J.K^{-1}.mol^{-1})	Reaction	$\log_{10} K°$	$\Delta_r G^0_m$ (kJ.mol^{-1})	$\Delta_r H^0_m$ (kJ.mol^{-1})	$\Delta_r S^0_m$ (J.K^{-1}.mol^{-1})
$UO_2PO_4^-$	**-2046.872**				$UO_2^{2+} + PO_4^{3-} \rightleftarrows UO_2PO_4^-$	13.230	-75.517		
	± 8.591					± 0.150	± 0.856		
						[2003GUI/FAN]	[2003GUI/FAN]		
UP_2O_7(cr)	-2659.272	-2852.000	204.000	184.000	UP_2O_7(cr) + 3 H_2O(l) $\rightleftarrows UO_2^{2+} + 2\ PO_4^{3-} + 6\ H^+ + 2\ e^-$	**-66.689**	**380.661**	**135.765**	**-824.794**
	± 5.369	± 4.000	± 12.000	± 18.000		**± 3.095**	**± 17.665**	**± 17.275**	**± 167.817**
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]					
$(UO_2)_2P_2O_7$(cr)	-3930.002	-4232.600	296.000	258.000	$(UO_2)_2P_2O_7$(cr) + H_2O(l) $\rightleftarrows 2\ UO_2^{2+} + 2\ PO_4^{3-} + 2\ H^+$	**-39.326**	**224.475**	**-74.312**	**-1005.827**
	± 6.861	± 2.800	± 21.000	± 26.000		**± 3.227**	**± 18.422**	**± 17.232**	**± 168.779**
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]					
$(UO_2)_3(PO_4)_2$(cr)	-5115.975	-5491.300	410.000	339.000	$(UO_2)_3(PO_4)_2$(cr) $\rightleftarrows 3\ UO_2^{2+} + 2\ PO_4^{3-}$	**-38.667**	**220.714**	**-120.450**	**-1148.104**
	± 5.452	± 3.500	± 14.000	± 17.000		**± 3.217**	**± 18.365**	**± 17.680**	**± 168.186**
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]					
UO_2HPO_4(aq)	**-2083.014**				$UO_2^{2+} + HPO_4^{2-} \rightleftarrows UO_2HPO_4$(aq)	7.240	-41.326		
	± 2.440					± 0.260	± 1.484		
						[2003GUI/FAN]	[2003GUI/FAN]		
$UO_2H_2PO_4^+$	**-2101.594**				$UO_2^{2+} + H_3PO_4$(aq) $\rightleftarrows UO_2H_2PO_4^+ + H^+$	1.120	-6.393		
	± 1.967					± 0.060	± 0.342		
						[2003GUI/FAN]	[2003GUI/FAN]		
$UO_2H_3PO_4^{2+}$	**-2099.539**				$UO_2^{2+} + H_3PO_4$(aq) $\rightleftarrows UO_2H_3PO_4^{2+}$	0.760	-4.338		
	± 2.118					± 0.150	± 0.856		
						[2003GUI/FAN]	[2003GUI/FAN]		
$UO_2(H_2PO_4)_2$(aq)	**-3241.505**				$UO_2^{2+} + 2\ H_3PO_4$(aq) $\rightleftarrows UO_2(H_2PO_4)_2$(aq) $+ 2\ H^+$	0.640	-3.653		
	± 2.499					± 0.110	± 0.628		
						[2003GUI/FAN]	[2003GUI/FAN]		
$UO_2(H_2PO_4)(H_3PO_4)^+$	**-3247.270**				$UO_2^{2+} + 2\ H_3PO_4$(aq) $\rightleftarrows UO_2(H_2PO_4)(H_3PO_4)^+ + H^+$	1.650	-9.418		
	± 2.499					± 0.110	± 0.628		
						[2003GUI/FAN]	[2003GUI/FAN]		
$UO_2HPO_4 \cdot 4H_2O$(cr)	**-3058.202**	-3469.968	346.000		$UO_2^{2+} + H_3PO_4$(aq) $+ 4\ H_2O$(l) $\rightleftarrows UO_2HPO_4 \cdot 4H_2O$(cr) $+ 2\ H^+$	2.500	-14.270		
	± 2.044	± 7.836	± 25.000			± 0.090	± 0.514		
		[2003GUI/FAN]	[2003GUI/FAN]			[2003GUI/FAN]	[2003GUI/FAN]		
$U(HPO_4)_2 \cdot 4H_2O$(cr)	**-3831.189**	-4334.818	372.000	460.000	$U^{4+} + 2\ H_3PO_4$(aq) $+ 4\ H_2O$(l) $\rightleftarrows U(HPO_4)_2 \cdot 4H_2O$(cr) $+ 4\ H^+$	11.790	-67.298		
	± 2.610	± 8.598	± 26.000	± 50.000		± 0.150	± 0.856		
		[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]		[2003GUI/FAN]	[2003GUI/FAN]		
$(UO_2)_3(PO_4)_2 \cdot 4H_2O$(cr)	**-6125.704**	-6739.105	589.000		$3\ UO_2^{2+} + 2\ H_3PO_4$(aq) $+ 4\ H_2O$(l)	5.960	-34.020		
	± 5.776	± 9.136	± 22.000		$\rightleftarrows (UO_2)_3(PO_4)_2 \cdot 4H_2O$(cr) $+ 6\ H^+$	± 0.300	± 1.712		
		[2003GUI/FAN]	[2003GUI/FAN]			[2003GUI/FAN]	[2003GUI/FAN]		
$(UO_2)_3(PO_4)_2 \cdot 6H_2O$(cr)	-6613.025	-7328.400	669.000		$(UO_2)_3(PO_4)_2 \cdot 6H_2O$(cr) $\rightleftarrows 3\ UO_2^{2+} + 2\ PO_4^{3-} + 6\ H_2O$(l)	**-51.623**	**294.668**	**1.620**	**-987.566**
	± 13.392	± 10.700	± 27.000			**± 3.867**	**± 22.074**	**± 20.377**	**± 169.763**
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]						
UAs(cr)	-237.908	-234.300	97.400	57.900	UAs(cr) $+ 4\ H_2O$(l) $\rightleftarrows U^{4+} + AsO_4^{3-} + 8\ H^+ + 9\ e^-$	**-1.475**	**8.418**	**-101.687**	**-368.732**
	± 8.024	± 8.000	± 2.000	± 1.200		**± 1.603**	**± 9.150**	**± 9.543**	**± 12.731**
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]					

Table A19 Selected thermodynamic data for uranium (U) in JAEA-TDB-RN in 2020 (17/25)

Species / compound	$\Delta_f G^0_m$ (kJ.mol^{-1})	$\Delta_f H^0_m$ (kJ.mol^{-1})	S^0_m (J.K^{-1}.mol^{-1})	$C^0_{p,m}$ (J.K^{-1}.mol^{-1})	Reaction	$\log_{10} K°$	$\Delta_r G^0_m$ (kJ.mol^{-1})	$\Delta_r H^0_m$ (kJ.mol^{-1})	$\Delta_r S^0_m$ (J.K^{-1}.mol^{-1})
UAs_2(cr)	-252.790	-252.000	123.050	79.960	$UAs_2(cr) + 8\ H_2O(l) \rightleftarrows U^{4+} + 2\ AsO_4^{3-} + 16\ H^+ + 14\ e^-$	**-56.704**	**323.671**	**171.227**	**-510.177**
	± 13.005	± 13.000	± 0.200	± 0.100		**± 2.698**	**± 15.400**	**± 15.639**	**± 12.632**
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]					
U_3As_4(cr)	-725.388	-720.000	309.070	187.530	$U_3As_4(cr) + 16\ H_2O(l) \rightleftarrows 3\ U^{4+} + 4\ AsO_4^{3-} + 32\ H^+ + 32\ e^-$	**-59.090**	**337.289**	**-32.747**	**-1238.861**
	± 18.016	± 18.000	± 0.600	± 0.200		**± 4.335**	**± 24.743**	**± 26.092**	**± 37.768**
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]					
$UAsO_5$(cr)				138.000					
				± 14.000					
				[2003GUI/FAN]					
$UO_2(AsO_3)_2$(cr)	-1944.911	-2156.600	231.000	201.000	$UO_2(AsO_3)_2(cr) + 2\ H_2O(l) \rightleftarrows UO_2^{2+} + 2\ AsO_4^{3-} + 4\ H^+$	**-29.783**	**170.005**	**-67.003**	**-794.646**
	± 12.006	± 8.000	± 30.000	± 20.000		**± 2.548**	**± 14.543**	**± 11.415**	**± 30.174**
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]					
$(UO_2)_2As_2O_7$(cr)	-3130.254	-3426.000	307.000	273.000	$(UO_2)_2As_2O_7(cr) + H_2O(l) \rightleftarrows 2\ UO_2^{2+} + 2\ AsO_4^{3-} + 2\ H^+$	**-29.014**	**165.615**	**-102.442**	**-898.923**
	± 12.006	± 8.000	± 30.000	± 27.000		**± 2.602**	**± 14.853**	**± 11.705**	**± 30.618**
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]					
$(UO_2)_3(AsO_4)_2$(cr)	-4310.789	-4689.400	387.000	364.000	$(UO_2)_3(AsO_4)_2(cr) \rightleftarrows 3\ UO_2^{2+} + 2\ AsO_4^{3-}$	**-27.403**	**156.416**	**-143.880**	**-1007.200**
	± 12.007	± 8.000	± 30.000	± 36.000		**± 2.691**	**± 15.359**	**± 12.176**	**± 31.344**
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]					
UO_2HAsO_4(aq)	-1707.994				$UO_2^{2+} + AsO_4^{3-} + H^+ \rightleftarrows UO_2HAsO_4(aq)$	18.760	-107.083		
	± 4.717					± 0.310	± 1.769		
	[2003GUI/FAN]					[2003GUI/FAN]	[2003GUI/FAN]		
$UO_2H_2AsO_4^+$	-1726.260				$UO_2^{2+} + AsO_4^{3-} + 2\ H^+ \rightleftarrows UO_2H_2AsO_4^+$	21.960	-125.349		
	± 4.582					± 0.240	± 1.370		
	[2003GUI/FAN]					[2003GUI/FAN]	[2003GUI/FAN]		
$UO_2(H_2AsO_4)_2$(aq)	-2486.326				$UO_2^{2+} + 2\ AsO_4^{3-} + 4\ H^+ \rightleftarrows UO_2(H_2AsO_4)_2(aq)$	41.530	-237.055		
	± 8.283					± 0.200	± 1.142		
	[2003GUI/FAN]					[2003GUI/FAN]	[2003GUI/FAN]		
UAsS(cr)			114.500	80.900					
			± 3.400	± 2.400					
			[2003GUI/FAN]	[2003GUI/FAN]					
UAsSe(cr)			131.900	83.500					
			± 4.000	± 2.500					
			[2003GUI/FAN]	[2003GUI/FAN]					
UAsTe(cr)			139.900	81.300					
			± 4.200	± 2.400					
			[2003GUI/FAN]	[2003GUI/FAN]					
USb(cr)	-140.969	-138.500	104.000	75.000	$USb(cr) + 3\ H_2O(l) \rightleftarrows U^{4+} + Sb(OH)_3(aq) + 3\ H^+ + 7\ e^-$	**56.140**	**-320.452**		
	± 7.711	± 7.500	± 6.000	± 7.000		**± 1.387**	**± 7.916**		
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]					
USb_2(cr)	-173.666	-173.600	141.460	80.200	$USb_2(cr) + 6\ H_2O(l) \rightleftarrows U^{4+} + 2\ Sb(OH)_3(aq) + 6\ H^+ + 10\ e^-$	**38.422**	**-219.315**		
	± 10.901	± 10.900	± 0.130	± 0.100		**± 1.938**	**± 11.059**		
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]					

Table A19 Selected thermodynamic data for uranium (U) in JAEA-TDB-RN in 2020 (18/25)

Species / compound	$\Delta_f G^0_m$ (kJ.mol^{-1})	$\Delta_f H^0_m$ (kJ.mol^{-1})	S^0_m (J.K^{-1}.mol^{-1})	$C^0_{p,m}$ (J.K^{-1}.mol^{-1})	Reaction	$\log_{10} K°$	$\Delta_r G^0_m$ (kJ.mol^{-1})	$\Delta_r H^0_m$ (kJ.mol^{-1})	$\Delta_r S^0_m$ (J.K^{-1}.mol^{-1})
U_4Sb_3(cr)			379.000 ± 2.000 [2003GUI/FAN]						
U_3Sb_4(cr)	-457.004 ± 22.602 [2003GUI/FAN]	-451.900 ± 22.600 [2003GUI/FAN]	349.800 ± 0.400 [2003GUI/FAN]	188.200 ± 0.200 [2003GUI/FAN]	U_3Sb_4(cr) + 12 H_2O(l) ⇄ 3 U^{4+} + 4 $Sb(OH)_3$(aq) + 12 H^+ + 24 e^-	**150.458 ± 4.072**	**-858.818 ± 23.245**		
UC(cr)	-98.900 ± 3.000 [2003GUI/FAN]	-97.900 ± 4.000 [2003GUI/FAN]	59.294 ± 16.772 [2003GUI/FAN]	50.100 ± 1.000 [2003GUI/FAN]	UC(cr) + 3 H_2O(l) ⇄ U^{4+} + HCO_3^- + 5 H^+ + 8 e^-	**53.670 ± 0.612**	**-306.352 ± 3.496**	**-325.718 ± 5.199**	**-64.793 ± 20.957**
α-$UC_{1.94}$	-87.400 ± 2.100 [2003GUI/FAN]	-85.324 ± 2.185 [2003GUI/FAN]	68.300 ± 2.000 [2003GUI/FAN]	60.800 ± 1.500 [2003GUI/FAN]	α-$UC_{1.94}$ + 5.82 H_2O(l) ⇄ U^{4+} + 1.94 HCO_3^- + 9.7 H^+ + 11.76 e^-	**35.165 ± 0.493**	**-200.721 ± 2.815**	**-180.767 ± 4.025**	**67.237 ± 12.759**
U_2C_3(cr)	-189.317 ± 10.002 [2003GUI/FAN]	-183.300 ± 10.000 [2003GUI/FAN]	137.800 ± 0.300 [2003GUI/FAN]	107.400 ± 2.000 [2003GUI/FAN]	U_2C_3(cr) + 9 H_2O(l) ⇄ 2 U^{4+} + 3 HCO_3^- + 15 H^+ + 20 e^-	**86.996 ± 1.866**	**-496.579 ± 10.652**	**-496.355 ± 12.035**	**1.240 ± 25.166**
UO_2CO_3(aq)	**-1537.272 ± 1.780**	**-1689.235 ± 2.541**	**58.871 ± 7.484**		UO_2^{2+} + CO_3^{2-} ⇄ UO_2CO_3(aq)	9.940 ± 0.030 [2003GUI/FAN]	-56.738 ± 0.171 [2003GUI/FAN]	5.000 ± 2.000 [2003GUI/FAN]	207.070 ± 6.733 [2003GUI/FAN]
UO_2CO_3(cr)	**-1564.785 ± 1.775**	-689.933 ± 0.209 [2003GUI/FAN]	181.846 ± 13.999 [2003GUI/FAN]	120.100 ± 0.100 [2003GUI/FAN]	UO_2^{2+} + CO_3^{2-} ⇄ UO_2CO_3(cr)	14.760 ± 0.020 [2003GUI/FAN]	-84.251 ± 0.114 [2003GUI/FAN]		
$UO_2(CO_3)_2^{2-}$	**-2103.328 ± 1.913**	**-2350.970 ± 4.367**	**181.848 ± 14.095**		UO_2^{2+} + 2 CO_3^{2-} ⇄ $UO_2(CO_3)_2^{2-}$	16.610 ± 0.090 [2003GUI/FAN]	-94.811 ± 0.514 [2003GUI/FAN]	18.500 ± 4.000 [2003GUI/FAN]	380.046 ± 13.526 [2003GUI/FAN]
$UO_2(CO_3)_3^{4-}$	**-2661.164 ± 1.969**	**-3083.905 ± 4.571**	**38.450 ± 14.623**		UO_2^{2+} + 3 CO_3^{2-} ⇄ $UO_2(CO_3)_3^{4-}$	21.840 ± 0.040 [2003GUI/FAN]	-124.664 ± 0.228 [2003GUI/FAN]	-39.200 ± 4.100 [2003GUI/FAN]	286.646 ± 13.773 [2003GUI/FAN]
$UO_2(CO_3)_3^{5-}$	**-2576.171 ± 2.837**				UO_2^+ + 3 CO_3^{2-} ⇄ $UO_2(CO_3)_3^{5-}$	6.950 ± 0.360 [2003GUI/FAN]	-39.671 ± 2.055 [2003GUI/FAN]		
$U(CO_3)_4^{4-}$	**-2841.842 ± 5.953**				U^{4+} + 4 CO_3^{2-} ⇄ $U(CO_3)_4^{4-}$	1.120 ± 0.250 [2003GUI/FAN]	-6.393 ± 1.427 [2003GUI/FAN]		
$U(CO_3)_5^{6-}$	**-3363.849 ± 5.626**	**-3987.374 ± 5.656**	**-83.044 ± 26.010**		U^{4+} + 5 CO_3^{2-} ⇄ $U(CO_3)_5^{6-}$	34.000 ± 0.900 [2003GUI/FAN]	-194.073 ± 5.137 [2003GUI/FAN]	-20.000 ± 4.000 [2003GUI/FAN]	583.845 ± 21.838 [2003GUI/FAN]
$(UO_2)_3(CO_3)_6^{6-}$	**-6333.786 ± 7.946**	**-7171.109 ± 5.776**	**228.933 ± 23.935**		3 UO_2^{2+} + 6 CO_3^{2-} ⇄ $(UO_2)_3(CO_3)_6^{6-}$	54.000 ± 1.000 [2003GUI/FAN]	-308.234 ± 5.708 [2003GUI/FAN]	-62.700 ± 2.400 [2003GUI/FAN]	823.526 ± 20.768 [2003GUI/FAN]
$U(CO_3)_2(OH)_2^{2-}$	**-2137.647 ± 6.005**				U^{4+} + 2 CO_3^{2-} + 2 H_2O(l) ⇄ $U(CO_3)_2(OH)_2^{2-}$ + 2 H^+	41.560 ± 1.000 [2010FUJ/KIT]	**-237.226 ± 5.708**		

Table A19 Selected thermodynamic data for uranium (U) in JAEA-TDB-RN in 2020 (19/25)

Species / compound	$\Delta_f G^0_m$ (kJ.mol^{-1})	$\Delta_f H^0_m$ (kJ.mol^{-1})	S^0_m (J.K^{-1}.mol^{-1})	$C^0_{p,m}$ (J.K^{-1}.mol^{-1})	Reaction	$\log_{10} K°$	$\Delta_r G^0_m$ (kJ.mol^{-1})	$\Delta_r H^0_m$ (kJ.mol^{-1})	$\Delta_r S^0_m$ (J.K^{-1}.mol^{-1})
$(UO_2)_2CO_3(OH)_3^-$	**-3139.681 ± 4.530**				$2\ UO_2^{2+} + CO_3^{2-} + 3\ H_2O(l) \rightleftarrows (UO_2)_2CO_3(OH)_3^- + 3\ H^+$	-19.010 ± 0.500 [2003GUI/FAN]	108.510 ± 2.854 [2003GUI/FAN]		
$(UO_2)_3O(OH)_2(HCO_3)^+$	**-4100.851 ± 5.982**				$3\ UO_2^{2+} + CO_3^{2-} + 3\ H_2O(l) \rightleftarrows (UO_2)_3O(OH)_2(HCO_3)^+ + 3\ H^+$	-17.500 ± 0.500 [2003GUI/FAN]	99.891 ± 2.854 [2003GUI/FAN]		
$(UO_2)_{11}(CO_3)_6(OH)_{12}^{2-}$	**-16699.667 ± 22.431**				$11\ UO_2^{2+} + 6\ CO_3^{2-} + 12\ H_2O(l) \rightleftarrows (UO_2)_{11}(CO_3)_6(OH)_{12}^{2-} + 12\ H^+$	-72.500 ± 2.000 [2003GUI/FAN]	413.833 ± 11.416 [2003GUI/FAN]		
$UO_2CO_3F^-$	**-1841.131 ± 1.962**				$UO_2^{2+} + CO_3^{2-} + F^- \rightleftarrows UO_2CO_3F^-$	13.750 ± 0.090 [2003GUI/FAN]	-78.846 ± 0.514 [2003GUI/FAN]		
$UO_2CO_3F_2^{2-}$	**-2132.819 ± 2.360**				$UO_2^{2+} + CO_3^{2-} + 2\ F^- \rightleftarrows UO_2CO_3F_2^{2-}$	15.570 ± 0.140 [2003GUI/FAN]	-88.784 ± 0.799 [2003GUI/FAN]		
$UO_2CO_3F_3^{3-}$	**-2419.284 ± 2.751**				$UO_2^{2+} + CO_3^{2-} + 3\ F^- \rightleftarrows UO_2CO_3F_3^{3-}$	16.380 ± 0.110 [2003GUI/FAN]	-93.498 ± 0.628 [2003GUI/FAN]		
$USCN^{3+}$	**-453.928 ± 8.559**	**-541.633 ± 12.038**	**-306.245 ± 30.804**		$U^{4+} + SCN^- \rightleftarrows USCN^{3+}$	2.970 ± 0.060 [2003GUI/FAN]	-16.953 ± 0.342 [2003GUI/FAN]	-27.000 ± 8.000 [2003GUI/FAN]	-33.698 ± 26.857 [2003GUI/FAN]
$U(SCN)_2^{2+}$	**-368.406 ± 16.860**	**-456.066 ± 17.521**	**-107.014 ± 25.091**		$U^{4+} + 2\ SCN^- \rightleftarrows U(SCN)_2^{2+}$	4.260 ± 0.180 [2003GUI/FAN]	-24.316 ± 1.027 [2003GUI/FAN]	-18.000 ± 4.000 [2003GUI/FAN]	21.185 ± 13.852 [2003GUI/FAN]
UO_2SCN^+	**-867.657 ± 8.649**	**-939.213 ± 8.502**	**83.751 ± 9.922**		$UO_2^{2+} + SCN^- \rightleftarrows UO_2SCN^+$	1.400 ± 0.230 [2003GUI/FAN]	-7.991 ± 1.313 [2003GUI/FAN]	3.220 ± 0.060 [2003GUI/FAN]	37.603 ± 4.408 [2003GUI/FAN]
$UO_2(SCN)_2(aq)$	**-773.859 ± 17.117**	**-856.966 ± 16.814**	**244.086 ± 20.100**		$UO_2^{2+} + 2\ SCN^- \rightleftarrows UO_2(SCN)_2(aq)$	1.240 ± 0.550 [2003GUI/FAN]	-7.078 ± 3.139 [2003GUI/FAN]	8.900 ± 0.600 [2003GUI/FAN]	53.590 ± 10.720 [2003GUI/FAN]
$UO_2(SCN)_3^-$	**-685.884 ± 25.326**	**-783.298 ± 25.177**	**395.172 ± 27.332**		$UO_2^{2+} + 3\ SCN^- \rightleftarrows UO_2(SCN)_3^-$	2.100 ± 0.500 [2003GUI/FAN]	-11.987 ± 2.854 [2003GUI/FAN]	6.000 ± 1.200 [2003GUI/FAN]	60.328 ± 10.384 [2003GUI/FAN]
$USiO_4(cr)$	-1883.600 ± 4.000 [2003GUI/FAN]	-1991.326 ± 5.367 [2003GUI/FAN]	118.000 ± 12.000 [2003GUI/FAN]		$USiO_4(cr) + 4\ H^+ \rightleftarrows U^{4+} + Si(OH)_4(aq)$	**-8.053 ± 0.830**	**45.968 ± 4.735**	**-56.798 ± 7.179**	**-345.098 ± 20.163**
$UO_2SiO(OH)_3^+$	**-2249.820 ± 2.586**				$UO_2^{2+} + Si(OH)_4(aq) \rightleftarrows UO_2SiO(OH)_3^+ + H^+$	-1.840 ± 0.100 [2003GUI/FAN]	10.503 ± 0.571 [2003GUI/FAN]		
$Tl_2U_4O_{11}(cr)$				360.200 ± 20.000 [2003GUI/FAN]					

Table A19 Selected thermodynamic data for uranium (U) in JAEA-TDB-RN in 2020 (20/25)

Species / compound	$\Delta_f G^0_m$ (kJ.mol^{-1})	$\Delta_f H^0_m$ (kJ.mol^{-1})	S^0_m (J.K^{-1}.mol^{-1})	$C^0_{p,m}$ (J.K^{-1}.mol^{-1})	Reaction	$\log_{10} K°$	$\Delta_r G^0_m$ (kJ.mol^{-1})	$\Delta_r H^0_m$ (kJ.mol^{-1})	$\Delta_r S^0_m$ (J.K^{-1}.mol^{-1})
$Zn_{0.12}UO_{2.95}$(cr)		-1938.070 ± 1.060 [2003GUI/FAN]			$Zn_{0.12}UO_{2.95}$(cr) + 1.9 H^+ ⇄ UO_2^{2+} + 0.12 Zn^{2+} + 0.95 H_2O(l) + 0.34 e^-			**629.117** **± 1.840**	
$(UO_2)_2(PuO_2)(CO_3)_6^{6-}$	**-6139.870** **± 9.550**				2 $UO_2(CO_3)_3^{4-}$ + $PuO_2(CO_3)_3^{4-}$ ⇄ $(UO_2)_2(PuO_2)(CO_3)_6^{6-}$ + 3 CO_3^{2-}	-8.200 ± 1.300 [2003GUI/FAN]	46.806 ± 7.420 [2003GUI/FAN]		
$(UO_2)_2(NpO_2)(CO_3)_6^{6-}$	-6176.973 ± 16.977 [2003GUI/FAN]				2 $UO_2(CO_3)_3^{4-}$ + $NpO_2(CO_3)_3^{4-}$ ⇄ $(UO_2)_2(NpO_2)(CO_3)_6^{6-}$ + 3 CO_3^{2-}	-8.998 ± 2.690 [2003GUI/FAN]	51.364 ± 15.355 [2003GUI/FAN]		
$Be_{13}U$(cr)	-165.508 ± 17.530 [2003GUI/FAN]	-163.600 ± 17.500 [2003GUI/FAN]	180.100 ± 3.300 [2003GUI/FAN]	242.300 ± 4.200 [2003GUI/FAN]					
α-$Mg_{0.17}UO_{2.95}$		-1291.440 ± 0.990 [2003GUI/FAN]			α-$Mg_{0.17}UO_{2.95}$ + 1.9 H^+ ⇄ UO_2^{2+} + 0.17 Mg^{2+} + 0.95 H_2O(l) + 0.44 e^-			**-78.320** **± 1.809**	
$MgUO_4$(cr)	-1749.601 ± 1.502 [2003GUI/FAN]	-1857.300 ± 1.500 [2003GUI/FAN]	131.950 ± 0.170 [2003GUI/FAN]	128.100 ± 0.300 [2003GUI/FAN]	$MgUO_4$(cr) + 4 H^+ ⇄ UO_2^{2+} + Mg^{2+} + 2 H_2O(l)	**23.003** **± 0.448**	**-131.300** **± 2.556**	**-199.336** **± 2.393**	**-228.376** **± 8.500**
MgU_3UO_{10}			338.600 ± 1.000 [2003GUI/FAN]	305.600 ± 5.000 [2003GUI/FAN]					
$MgUO_2(CO_3)_3^{2-}$	**-3139.522** **± 3.627**				UO_2^{2+} + Mg^{2+} + 3 CO_3^{2-} ⇄ $MgUO_2(CO_3)_3^{2-}$	26.110 ± 0.500 [14THO/HUM]	**-149.037** **± 2.854**		
β-$CaUO_4$				124.700 ± 2.700 [2003GUI/FAN]					
$CaUO_4$(cr)	-1888.706 ± 2.421 [2003GUI/FAN]	-2002.300 ± 2.300 [2003GUI/FAN]	121.100 ± 2.500 [2003GUI/FAN]	123.800 ± 2.500 [2003GUI/FAN]	$CaUO_4$(cr) + 4 H^+ ⇄ UO_2^{2+} + Ca^{2+} + 2 H_2O(l)	**15.942** **± 0.542**	**-91.000** **± 3.096**	**-131.460** **± 2.866**	**-135.938** **± 3.931**
Ca_3UO_6(cr)		-3305.400 ± 4.100 [2003GUI/FAN]			Ca_3UO_6(cr) + 8 H^+ ⇄ UO_2^{2+} + 3 Ca^{2+} + 4 H_2O(l)			**-486.203** **± 4.992**	
$CaU_6O_{19}·11H_2O$(cr)	**-10306.207** **± 14.042**				6 UO_2^{2+} + Ca^{2+} + 18 H_2O(l) ⇄ $CaU_6O_{19}·11H_2O$(cr) + 14 H^+	-40.500 ± 1.600 [2003GUI/FAN]	231.176 ± 9.133 [2003GUI/FAN]		
$CaUO_2(CO_3)_3^{2-}$	**-3244.435** **± 3.550**				UO_2^{2+} + Ca^{2+} + 3 CO_3^{2-} ⇄ $CaUO_2(CO_3)_3^{2-}$	27.180 ± 0.500 [14THO/HUM]	**-155.145** **± 2.854**		
$Ca_2UO_2(CO_3)_3$(aq)	**-3808.870** **± 2.896**				UO_2^{2+} + 2 Ca^{2+} + 3 CO_3^{2-} ⇄ $Ca_2UO_2(CO_3)_3$(aq)	29.220 ± 0.250 [14THO/HUM]	**-166.789** **± 1.427**		

Table A19 Selected thermodynamic data for uranium (U) in JAEA-TDB-RN in 2020 (21/25)

Species / compound	$\Delta_f G^0_m$ (kJ.mol^{-1})	$\Delta_f H^0_m$ (kJ.mol^{-1})	S^0_m (J.K^{-1}.mol^{-1})	$C^0_{p,m}$ (J.K^{-1}.mol^{-1})	Reaction	$\log_{10} K°$	$\Delta_r G^0_m$ (kJ.mol^{-1})	$\Delta_r H^0_m$ (kJ.mol^{-1})	$\Delta_r S^0_m$ (J.K^{-1}.mol^{-1})
$SrUO_3$(cr)		-1672.600 ± 8.600 [2003GUI/FAN]			$SrUO_3(cr) + 6\ H^+ \rightleftarrows U^{4+} + Sr^{2+} + 3\ H_2O(l)$			**-327.022 ± 9.230**	
α-$SrUO_4$	-1881.355 ± 2.802 [2003GUI/FAN]	-1989.600 ± 2.800 [2003GUI/FAN]	153.150 ± 0.170 [2003GUI/FAN]	130.620 ± 0.200 [2003GUI/FAN]	$\alpha\text{-}SrUO_4 + 4\ H^+ \rightleftarrows UO_2^{2+} + Sr^{2+} + 2\ H_2O(l)$	**19.165 ± 0.596**	**-109.397 ± 3.402**	**-151.984 ± 3.223**	**-143.010 ± 3.618**
β-$SrUO_4$		-1988.400 ± 5.400 [2003GUI/FAN]			$\beta\text{-}SrUO_4 + 4\ H^+ \rightleftarrows UO_2^{2+} + Sr^{2+} + 2\ H_2O(l)$			**-153.184 ± 5.631**	
$Sr_2UO_{4.5}$(cr)		-2494.000 ± 2.800 [2003GUI/FAN]			$Sr_2UO_{4.5}(cr)$			**-341.410 ± 3.342**	
Sr_2UO_5(cr)		-2632.900 ± 1.900 [2003GUI/FAN]			$Sr_2UO_5(cr) + 6\ H^+ \rightleftarrows UO_2^{2+} + 2\ Sr^{2+} + 3\ H_2O(l)$			**-345.430 ± 2.639**	
Sr_3UO_6(cr)		-3263.500 ± 3.000 [2003GUI/FAN]			$Sr_3UO_6(cr) + 8\ H^+ \rightleftarrows UO_2^{2+} + 3\ Sr^{2+} + 4\ H_2O(l)$			**-551.575 ± 3.701**	
$Sr_3U_2O_9$(cr)		-4620.000 ± 8.000 [2003GUI/FAN]		301.800 ± 3.000 [2003GUI/FAN]	$Sr_3U_2O_9(cr) + 10\ H^+ \rightleftarrows 2\ UO_2^{2+} + 3\ Sr^{2+} + 5\ H_2O(l)$			**-499.913 ± 8.692**	
$Sr_2U_3O_{11}$(cr)		-5243.700 ± 5.000 [2003GUI/FAN]			$Sr_2U_3O_{11}(cr) + 10\ H^+ \rightleftarrows 3\ UO_2^{2+} + 2\ Sr^{2+} + 5\ H_2O(l)$			**-344.306 ± 6.821**	
SrU_4O_{13}(cr)		-5920.000 ± 20.000 [2003GUI/FAN]			$SrU_4O_{13}(cr) + 10\ H^+ \rightleftarrows 4\ UO_2^{2+} + Sr^{2+} + 5\ H_2O(l)$			**-136.099 ± 20.893**	
$Sr_5U_3O_{14}$(cr)		-7248.600 ± 7.500 [2003GUI/FAN]			$Sr_5U_3O_{14}(cr) + 16\ H^+ \rightleftarrows 3\ UO_2^{2+} + 5\ Sr^{2+} + 8\ H_2O(l)$			**-849.643 ± 9.138**	
$Sr_3U_{11}O_{36}$(cr)		- 15903.800 ± 16.500 [2003GUI/FAN]		1064.200 ± 10.600 [2003GUI/FAN]	$Sr_3U_{11}O_{36}(cr) + 28\ H^+ \rightleftarrows 11\ UO_2^{2+} + 3\ Sr^{2+} + 14\ H_2O(l)$			**-959.658 ± 23.429**	
$SrUO_2(CO_3)_3^{2-}$	**-3253.654 ± 3.550**				$UO_2^{2+} + Sr^{2+} + 3\ CO_3^{2-} \rightleftarrows SrUO_2(CO_3)_3^{2-}$	26.860 ± 0.500 [14THO/HUM]	**-153.318 ± 2.854**		
$BaUO_3$(cr)		-1690.000 ± 10.000 [2003GUI/FAN]			$BaUO_3(cr) + 6\ H^+ \rightleftarrows U^{4+} + Ba^{2+} + 3\ H_2O(l)$			**-293.347 ± 10.667**	
$BaUO_4$(cr)	-1883.805 ± 3.393 [2003GUI/FAN]	-1993.800 ± 3.300 [2003GUI/FAN]	154.000 ± 2.500 [2003GUI/FAN]	125.300 ± 2.500 [2003GUI/FAN]	$BaUO_4(cr) + 4\ H^+ \rightleftarrows UO_2^{2+} + Ba^{2+} + 2\ H_2O(l)$	**17.644 ± 0.731**	**-100.713 ± 4.172**	**-131.508 ± 3.998**	**-103.568 ± 3.931**

Table A19 Selected thermodynamic data for uranium (U) in JAEA-TDB-RN in 2020 (22/25)

Species / compound	$\Delta_f G^0_m$ (kJ.mol^{-1})	$\Delta_f H^0_m$ (kJ.mol^{-1})	S^0_m (J.K^{-1}.mol^{-1})	$C^0_{p,m}$ (J.K^{-1}.mol^{-1})	Reaction	$\log_{10} K°$	$\Delta_r G^0_m$ (kJ.mol^{-1})	$\Delta_r H^0_m$ (kJ.mol^{-1})	$\Delta_r S^0_m$ (J.K^{-1}.mol^{-1})
Ba_3UO_6(cr)	-3044.951 ± 9.196 [2003GUI/FAN]	-3210.400 ± 8.000 [2003GUI/FAN]	298.000 ± 15.000 [2003GUI/FAN]		$Ba_3UO_6(cr) + 8\ H^+ \rightleftarrows UO_2^{2+} + 3\ Ba^{2+} + 4\ H_2O(l)$	**92.700 ± 1.862**	**-529.135 ± 10.630**	**-555.848 ± 9.573**	**-90.149 ± 15.352**
BaU_2O_7(cr)	-3052.093 ± 6.714 [2003GUI/FAN]	-3237.200 ± 5.000 [2003GUI/FAN]	260.000 ± 15.000 [2003GUI/FAN]		$BaU_2O_7(cr) + 6\ H^+ \rightleftarrows 2\ UO_2^{2+} + Ba^{2+} + 3\ H_2O(l)$	**21.401 ± 1.359**	**-122.158 ± 7.757**	**-192.947 ± 6.074**	**-237.845 ± 16.163**
$Ba_2U_2O_7$(cr)	-3547.015 ± 7.743 [2003GUI/FAN]	-3740.000 ± 6.300 [2003GUI/FAN]	296.000 ± 15.000 [2003GUI/FAN]		$Ba_2U_2O_7(cr) + 6\ H^+ \rightleftarrows 2\ UO_2^{+} + 2\ Ba^{2+} + 3\ H_2O(l)$	**35.350 ± 1.601**	**-201.778 ± 9.139**	**-237.032 ± 9.276**	**-118.658 ± 21.949**
$BaUO_2(CO_3)_3^{2-}$	**-3246.393 ± 3.843**				$UO_2^{2+} + Ba^{2+} + 3\ CO_3^{2-} \rightleftarrows BaUO_2(CO_3)_3^{2-}$	26.680 ± 0.500 [14THO/HUM]	**-152.291 ± 2.854**		
$Ba_2UO_2(CO_3)_3$(aq)	**-3821.518 ± 4.814**				$UO_2^{2+} + 2\ Ba^{2+} + 3\ CO_3^{2-} \rightleftarrows Ba_2UO_2(CO_3)_3$(aq)	29.75 ± 0.500 [14THO/HUM]	**-169.814 ± 2.854**		
Ba_2MgUO_6(cr)		-3245.900 ± 6.500 [2003GUI/FAN]			$Ba_2MgUO_6(cr) + 8\ H^+ \rightleftarrows UO_2^{2+} + 2\ Ba^{2+} + Mg^{2+} + 4\ H_2O(l)$			**-451.676 ± 7.554**	
Ba_2CaUO_6(cr)		-3295.800 ± 5.900 [2003GUI/FAN]			$Ba_2CaUO_6(cr) + 8\ H^+ \rightleftarrows UO_2^{2+} + 2\ Ba^{2+} + Ca^{2+} + 4\ H_2O(l)$			**-478.900 ± 7.005**	
Ba_2SrUO_6(cr)		-3257.300 ± 5.700 [2003GUI/FAN]			$Ba_2SrUO_6(cr) + 8\ H^+ \rightleftarrows UO_2^{2+} + 2\ Ba^{2+} + Sr^{2+} + 4\ H_2O(l)$			**-525.224 ± 6.810**	
$Li_{0.12}UO_{2.95}$(cr)		-1254.970 ± 1.225 [2003GUI/FAN]			$Li_{0.12}UO_{2.95}(cr) + 1.9\ H^+ \rightleftarrows UO_2^{2+} + 0.12\ Li^+ + 0.95\ H_2O(l) + 0.22\ e^-$			**-68.991 ± 1.939**	
γ-$Li_{0.55}UO_3$(cr)		-1394.535 ± 2.779 [2003GUI/FAN]			$\gamma\text{-}Li_{0.55}UO_3(cr) + 2\ H^+ \rightleftarrows UO_2^{2+} + 0.55\ Li^+ + H_2O(l) + 0.55\ e^-$			**-63.453 ± 3.160**	
δ-$Li_{0.69}UO_3$(cr)		-1434.525 ± 2.367 [2003GUI/FAN]			$\delta\text{-}Li_{0.69}UO_3(cr) + 2\ H^+ \rightleftarrows UO_2^{2+} + 0.69\ Li^+ + H_2O(l) + 0.69\ e^-$			**-62.446 ± 2.805**	
$LiUO_3$(cr)		-1522.300 ± 1.800 [2003GUI/FAN]			$LiUO_3(cr) + 2\ H^+ \rightleftarrows UO_2^{+} + Li^+ + H_2O(l)$			**-67.119 ± 2.347**	
Li_2UO_4(cr)	-1853.190 ± 2.215 [2003GUI/FAN]	-1968.200 ± 1.300 [2003GUI/FAN]	133.000 ± 6.000 [2003GUI/FAN]		$Li_2UO_4(cr) + 4\ H^+ \rightleftarrows UO_2^{2+} + 2\ Li^+ + 2\ H_2O(l)$	**27.845 ± 0.496**	**-158.942 ± 2.833**	**-179.384 ± 2.003**	**-68.752 ± 6.723**
Li_4UO_5(cr)		-2639.400 ± 1.700 [2003GUI/FAN]			$Li_4UO_5(cr) + 6\ H^+ \rightleftarrows UO_2^{2+} + 4\ Li^+ + 3\ H_2O(l)$			**-350.929 ± 2.313**	

Table A19 Selected thermodynamic data for uranium (U) in JAEA-TDB-RN in 2020 (23/25)

Species / compound	$\Delta_f G^0_m$ (kJ.mol^{-1})	$\Delta_f H^0_m$ (kJ.mol^{-1})	S^0_m (J.K^{-1}.mol^{-1})	$C^0_{p,m}$ (J.K^{-1}.mol^{-1})	Reaction	$\log_{10} K°$	$\Delta_r G^0_m$ (kJ.mol^{-1})	$\Delta_r H^0_m$ (kJ.mol^{-1})	$\Delta_r S^0_m$ (J.K^{-1}.mol^{-1})
$Li_2U_2O_7$(cr)		-3213.600 ± 5.300 [2003GUI/FAN]			$Li_2U_2O_7$(cr) + 6 H^+ ⇄ 2 UO_2^{2+} + 2 Li^+ + 3 H_2O(l)			**-238.822 ± 6.101**	
$Li_{0.19}U_3O_8$(cr)		-3632.955 ± 3.113 [2003GUI/FAN]			$Li_{0.19}U_3O_8$(cr) + 4 H^+ ⇄ 3 UO_2^{2+} + 0.19 Li^+ + 2 H_2O(l) + 2.19 e^-			**-48.628 ± 5.476**	
$Li_{0.88}U_3O_8$(cr)		-3837.090 ± 3.748 [2003GUI/FAN]			$Li_{0.88}U_3O_8$(cr) + 4 H^+ ⇄ 3 UO_2^{2+} + 0.88 Li^+ + 2 H_2O(l) + 2.88 e^-			**-36.626 ± 5.861**	
$Li_2U_3O_{10}$(cr)		-4437.400 ± 4.100 [2003GUI/FAN]			$Li_2U_3O_{10}$(cr) + 8 H^+ ⇄ 3 UO_2^{2+} + 2 Li^+ + 4 H_2O(l)			**-319.860 ± 6.104**	
$Na_{0.12}UO_{2.95}$(cr)		-1247.372 ± 1.877 [2003GUI/FAN]			$Na_{0.12}UO_{2.95}$(cr) + 1.9 H^+ ⇄ UO_2^{2+} + 0.12 Na^+ + 0.95 H_2O(l) + 0.22 e^-			**-72.010 ± 2.405**	
α-$Na_{0.14}UO_3$(cr)		-1267.234 ± 1.804 [2003GUI/FAN]			α-$Na_{0.14}UO_3$(cr) + 2 H^+ ⇄ UO_2^{2+} + 0.14 Na^+ + H_2O(l) + 0.14 e^-			**-71.246 ± 2.349**	
δ-$Na_{0.54}UO_3$(cr)		-1376.954 ± 5.482 [2003GUI/FAN]			δ-$Na_{0.54}UO_3$(cr) + 2 H^+ ⇄ UO_2^{2+} + 0.54 Na^+ + H_2O(l) + 0.54 e^-			**-57.644 ± 5.685**	
$NaUO_3$(cr)	-1412.495 ± 10.001 [2003GUI/FAN]	-1494.900 ± 10.000 [2003GUI/FAN]	132.840 ± 0.400 [2003GUI/FAN]	108.870 ± 0.400 [2003GUI/FAN]	$NaUO_3$(cr) + 2 H^+ ⇄ UO_2^+ + Na^+ + H_2O(l)	**8.337 ± 1.779**	**-47.589 ± 10.155**	**-56.361 ± 10.430**	**-29.508 ± 8.013**
α-Na_2UO_4	-1779.303 ± 3.506 [2003GUI/FAN]	-1897.700 ± 3.500 [2003GUI/FAN]	166.000 ± 0.500 [2003GUI/FAN]	146.700 ± 0.500 [2003GUI/FAN]	α-Na_2UO_4 + 4 H^+ ⇄ UO_2^{2+} + 2 Na^+ + 2 H_2O(l)	**30.023 ± 0.689**	**-171.375 ± 3.930**	**-173.568 ± 3.817**	**-7.537 ± 3.075**
β-Na_2UO_4		-1884.600 ± 3.600 [2003GUI/FAN]			β-Na_2UO_4 + 4 H^+ ⇄ UO_2^{2+} + 2 Na^+ + 2 H_2O(l)			**-186.668 ± 3.909**	
Na_3UO_4(cr)	-1899.909 ± 8.003 [2003GUI/FAN]	-2024.000 ± 8.000 [2003GUI/FAN]	198.200 ± 0.400 [2003GUI/FAN]	173.000 ± 0.400 [2003GUI/FAN]	Na_3UO_4(cr) + 4 H^+ ⇄ UO_2^+ + 3 Na^+ + 2 H_2O(l)	**56.257 ± 1.437**	**-321.119 ± 8.204**	**-293.690 ± 8.536**	**91.872 ± 8.036**
Na_4UO_5(cr)		-2457.000 ± 2.200 [2003GUI/FAN]			Na_4UO_5(cr) + 6 H^+ ⇄ UO_2^{2+} + 4 Na^+ + 3 H_2O(l)			**-386.824 ± 3.716**	
$Na_2U_2O_7$(cr)	-3011.454 ± 4.015 [2003GUI/FAN]	-3203.800 ± 4.000 [2003GUI/FAN]	275.900 ± 1.000 [2003GUI/FAN]	227.300 ± 1.000 [2003GUI/FAN]	$Na_2U_2O_7$(cr) + 6 H^+ ⇄ 2 UO_2^{2+} + 2 Na^+ + 3 H_2O(l)	**22.592 ± 0.935**	**-128.957 ± 5.337**	**-172.306 ± 5.013**	**-145.714 ± 6.102**
$Na_{0.20}U_3O_8$(cr)		-3626.450 ± 3.252 [2003GUI/FAN]			$Na_{0.20}U_3O_8$(cr) + 4 H^+ ⇄ 3 UO_2^{2+} + 0.2 Na^+ + 2 H_2O(l) + 2.2 e^-			**-50.286 ± 5.556**	

Table A19 Selected thermodynamic data for uranium (U) in JAEA-TDB-RN in 2020 (24/25)

Species / compound	$\Delta_f G^0_m$ (kJ.mol^{-1})	$\Delta_f H^0_m$ (kJ.mol^{-1})	S^0_m (J.K^{-1}.mol^{-1})	$C^0_{p,m}$ (J.K^{-1}.mol^{-1})	Reaction	$\log_{10} K°$	$\Delta_r G^0_m$ (kJ.mol^{-1})	$\Delta_r H^0_m$ (kJ.mol^{-1})	$\Delta_r S^0_m$ (J.K^{-1}.mol^{-1})
$Na_6U_7O_{24}$(cr)		-10841.700 ± 10.000 [2003GUI/FAN]			$Na_6U_7O_{24}$(cr) + 20 H^+ ⇄ 7 UO_2^{2+} + 6 Na^+ + 10 H_2O(l)			**-591.456 ± 14.546**	
$Na_4UO_2(CO_3)_3$(cr)	**-3738.918 ± 2.359**				$UO_2(CO_3)_3^{4-}$ + 4 Na^+ ⇄ $Na_4UO_2(CO_3)_3$(cr)	5.340 ± 0.160 [2003GUI/FAN]	-30.481 ± 0.913 [2003GUI/FAN]		
KUO_3(cr)		-1522.900 ± 1.700 [2003GUI/FAN]		137.000 ± 10.000 [2003GUI/FAN]	KUO_3(cr) + 2 H^+ ⇄ UO_2^+ + K^+ + H_2O(l)			**-40.235 ± 3.416**	
K_2UO_4(cr)	-1798.499 ± 3.248 [2003GUI/FAN]	-1920.700 ± 2.200 [2003GUI/FAN]	180.000 ± 8.000 [2003GUI/FAN]		K_2UO_4(cr) + 4 H^+ ⇄ UO_2^{2+} + 2 K^+ + 2 H_2O(l)	**33.872 ± 0.649**	**-193.341 ± 3.702**	**-174.316 ± 2.676**	**63.733 ± 8.560**
$K_2U_2O_7$(cr)		-3250.500 ± 4.500 [2003GUI/FAN]		229.000 ± 20.000 [2003GUI/FAN]	$K_2U_2O_7$(cr) + 6 H^+ ⇄ 2 UO_2^{2+} + 2 K^+ + 3 H_2O(l)			**-149.354 ± 5.420**	
$K_2U_4O_{13}$(cr)				425.000 ± 50.000 [2003GUI/FAN]					
$K_2U_6O_{19}$·11H_2O(cr)	**-10337.748 ± 11.077**				6 UO_2^{2+} + 2 K^+ + 18 H_2O(l) ⇄ $K_2U_6O_{19}$·11H_2O(cr) + 14 H^+	-37.100 ± 0.540 [2003GUI/FAN]	211.768 ± 3.082 [2003GUI/FAN]		
$RbUO_3$(cr)		-1520.900 ± 1.800 [2003GUI/FAN]			$RbUO_3$(cr) + 2 H^+ ⇄ UO_2^+ + Rb^+ + H_2O(l)			**-41.189 ± 3.468**	
Rb_2UO_4(cr)	-1800.141 ± 3.250 [2003GUI/FAN]	-1922.700 ± 2.200 [2003GUI/FAN]	203.000 ± 8.000 [2003GUI/FAN]		Rb_2UO_4(cr) + 4 H^+ ⇄ UO_2^{2+} + 2 Rb^+ + 2 H_2O(l)	**34.009 ± 0.652**	**-194.126 ± 3.719**	**-170.224 ± 2.683**	**79.644 ± 8.556**
$Rb_2U_2O_7$(cr)		-3232.000 ± 4.300 [2003GUI/FAN]			$Rb_2U_2O_7$(cr) + 6 H^+ ⇄ 2 UO_2^{2+} + 2 Rb^+ + 3 H_2O(l)			**-170.224 ± 2.683**	
$Rb_2U_4O_{11}$(cr)				365.600 ± 25.000 [2003GUI/FAN]					
$Rb_2U_4O_{13}$(cr)				420.000 ± 50.000 [2003GUI/FAN]					
$Rb_2U(SO_4)_3$(cr)				348.000 ± 30.000 [2003GUI/FAN]					
Cs_2UO_4(cr)	-1805.370 ± 1.232 [2003GUI/FAN]	-1928.000 ± 1.200 [2003GUI/FAN]	219.660 ± 0.440 [2003GUI/FAN]	152.760 ± 0.310 [2003GUI/FAN]	Cs_2UO_4(cr) + 4 H^+ ⇄ UO_2^{2+} + 2 Cs^+ + 2 H_2O(l)	**35.893 ± 0.383**	**-204.879 ± 2.188**	**-178.731 ± 1.949**	**87.670 ± 3.038**

Table A19 Selected thermodynamic data for uranium (U) in JAEA-TDB-RN in 2020 (25/25)

Species / compound	$\Delta_f G^0_m$ (kJ.mol^{-1})	$\Delta_f H^0_m$ (kJ.mol^{-1})	S^0_m (J.K^{-1}.mol^{-1})	$C^0_{p,m}$ (J.K^{-1}.mol^{-1})	Reaction	$\log_{10} K°$	$\Delta_r G^0_m$ (kJ.mol^{-1})	$\Delta_r H^0_m$ (kJ.mol^{-1})	$\Delta_r S^0_m$ (J.K^{-1}.mol^{-1})
$Cs_2U_2O_7$(cr)	-3022.881	-3220.000	327.750	231.200	$Cs_2U_2O_7(cr) + 6\ H^+ \rightleftarrows 2\ UO_2^{2+} + 2\ Cs^+ + 3\ H_2O(l)$	**31.027**	**-177.102**	**-191.570**	**-48.697**
	± 10.005	± 10.000	± 0.660	± 0.500		**± 1.859**	**± 10.610**	**± 10.448**	**± 6.042**
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]					
$Cs_2U_4O_{12}$(cr)	-5251.058	-5571.800	526.400	384.000	$Cs_2U_4O_{12}(cr) + 8\ H^+ \rightleftarrows 4\ UO_2^{2+} + 2\ Cs^+ + 4\ H_2O(l) + 2\ e^-$	**15.979**	**-91.210**	**-163.608**	**-243.145**
	± 3.628	± 3.600	± 1.000	± 1.000		**± 1.383**	**± 7.895**	**± 7.014**	**± 12.047**
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]					
$Cs_4U_5O_{17}$(cr)				750.000	$Cs_4U_5O_{17}$(cr)				
				± 50.000					
				[2003GUI/FAN]					

[2003GUI/FAN] Guillaumont et al. [A15)]
[2010FUJ/KIT] Fujiwara et al. [A33)]
[14THO/HUM] Thoenen et al. [A34)]

Table A20 Selected thermodynamic data for neptunium (Np) in JAEA-TDB-RN in 2020 (1/8)

Values indicated by **boldface** are calculated and selected in the present report.

Species / compound	$\Delta_f G^0_m$ (kJ.mol^{-1})	$\Delta_f H^0_m$ (kJ.mol^{-1})	S^0_m (J.K^{-1}.mol^{-1})	$C^0_{p,m}$ (J.K^{-1}.mol^{-1})	Reaction	$\log_{10} K°$	$\Delta_r G^0_m$ (kJ.mol^{-1})	$\Delta_r H^0_m$ (kJ.mol^{-1})	$\Delta_r S^0_m$ (J.K^{-1}.mol^{-1})
Np(cr)	0.000	0.000	50.460	29.620	$Np^{4+} + 4\ e^- \rightleftarrows Np(cr)$	**-86.155**	**491.774**	**556.022**	**215.492**
			± 0.800	± 0.800		**± 0.979**	**± 5.586**	**± 4.185**	**± 12.412**
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]					
Np(g)	421.195	465.100	197.719	20.824	$Np^{4+} + 4\ e^- \rightleftarrows Np(g)$	**-159.944**	**912.969**	**1021.122**	**362.751**
	± 3.009	± 3.000	± 0.005	± 0.020		**± 1.112**	**± 6.345**	**± 5.149**	**± 12.386**
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]					
Np^{3+}	-512.866	-527.184	-193.584		$Np^{4+} + 0.5\ H_2(g) \rightleftarrows Np^{3+} + H^+$ ($Np^{4+} + e^- \rightleftarrows Np^{3+}$)	3.695	-21.091	**28.838**	**167.467**
	± 5.669	± 2.092	± 20.253			± 0.169	± 0.965	**± 4.679**	**± 23.740**
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]			[2003GUI/FAN]	[2003GUI/FAN]		
Np^{4+}	-491.774	-556.022	-426.390						
	± 5.586	± 4.185	± 12.386						
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]						
NpO_2(cr)	-1021.731	-1074.000	80.300	66.200	$NpO_2(cr) + 4\ H^+ \rightleftarrows Np^{4+} + 2\ H_2O(l)$	**-9.739**	**55.592**	**-53.699**	**-366.844**
	± 2.514	± 2.500	± 0.400	± 0.500		**± 1.074**	**± 6.129**	**± 4.879**	**± 12.394**
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]					
NpO_2(am,hyd)	**-962.824**				$Np^{4+} + 4\ OH^- \rightleftarrows NpO_2(am,hyd) + 2\ H_2O(l)$	55.400	**-316.226**		
	± 7.995					± 1.000	**± 5.708**		
						[2010FUJ/KIT]			
NpO_2^+	-907.765	-978.181	-45.904	-4.000	$Np^{4+} + 2\ H_2O(l) \rightleftarrows NpO_2^+ + 4\ H^+ + e^-$	**-10.227**	**58.374**	**149.518**	**305.979**
	± 5.628	± 4.629	± 10.706	± 25.000		**± 1.390**	**± 7.932**	**± 6.244**	**± 16.373**
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]					
NpO_2^{2+}	-795.939	-860.733	-92.387		$Np^{4+} + 2\ H_2O(l) \rightleftarrows NpO_2^{2+} + 4\ H^+ + 2\ e^-$	**-29.818**	**170.200**	**266.966**	**324.836**
	± 5.615	± 4.662	± 10.464			**± 1.388**	**± 7.923**	**± 6.268**	**± 16.215**
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]						
Np_2O_5(cr)	-2031.574	-2162.700	174.000	128.600	$Np_2O_5(cr) + 2\ H^+ \rightleftarrows 2\ NpO_2^+ + H_2O(l)$	**3.703**	**-21.139**	**-79.500**	**-195.885**
	± 11.227	± 9.500	± 20.000	± 5.000		**± 2.785**	**± 15.898**	**± 13.265**	**± 29.300**
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]					
$NpOH^{2+}$	**-711.234**				$Np^{3+} + H_2O(l) \rightleftarrows NpOH^{2+} + H^+$	-6.800	38.815		
	± 5.923					± 0.300	± 1.712		
						[2003GUI/FAN]	[2003GUI/FAN]		
$NpOH^{3+}$	**-728.470**				$Np^{4+} + OH^- \rightleftarrows NpOH^{3+}$	13.910	**-79.399**		
	± 5.739					± 0.230	**± 1.313**		
						[2010FUJ/KIT]			
$Np(OH)_2^{2+}$	**-961.228**				$Np^{4+} + 2\ OH^- \rightleftarrows Np(OH)_2^{2+}$	27.130	**-154.859**		
	± 5.596					± 0.050	**± 0.285**		
						[2010FUJ/KIT]			
NpO_2OH(am,aged)	**-1118.120**				$NpO_2^+ + H_2O(l) \rightleftarrows NpO_2OH(am, aged) + H^+$	-4.700	26.828		
	± 6.311					± 0.500	± 2.854		
						[2003GUI/FAN]	[2003GUI/FAN]		

Table A20 Selected thermodynamic data for neptunium (Np) in JAEA-TDB-RN in 2020 (2/8)

Species / compound	$\Delta_f G^0_m$ (kJ.mol^{-1})	$\Delta_f H^0_m$ (kJ.mol^{-1})	S^0_m (J.K^{-1}.mol^{-1})	$C^0_{p,m}$ (J.K^{-1}.mol^{-1})	Reaction	$\log_{10} K°$	$\Delta_r G^0_m$ (kJ.mol^{-1})	$\Delta_r H^0_m$ (kJ.mol^{-1})	$\Delta_r S^0_m$ (J.K^{-1}.mol^{-1})
NpO_2OH(am,fresh)	**-1114.695**				$NpO_2^+ + H_2O(l) \rightleftarrows NpO_2OH(am, fresh) + H^+$	-5.300	30.253		
	± 5.743					± 0.200	± 1.142		
						[2003GUI/FAN]	[2003GUI/FAN]		
$NpO_2OH(aq)$	**-1080.447**	-1199.226	25.000		$NpO_2^+ + H_2O(l) \rightleftarrows NpO_2OH(aq) + H^+$	-11.300	64.501		
	± 6.903	± 19.176	± 60.000			± 0.700	± 3.996		
		[2003GUI/FAN]	[2003GUI/FAN]			[2003GUI/FAN]	[2003GUI/FAN]		
NpO_2OH^+	**-1004.011**				$NpO_2^{2+} + H_2O(l) \rightleftarrows NpO_2OH^+ + H^+$	-5.100	29.111		
	± 6.062					± 0.400	± 2.283		
						[2003GUI/FAN]	[2003GUI/FAN]		
$NpO_2(OH)_2$(cr)	-1239.000	-1377.000	128.590	120.000	$NpO_2(OH)_2(cr) + 2\ H^+ \rightleftarrows NpO_2^{2+} + 2\ H_2O(l)$	**5.484**	**-31.304**	**-55.410**	**-81.131**
	± 6.400	± 5.000	± 27.252	± 20.000		**± 1.492**	**± 8.516**	**± 6.839**	**± 29.192**
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]					
$NpO_2(OH)_2^-$	**-1247.420**	-1431.230	40.000		$NpO_2^+ + 2\ H_2O(l) \rightleftarrows NpO_2(OH)_2^- + 2\ H^+$	-23.600	134.710		
	± 6.313	± 30.476	± 100.000			± 0.500	± 2.854		
		[2003GUI/FAN]	[2003GUI/FAN]			[2003GUI/FAN]	[2003GUI/FAN]		
$Np(OH)_3^+$	**-1178.860**				$Np^{4+} + 3\ OH^- \rightleftarrows Np(OH)_3^+$	37.700	**-215.193**		
	± 5.847					± 0.300	**± 1.712**		
						[2010FUJ/KIT]			
$Np(OH)_4$(aq)	**-1385.817**				$Np^{4+} + 4\ OH^- \rightleftarrows Np(OH)_4(aq)$	46.400	**-264.853**		
	± 8.410					± 1.100	**± 6.279**		
						[2010FUJ/KIT]			
$(NpO_2)_2(OH)_2^{2+}$	**-2030.454**				$2\ NpO_2^{2+} + 2\ H_2O(l) \rightleftarrows (NpO_2)_2(OH)_2^{2+} + 2\ H^+$	-6.270	35.789		
	± 11.296					± 0.210	± 1.199		
						[2003GUI/FAN]	[2003GUI/FAN]		
$(NpO_2)_3(OH)_5^+$	**-3476.008**				$3\ NpO_2^{2+} + 5\ H_2O(l) \rightleftarrows (NpO_2)_3(OH)_5^+ + 5\ H^+$	-17.120	97.722		
	± 16.899					± 0.220	± 1.256		
						[2003GUI/FAN]	[2003GUI/FAN]		
NpF(g)	-109.560	-80.000	251.000	33.800	$NpF(g) \rightleftarrows Np^{4+} + F^- + 3\ e^-$	**116.321**	**-663.965**	**-811.370**	**-494.551**
	± 25.046	± 25.000	± 5.000	± 3.000		**± 4.497**	**± 25.670**	**± 25.357**	**± 13.368**
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]					
NpF^{3+}	**-824.669**	**-889.870**	**-263.000**		$Np^{4+} + F^- \rightleftarrows NpF^{3+}$	8.960	-51.144	1.500	176.570
	± 5.682	**± 4.686**	**± 14.349**			± 0.140	± 0.799	± 2.000	± 7.224
						[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]
$NpF_2(g)$	-590.131	-575.000	304.000	55.900	$NpF_2(g) \rightleftarrows Np^{4+} + 2\ F^- + 2\ e^-$	**81.489**	**-465.144**	**-651.717**	**-626.070**
	± 30.149	± 30.000	± 10.000	± 5.000		**± 5.377**	**± 30.691**	**± 30.320**	**± 15.956**
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]					
NpF_2^{2+}	**-1144.891**				$Np^{4+} + 2\ F^- \rightleftarrows NpF_2^{2+}$	15.700	-89.616		
	± 5.994					± 0.300	± 1.712		
						[2003GUI/FAN]	[2003GUI/FAN]		
NpF_3(cr)	-1460.501	-1529.000	124.900	94.200	$NpF_3(cr) \rightleftarrows Np^{3+} + 3\ F^-$	**-17.937**	**102.383**	**-4.227**	**-358.023**
	± 8.325	± 8.300	± 2.000	± 3.000		**± 1.799**	**± 10.270**	**± 8.792**	**± 20.417**
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]					

Table A20 Selected thermodynamic data for neptunium (Np) in JAEA-TDB-RN in 2020 (3/8)

Species / compound	$\Delta_f G^0_m$ (kJ.mol^{-1})	$\Delta_f H^0_m$ (kJ.mol^{-1})	S^0_m (J.K^{-1}.mol^{-1})	$C^0_{p,m}$ (J.K^{-1}.mol^{-1})	Reaction	$\log_{10} K°$	$\Delta_r G^0_m$ (kJ.mol^{-1})	$\Delta_r H^0_m$ (kJ.mol^{-1})	$\Delta_r S^0_m$ (J.K^{-1}.mol^{-1})
$NpF_3(g)$	-1107.801	-1115.000	330.500	72.200	$NpF_3(g) \rightleftarrows Np^{3+} + 3\ F^-$	**43.853**	**-250.317**	**-418.227**	**-563.623**
	± 25.178	± 25.000	± 10.000	± 5.000		**± 4.535**	**± 25.886**	**± 25.168**	**± 22.646**
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]					
$NpF_4(cr)$	-1783.797	-1874.000	153.500	116.100	$NpF_4(cr) \rightleftarrows Np^{4+} + 4\ F^-$	**-28.910**	**165.021**	**-23.412**	**-632.608**
	± 16.046	± 16.000	± 4.000	± 4.000		**± 3.013**	**± 17.200**	**± 16.754**	**± 13.196**
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]					
$NpF_4(g)$	-1535.287	-1561.000	369.800	95.300	$NpF_4(g) \rightleftarrows Np^{4+} + 4\ F^-$	**14.627**	**-83.489**	**-336.412**	**-848.908**
	± 22.202	± 22.000	± 10.000	± 5.000		**± 4.038**	**± 23.050**	**± 22.554**	**± 16.067**
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]					
$NpF_5(cr)$	-1834.430	-1941.000	200.000	132.800	$NpF_5(cr) + 2\ H_2O(l) \rightleftarrows NpO_2^+ + 5\ F^- + 4\ H^+$	**1.353**	**-7.723**	**-142.242**	**-451.648**
	± 25.398	± 25.000	± 15.000	± 8.000		**± 4.595**	**± 26.229**	**± 25.645**	**± 18.629**
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]					
$NpF_6(cr)$	-1841.872	-1970.000	229.090	167.440	$NpF_6(cr) + 2\ H_2O(l) \rightleftarrows NpO_2^{2+} + 6\ F^- + 4\ H^+$	**29.818**	**-170.205**	**-331.142**	**-540.401**
	± 20.002	± 20.000	± 0.500	± 0.400		**± 3.707**	**± 21.161**	**± 20.926**	**± 10.974**
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]					
$NpF_6(g)$	-1837.525	-1921.660	376.643	129.072	$NpF_6(g) + 2\ H_2O(l) \rightleftarrows NpO_2^{2+} + 6\ F^- + 4\ H^+$	**30.580**	**-174.552**	**-379.482**	**-687.954**
	± 20.002	± 20.000	± 0.500	± 1.000		**± 3.707**	**± 21.161**	**± 20.926**	**± 10.974**
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]					
$NpO_2F(aq)$	**-1196.365**				$NpO_2^+ + F^- \rightleftarrows NpO_2F(aq)$	1.200	-6.850		
	± 5.921					± 0.300	± 1.712		
						[2003GUI/FAN]	[2003GUI/FAN]		
NpO_2F^+	**-1103.775**				$NpO_2^{2+} + F^- \rightleftarrows NpO_2F^+$	4.570	-26.086		
	± 5.669					± 0.070	± 0.400		
						[2003GUI/FAN]	[2003GUI/FAN]		
$NpO_2F_2(aq)$	**-1402.821**				$NpO_2^{2+} + 2\ F^- \rightleftarrows NpO_2F_2(aq)$	7.600	-43.381		
	± 5.790					± 0.080	± 0.457		
						[2003GUI/FAN]	[2003GUI/FAN]		
$NpCl^{3+}$	**-631.626**				$Np^{4+} + Cl^- \rightleftarrows NpCl^{3+}$	1.500	-8.562		
	± 5.843					± 0.300	± 1.712		
						[2003GUI/FAN]	[2003GUI/FAN]		
$NpCl_3(cr)$	-829.811	-896.800	160.400	101.850	$NpCl_3(cr) \rightleftarrows Np^{3+} + 3\ Cl^-$	**13.476**	**-76.924**	**-131.623**	**-183.779**
	± 3.237	± 3.000	± 4.000	± 4.000		**± 1.145**	**± 6.535**	**± 3.667**	**± 20.650**
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]					
$NpCl_3(g)$	-582.357	-589.000	362.800	78.500	$NpCl_3(g) \rightleftarrows Np^{3+} + 3\ Cl^-$	**56.828**	**-324.378**	**-439.423**	**-386.179**
	± 10.822	± 10.400	± 10.000	± 5.000		**± 2.141**	**± 12.221**	**± 10.612**	**± 22.593**
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]					
$NpCl_4(cr)$	-895.562	-984.000	200.000	122.000	$NpCl_4(cr) \rightleftarrows Np^{4+} + 4\ Cl^-$	**21.263**	**-121.371**	**-240.341**	**-399.450**
	± 2.998	± 1.800	± 8.000	± 6.000		**± 1.113**	**± 6.352**	**± 4.569**	**± 14.760**
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]					
$NpCl_4(g)$	-765.050	-787.000	423.000	105.000	$NpCl_4(g) \rightleftarrows Np^{4+} + 4\ Cl^-$	**44.128**	**-251.883**	**-437.341**	**-622.450**
	± 5.487	± 4.600	± 10.000	± 5.000		**± 1.374**	**± 7.840**	**± 6.229**	**± 15.933**
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]					

Table A20 Selected thermodynamic data for neptunium (Np) in JAEA-TDB-RN in 2020 (4/8)

Species / compound	$\Delta_f G^0_m$ (kJ.mol^{-1})	$\Delta_f H^0_m$ (kJ.mol^{-1})	S^0_m (J.K^{-1}.mol^{-1})	$C^0_{p,m}$ (J.K^{-1}.mol^{-1})	Reaction	$\log_{10} K°$	$\Delta_r G^0_m$ (kJ.mol^{-1})	$\Delta_r H^0_m$ (kJ.mol^{-1})	$\Delta_r S^0_m$ (J.K^{-1}.mol^{-1})
$NpOCl_2$(cr)	-960.645	-1030.000	143.500	95.000	$NpOCl_2(cr) + 2\ H^+ \rightleftarrows Np^{4+} + 2\ Cl^- + H_2O(l)$	**5.412**	**-30.891**	**-146.020**	**-386.497**
	± 8.141	± 8.000	± 5.000	± 4.000		**± 1.730**	**± 9.876**	**± 9.031**	**± 13.362**
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]					
NpO_2Cl^+	**-929.512**				$NpO_2^{2+} + Cl^- \rightleftarrows NpO_2Cl^+$	0.400	-2.283		
	± 5.699					± 0.170	± 0.970		
						[2003GUI/FAN]	[2003GUI/FAN]		
NpO_2ClO_4(aq)				-32.000					
				± 25.000					
				[2003GUI/FAN]					
$NpBr_3$(cr)	-705.521	-730.200	196.000	103.800	$NpBr_3(cr) \rightleftarrows Np^{3+} + 3\ Br^-$	**20.931**	**-119.476**	**-161.494**	**-141.054**
	± 3.765	± 2.900	± 8.000	± 6.000		**± 1.195**	**± 6.824**	**± 3.604**	**± 21.785**
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]					
$NpBr_4$(cr)	-737.843	-771.200	243.000	128.000	$NpBr_4(cr) \rightleftarrows Np^{4+} + 4\ Br^-$	**29.801**	**-170.105**	**-270.835**	**-338.017**
	± 3.495	± 1.800	± 10.000	± 4.000		**± 1.160**	**± 6.623**	**± 4.595**	**± 15.941**
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]					
$NpOBr_2$(cr)	-906.933	-950.000	160.800	98.200	$NpOBr_2(cr) + 2\ H^+ \rightleftarrows Np^{4+} + 2\ Br^- + H_2O(l)$	**5.275**	**-30.111**	**-134.867**	**-351.581**
	± 11.067	± 11.000	± 4.000	± 4.000		**± 2.173**	**± 12.402**	**± 11.774**	**± 13.023**
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]					
NpI^{3+}	**-552.260**				$Np^{4+} + I^- \rightleftarrows NpI^{3+}$	1.500	-8.562		
	± 6.092					± 0.400	± 2.283		
						[2003GUI/FAN]	[2003GUI/FAN]		
NpI_3(cr)	-512.498	-512.400	225.000	110.000	$NpI_3(cr) \rightleftarrows Np^{3+} + 3\ I^-$	**27.354**	**-156.138**	**-185.491**	**-98.508**
	± 3.715	± 2.200	± 10.000	± 8.000		**± 1.266**	**± 7.228**	**± 3.939**	**± 22.596**
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]					
NpO_2IO_3(aq)	**-1038.649**				$NpO_2^+ + IO_3^- \rightleftarrows NpO_2IO_3$(aq)	0.500	-2.854		
	± 10.229					± 0.300	± 1.712		
						[2003GUI/FAN]	[2003GUI/FAN]		
$NpO_2IO_3^+$	**-930.819**				$NpO_2^{2+} + IO_3^- \rightleftarrows NpO_2IO_3^+$	1.200	-6.850		
	± 10.222					± 0.300	± 1.712		
						[2003GUI/FAN]	[2003GUI/FAN]		
$NpSO_4^{2+}$	**-1275.328**	**-1437.722**	**-182.815**		$Np^{4+} + HSO_4^- \rightleftarrows NpSO_4^{2+} + H^+$	4.870	-27.798	7.400	118.055
						± 0.150	± 0.856	± 8.800	± 29.655
						[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]
NpO_2SO_4(aq)	**-1559.120**	**-1753.635**	**45.248**		$NpO_2^{2+} + SO_4^{2-} \rightleftarrows NpO_2SO_4$(aq)	3.280	-18.722	16.700	118.807
	± 5.644	**± 4.707**	**± 10.671**			± 0.060	± 0.342	± 0.500	± 2.033
						[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]
$NpO_2SO_4^-$	**-1654.736**	**-1864.583**	**59.161**		$NpO_2^+ + SO_4^{2-} \rightleftarrows NpO_2SO_4^-$	0.440	-2.512	23.200	86.237
	± 5.853	**± 8.570**	**± 26.921**			± 0.270	± 1.541	± 7.200	± 24.696
						[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]
$Np(SO_4)_2$(aq)	**-2043.756**	**-2323.722**	**-4.396**		$Np^{4+} + 2\ HSO_4^- \rightleftarrows Np(SO_4)_2(aq) + 2\ H^+$	7.090	-40.470	10.500	170.954
						± 0.250	± 1.427	± 3.600	± 12.988
						[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]

Table A20 Selected thermodynamic data for neptunium (Np) in JAEA-TDB-RN in 2020 (5/8)

Species / compound	$\Delta_f G^0_m$ (kJ.mol^{-1})	$\Delta_f H^0_m$ (kJ.mol^{-1})	S^0_m (J.K^{-1}.mol^{-1})	$C^0_{p,m}$ (J.K^{-1}.mol^{-1})	Reaction	$\log_{10} K°$	$\Delta_r G^0_m$ (kJ.mol^{-1})	$\Delta_r H^0_m$ (kJ.mol^{-1})	$\Delta_r S^0_m$ (J.K^{-1}.mol^{-1})
$NpO_2(SO_4)_2^{2-}$	**-1567.226**	**-1744.335**	**103.626**		$NpO_2^{2+} + 2\ SO_4^{2-} \rightleftarrows NpO_2(SO_4)_2^{2-}$	4.700	-26.828	26.000	177.185
	± 5.663	**± 4.832**	**± 11.385**			± 0.100	± 0.571	± 1.200	± 4.457
						[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]
NpN(cr)	-280.443	-305.000	63.900	48.700	$NpN(cr) + 3\ H_2O(l) \rightleftarrows Np^{4+} + NO_3^- + 6\ H^+ + 9\ e^-$	**-68.202**	**389.299**	**399.594**	**34.938**
	± 10.013	± 10.000	± 1.500	± 0.900		**± 2.057**	**± 11.741**	**± 10.853**	**± 12.508**
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]					
$NpNO_3^{3+}$	**-613.537**				$Np^{4+} + NO_3^- \rightleftarrows NpNO_3^{3+}$	1.900	-10.845		
	± 6.184					± 0.150	± 0.856		
						[2003GUI/FAN]	[2003GUI/FAN]		
$NpO_2(NO_3)_2{\cdot}6H_2O(s)$	-2428.069	-3008.241	516.306		$NpO_2(NO_3)_2{\cdot}6H_2O(s) \rightleftarrows NpO_2^{2+} + 2\ NO_3^- + 6\ H_2O(l)$	**2.243**	**-12.801**	**18.680**	**104.729**
	± 5.565	± 5.022	± 8.000			**± 1.644**	**± 9.385**	**± 6.932**	**± 13.287**
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]						
$NpO_2HPO_4(aq)$	**-1920.466**				$NpO_2^{2+} + HPO_4^{2-} \rightleftarrows NpO_2HPO_4(aq)$	6.200	-35.390		
	± 6.942					± 0.700	± 3.996		
						[2003GUI/FAN]	[2003GUI/FAN]		
$NpO_2HPO_4^-$	**-2013.741**				$NpO_2^+ + HPO_4^{2-} \rightleftarrows NpO_2HPO_4^-$	2.950	-16.839		
	± 5.718					± 0.100	± 0.571		
						[2003GUI/FAN]	[2003GUI/FAN]		
$NpO_2H_2PO_4^+$	**-1945.155**				$NpO_2^{2+} + H_2PO_4^- \rightleftarrows NpO_2H_2PO_4^+$	3.320	-18.951		
	± 6.354					± 0.500	± 2.854		
						[2003GUI/FAN]	[2003GUI/FAN]		
$NpO_2(HPO_4)_2^{2-}$	**-3028.439**				$NpO_2^{2+} + 2\ HPO_4^{2-} \rightleftarrows NpO_2(HPO_4)_2^{2-}$	9.500	-54.226		
	± 8.180					± 1.000	± 5.708		
						[2003GUI/FAN]	[2003GUI/FAN]		
NpSb(cr)			101.400	48.900					
			± 6.100	± 2.900					
			[2003GUI/FAN]	[2003GUI/FAN]					
$NpC_{0.91}(cr)$	-76.024	-71.100	72.200	50.000	$NpC_{0.91}(cr) + 2.73\ H_2O(l)$	**52.970**	**-302.357**	**-332.423**	**-100.697**
	± 10.028	± 10.000	± 2.400	± 1.000	$\rightleftarrows Np^{4+} + 0.91\ HCO_3^- + 4.55\ H^+ + 7.64\ e^-$	**± 2.012**	**± 11.483**	**± 10.846**	**± 12.627**
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]					
$Np_2C_3(cr)$	-192.427	-187.400	135.000	110.000	$Np_2C_3(cr) + 9\ H_2O(l) \rightleftarrows 2\ Np^{4+} + 3\ HCO_3^- + 15\ H^+ + 20\ e^-$	**73.107**	**-417.297**	**-421.899**	**-14.950**
	± 19.436	± 19.200	± 10.000	± 8.000		**± 3.931**	**± 22.439**	**± 20.976**	**± 26.769**
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]					
$NpO_2CO_3(aq)$	**-1377.121**				$NpO_2^{2+} + CO_3^{2-} \rightleftarrows NpO_2CO_3(aq)$	9.320	-53.199		
	± 6.613					± 0.610	± 3.482		
						[2003GUI/FAN]	[2003GUI/FAN]		
$NpO_2CO_3(s)$	**-1407.237**				$NpO_2^{2+} + CO_3^{2-} \rightleftarrows NpO_2CO_3(s)$	14.596	-83.315		
	± 6.227					± 0.469	± 2.677		
						[2003GUI/FAN]	[2003GUI/FAN]		
$NpO_2CO_3^-$	**-1464.071**				$NpO_2^+ + CO_3^{2-} \rightleftarrows NpO_2CO_3^-$	4.962	-28.323		
	± 5.646					± 0.061	± 0.348		
						[2003GUI/FAN]	[2003GUI/FAN]		

Table A20 Selected thermodynamic data for neptunium (Np) in JAEA-TDB-RN in 2020 (6/8)

Species / compound	$\Delta_f G^0_m$ (kJ.mol^{-1})	$\Delta_f H^0_m$ (kJ.mol^{-1})	S^0_m (J.K^{-1}.mol^{-1})	$C^0_{p,m}$ (J.K^{-1}.mol^{-1})	Reaction	$\log_{10} K°$	$\Delta_r G^0_m$ (kJ.mol^{-1})	$\Delta_r H^0_m$ (kJ.mol^{-1})	$\Delta_r S^0_m$ (J.K^{-1}.mol^{-1})
$NpO_2(CO_3)_2^{2-}$	**-1946.179 ± 7.013**				$NpO_2^{2+} + 2\ CO_3^{2-} \rightleftarrows NpO_2(CO_3)_2^{2-}$	16.516 ± 0.729 [2003GUI/FAN]	-94.274 ± 4.161 [2003GUI/FAN]		
$NpO_2(CO_3)_2^{3-}$	**-2001.028 ± 5.674**				$NpO_2CO_3^- + CO_3^{2-} \rightleftarrows NpO_2(CO_3)_2^{3-}$	1.572 ± 0.083 [2003GUI/FAN]	-8.973 ± 0.474 [2003GUI/FAN]		
$Np(CO_3)_3^{3-}$	-2185.949 ± 15.451 [2003GUI/FAN]				$Np(CO_3)_5^{6-} + e^- \rightleftarrows Np(CO_3)_3^{3-} + 2\ CO_3^{2-}$	-16.261 ± 2.265 [2003GUI/FAN]	92.818 ± 12.929 [2003GUI/FAN]		
$NpO_2(CO_3)_3^{4-}$		**-2928.338 ± 6.355**			$NpO_2^{2+} + 3\ CO_3^{2-} \rightleftarrows NpO_2(CO_3)_3^{4-}$			-41.900 ± 4.100 [2003GUI/FAN]	
	-2490.459 ± 5.742		-12.070 ± 17.917 [2003GUI/FAN]		$NpO_2(CO_3)_3^{5-} \rightleftarrows NpO_2(CO_3)_3^{4-} + e^-$	-5.720 ± 0.095 [2003GUI/FAN]	32.650 ± 0.542 [2003GUI/FAN]	88.800 ± 2.900 [2003GUI/FAN]	**188.319 ± 27.201**
$NpO_2(CO_3)_3^{5-}$	**-2523.109 ± 5.716**		-135.050 ± 20.467 [2003GUI/FAN]		$NpO_2(CO_3)_2^{3-} + CO_3^{2-} \rightleftarrows NpO_2(CO_3)_3^{5-}$	-1.034 ± 0.110 [2003GUI/FAN]	5.902 ± 0.628 [2003GUI/FAN]		
		-3017.138 ± 6.985			$NpO_2(CO_3)_3^{4-} + e^- \rightleftarrows NpO_2(CO_3)_3^{5-}$		See above.		
$Np(CO_3)_4^{4-}$	-2812.775 ± 8.240 [2003GUI/FAN]				$Np^{4+} + 4\ CO_3^{2-} \rightleftarrows Np(CO_3)_4^{4-}$	**-4.688 ± 1.746**	**26.759 ± 9.968**		
$Np(CO_3)_5^{6-}$	**-3334.651 ± 8.421**				$Np(CO_3)_4^{4-} + CO_3^{2-} \rightleftarrows Np(CO_3)_5^{6-}$	-1.070 ± 0.300 [2003GUI/FAN]	6.108 ± 1.712 [2003GUI/FAN]		
$(NpO_2)_3(CO_3)_6^{6-}$	**-5840.210 ± 19.123**				$3\ NpO_2(CO_3)_3^{4-} \rightleftarrows (NpO_2)_3(CO_3)_6^{6-} + 3\ CO_3^{2-}$	-8.272 ± 1.447 [2003GUI/FAN]	47.217 ± 8.260 [2003GUI/FAN]		
$Np(CO_3)_2(OH)_2^{2-}$	**-2115.715 ± 8.904**				$Np^{4+} + 2\ CO_3^{2-} + 2\ OH^- \rightleftarrows Np(CO_3)_2(OH)_2^{2-}$	44.390 ± 1.210 [2010FUJ/KIT]	**-253.380 ± 6.907**		
$NpO_2(CO_3)_2OH^{4-}$	**-2170.660 ± 8.770**				$NpO_2(CO_3)_3^{5-} + OH^- \rightleftarrows NpO_2(CO_3)_2OH^{4-} + CO_3^{2-}$	3.195 ± 1.164 [2003GUI/FAN]	-18.237 ± 6.644 [2003GUI/FAN]		
$(NpO_2)_2CO_3(OH)_3^-$	**-2815.400 ± 14.630**				$2\ NpO_2(CO_3)_3^{4-} + 7\ H^+ \rightleftarrows (NpO_2)_2CO_3(OH)_3^- + 5\ CO_2(g) + 2\ H_2O(l)$	49.166 ± 1.586 [2003GUI/FAN]	-280.642 ± 9.053 [2003GUI/FAN]		
$(NH_4)_4NpO_2(CO_3)_3(s)$	**-2850.760 ± 6.135**				$NpO_2(CO_3)_3^{4-} + 4\ NH_4^+ \rightleftarrows (NH_4)_4NpO_2(CO_3)_3(s)$	7.443 ± 0.297 [2003GUI/FAN]	-42.485 ± 1.695 [2003GUI/FAN]		

Table A20 Selected thermodynamic data for neptunium (Np) in JAEA-TDB-RN in 2020 (7/8)

Species / compound	$\Delta_f G^0_m$ (kJ.mol^{-1})	$\Delta_f H^0_m$ (kJ.mol^{-1})	S^0_m (J.K^{-1}.mol^{-1})	$C^0_{p,m}$ (J.K^{-1}.mol^{-1})	Reaction	$\log_{10} K°$	$\Delta_r G^0_m$ (kJ.mol^{-1})	$\Delta_r H^0_m$ (kJ.mol^{-1})	$\Delta_r S^0_m$ (J.K^{-1}.mol^{-1})
$NpSCN^{3+}$	**-416.013**	**-486.455**	**-248.086**		$Np^{4+} + SCN^- \rightleftarrows NpSCN^{3+}$	3.000	-17.124	-7.000	33.956
	± 10.206	**± 9.825**	**± 18.912**			± 0.300	± 1.712	± 3.000	± 11.586
						[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]
$Np(SCN)_2^{2+}$	**-329.407**	**-411.888**	**-89.386**		$Np^{4+} + 2\ SCN^- \rightleftarrows Np(SCN)_2^{2+}$	4.100	-23.403	-9.000	48.308
	± 17.873	**± 19.458**	**± 37.899**			± 0.500	± 2.854	± 9.000	± 31.668
						[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]
$Np(SCN)_3^+$	**-240.518**	**-339.320**	**54.947**		$Np^{4+} + 3\ SCN^- \rightleftarrows Np(SCN)_3^+$	4.800	-27.399	-13.000	48.293
	± 25.876	**± 26.995**	**± 42.267**			± 0.500	± 2.854	± 9.000	± 31.668
						[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]
Sr_3NpO_6(cr)		-3125.800			$Sr_3NpO_6(cr) + 8\ H^+ \rightleftarrows NpO_2^{2+} + 3\ Sr^{2+} + 4\ H_2O(l)$			**-531.008**	
		± 5.900						**± 7.680**	
		[2003GUI/FAN]							
Ba_3NpO_6(cr)		-3085.600			$Ba_3NpO_6(cr) + 8\ H^+ \rightleftarrows NpO_2^{2+} + 3\ Ba^{2+} + 4\ H_2O(l)$			**-522.381**	
		± 9.600						**± 11.802**	
		[2003GUI/FAN]							
Ba_2MgNpO_6(cr)		-3096.900			$Ba_2MgNpO_6(cr) + 8\ H^+ \rightleftarrows NpO_2^{2+} + Mg^{2+} + 2\ Ba^{2+} + 4\ H_2O(l)$			**-442.409**	
		± 8.200						**± 10.077**	
		[2003GUI/FAN]							
Ba_2CaNpO_6(cr)		-3159.300			$Ba_2CaNpO_6(cr) + 8\ H^+ \rightleftarrows NpO_2^{2+} + Ca^{2+} + 2\ Ba^{2+} + 4\ H_2O(l)$			**-457.133**	
		± 7.900						**± 9.806**	
		[2003GUI/FAN]							
Ba_2SrNpO_6(cr)		-3122.500			$Ba_2SrNpO_6(cr) + 8\ H^+ \rightleftarrows NpO_2^{2+} + Sr^{2+} + 2\ Ba^{2+} + 4\ H_2O(l)$			**-501.757**	
		± 7.800						**± 9.706**	
		[2003GUI/FAN]							
Li_2NpO_4(cr)		-1828.200			$Li_2NpO_4(cr) + 4\ H^+ \rightleftarrows NpO_2^{2+} + 2\ Li^+ + 2\ H_2O(l)$			**-161.117**	
		± 5.800						**± 7.446**	
		[2003GUI/FAN]							
α-Na_2NpO_4		-1763.800			$\alpha\text{-}Na_2NpO_4 + 4\ H^+ \rightleftarrows NpO_2^{2+} + 2\ Na^+ + 2\ H_2O(l)$			**-149.201**	
		± 5.700						**± 7.369**	
		[2003GUI/FAN]							
β-Na_2NpO_4		-1748.500			$\beta\text{-}Na_2NpO_4 + 4\ H^+ \rightleftarrows NpO_2^{2+} + 2\ Na^+ + 2\ H_2O(l)$			**-164.501**	
		± 6.100						**± 7.682**	
		[2003GUI/FAN]							
β-Na_4NpO_5		-2315.400			$\beta\text{-}Na_4NpO_5 + 6\ H^+ \rightleftarrows NpO_2^{2+} + 4\ Na^+ + 3\ H_2O(l)$			**-2679.430**	
		± 5.700						**± 4.685**	
		[2003GUI/FAN]							
$Na_2Np_2O_7$(cr)		-2894.000			$Na_2Np_2O_7(cr) + 6\ H^+ \rightleftarrows 2\ NpO_2^{2+} + 2\ Na^+ + 3\ H_2O(l)$			**-165.572**	
		± 11.000						**± 14.424**	
		[2003GUI/FAN]							
Na_3NpF_8(cr)	-3521.239	-3714.000	369.000	272.250	$Na_3NpF_8(cr) + e^- \rightleftarrows Np^{4+} + 3\ Na^+ + 8\ F^-$	**1.784**	**-10.182**	**-245.689**	**-790.940**
	± 21.305	± 21.000	± 12.000	± 12.000		**± 3.972**	**± 22.670**	**± 22.074**	**± 17.797**
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]					

Table A20 Selected thermodynamic data for neptunium (Np) in JAEA-TDB-RN in 2020 (8/8)

Species / compound	$\Delta_f G^0_m$ (kJ.mol^{-1})	$\Delta_f H^0_m$ (kJ.mol^{-1})	S^0_m (J.K^{-1}.mol^{-1})	$C^0_{p,m}$ (J.K^{-1}.mol^{-1})	Reaction	$\log_{10} K°$	$\Delta_r G^0_m$ (kJ.mol^{-1})	$\Delta_r H^0_m$ (kJ.mol^{-1})	$\Delta_r S^0_m$ (J.K^{-1}.mol^{-1})
$Na_3NpO_2(CO_3)_2$(cr)	**-2830.542 ± 6.349**				$NpO_2^+ + 2\ CO_3^{2-} + 3\ Na^+ \rightleftarrows Na_3NpO_2(CO_3)_2$(cr)	14.220 ± 0.500 [2003GUI/FAN]	-81.168 ± 2.854 [2003GUI/FAN]		
$NaNpO_2CO_3 \cdot 3.5H_2O$(cr)	**-2590.556 ± 5.812**				$NpO_2^+ + CO_3^{2-} + 3.5\ H_2O + Na^+ \rightleftarrows NaNpO_2CO_3 \bullet 3.5H_2O$(cr)	11.000 ± 0.240 [2003GUI/FAN]	-62.788 ± 1.370 [2003GUI/FAN]		
K_2NpO_4(cr)		-1784.300 ± 6.400 [2003GUI/FAN]			K_2NpO_4(cr) + 4 $H^+ \rightleftarrows NpO_2^{2+} + 2\ K^+ + 2\ H_2O$(l)			**-152.449 ± 7.923**	
$K_2Np_2O_7$(cr)		-2932.000 ± 11.000 [2003GUI/FAN]			$K_2Np_2O_7$(cr) + 6 $H^+ \rightleftarrows 2\ NpO_2^{2+} + 2\ K^+ + 3\ H_2O$(l)			**-151.320 ± 14.424**	
$KNpO_2CO_3$(s)	**-1793.271 ± 5.740**				$NpO_2^+ + CO_3^{2-} + K^+ \rightleftarrows KNpO_2CO_3$(s)	13.150 ± 0.190 [2003GUI/FAN]	-75.061 ± 1.085 [2003GUI/FAN]		
$K_3NpO_2(CO_3)_2$(s)	**-2899.363 ± 5.744**				$NpO_2^+ + 2\ CO_3^{2-} + 3\ K^+ \rightleftarrows K_3NpO_2(CO_3)_2$(s)	15.460 ± 0.160 [2003GUI/FAN]	-88.246 ± 0.913 [2003GUI/FAN]		
$K_4NpO_2(CO_3)_3$(s)	**-3660.451 ± 7.630**				$NpO_2(CO_3)_3^{4-} + 4\ K^+ \rightleftarrows K_4NpO_2(CO_3)_3$(s)	7.033 ± 0.876 [2003GUI/FAN]	-40.145 ± 5.000 [2003GUI/FAN]		
$Rb_2Np_2O_7$(cr)		-2914.000 ± 12.000 [2003GUI/FAN]			$Rb_2Np_2O_7$(cr) + 6 $H^+ \rightleftarrows 2\ NpO_2^{2+} + 2\ Rb^+ + 3\ H_2O$(l)			**-167.228 ± 15.202**	
Cs_2NpO_4(cr)		-1788.100 ± 5.700 [2003GUI/FAN]			Cs_2NpO_4(cr) + 4 $H^+ \rightleftarrows NpO_2^{2+} + 2\ Cs^+ + 2\ H_2O$(l)			**-160.364 ± 7.371**	
Cs_2NpCl_6(cr)	-1833.039 ± 4.871 [2003GUI/FAN]	-1976.200 ± 1.900 [2003GUI/FAN]	410.000 ± 15.000 [2003GUI/FAN]		Cs_2NpCl_6(cr) $\rightleftarrows Np^{4+} + 2\ Cs^+ + 6\ Cl^-$	**5.222 ± 1.305**	**-29.807 ± 7.448**	**-98.355 ± 4.633**	**-230.296 ± 19.479**
$Cs_2NpO_2Cl_4$(cr)		-2056.100 ± 5.400 [2003GUI/FAN]			$Cs_2NpO_2Cl_4$(cr) $\rightleftarrows NpO_2^{2+} + 2\ Cs^+ + 4\ Cl^-$			**10.994 ± 7.147**	
$Cs_3NpO_2Cl_4$(cr)		-2449.100 ± 4.800 [2003GUI/FAN]			$Cs_3NpO_2Cl_4$(cr) $\rightleftarrows NpO_2^+ + 3\ Cs^+ + 4\ Cl^-$			**28.518 ± 6.688**	
Cs_2NpBr_6(cr)	-1620.121 ± 3.616 [2003GUI/FAN]	-1682.300 ± 2.000 [2003GUI/FAN]	469.000 ± 10.000 [2003GUI/FAN]		Cs_2NpBr_6(cr) $\rightleftarrows Np^{4+} + 2\ Cs^+ + 6\ Br^-$	**13.883 ± 1.181**	**-79.247 ± 6.743**	**-118.797 ± 4.732**	**-132.647 ± 15.969**
$Cs_2NaNpCl_6$(cr)		-2217.200 ± 3.100 [2003GUI/FAN]			$Cs_2NaNpCl_6$(cr) $\rightleftarrows Np^{3+} + Na^+ + 2\ Cs^+ + 6\ Cl^-$			**-68.812 ± 3.786**	

[2003GUI/FAN] Guillaumont et al. [A15)]
[2010FUJ/KIT] Fujiwara et al. [A33)]

Table A21 Selected thermodynamic data for plutonium (Pu) in JAEA-TDB-RN in 2020 (1/9)

Values indicated by **boldface** are calculated and selected in the present report.

Species / compound	$\Delta_f G^0_m$ (kJ.mol^{-1})	$\Delta_f H^0_m$ (kJ.mol^{-1})	S^0_m (J.K^{-1}.mol^{-1})	$C^0_{p,m}$ (J.K^{-1}.mol^{-1})	Reaction	$\log_{10} K°$	$\Delta_r G^0_m$ (kJ.mol^{-1})	$\Delta_r H^0_m$ (kJ.mol^{-1})	$\Delta_r S^0_m$ (J.K^{-1}.mol^{-1})
Pu(cr)	0.000	0.000	54.460	31.490	Pu(cr) ⇄ Pu^{4+} + 4 e^-	**83.739**	**-477.988**	**-539.895**	**-207.637**
			± 0.800	± 0.400		**± 0.474**	**± 2.705**	**± 3.103**	**± 10.224**
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]					
Pu(g)	312.415	349.000	177.167	20.854	Pu(g) ⇄ Pu^{4+} + 4 e^-	**138.472**	**-790.403**	**-888.895**	**-330.344**
	± 3.009	± 3.000	± 0.005	± 0.010		**± 0.709**	**± 4.046**	**± 4.316**	**± 10.192**
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]					
Pu^{3+}	-578.984	-591.790	-184.510		Pu^{4+} + e^- ⇄ Pu^{3+}	**17.694**	**-100.996**	**-51.895**	**164.686**
	± 2.688	± 1.964	± 6.154			**± 0.668**	**± 3.813**	**± 3.672**	**± 11.906**
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]						
Pu^{4+}	-477.988	-539.895	-414.535						
	± 2.705	± 3.103	± 10.192						
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]						
$PuO_{1.61}$(bcc)	-834.771	-875.500	83.000	61.200	$PuO_{1.61}$(bcc) + 3.22 H^+ ⇄ Pu^{4+} + 1.61 H_2O(l) + 0.78 e^-	**4.394**	**-25.081**	**-124.595**	**-333.994**
	± 10.113	± 10.000	± 5.000	± 5.000		**± 1.834**	**± 10.470**	**± 10.472**	**± 11.353**
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]					
PuO_2(cr)	-998.113	-1055.800	66.130	66.250	PuO_2(cr) + 4 H^+ ⇄ Pu^{4+} + 2 H_2O(l)	**-8.017**	**45.760**	**-55.772**	**-340.819**
	± 1.031	± 1.000	± 0.260	± 0.260		**± 0.508**	**± 2.902**	**± 3.267**	**± 10.197**
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]					
PuO_2(am,hyd)	**-965.763**				Pu^{4+} + 4 OH^- ⇄ PuO_2(am,hyd) + 2 H_2O(l)	58.330	-332.950		
	± 4.033					± 0.520	± 2.968		
						[2003GUI/FAN]	[2003GUI/FAN]		
PuO_2^+	-852.646	-910.127	1.480		PuO_2^{2+} + 0.5 H_2(g) ⇄ PuO_2^+ + H^+	15.819	-90.296	-88.091	7.386
	± 2.868	± 8.920	± 30.013			± 0.090	± 0.514	± 6.026	± 20.285
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]			[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]
PuO_2^{2+}	-762.353	-822.036	-71.246		Pu^{4+} + 2 H_2O(l) ⇄ PuO_2^{2+} + 4 H^+ + 2 e^-	**-33.286**	**190.000**	**289.536**	**334.122**
	± 2.821	± 6.577	± 22.120			**± 0.686**	**± 3.913**	**± 7.275**	**± 24.356**
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]						
Pu_2O_3(cr)	-1580.375	-1656.000	163.000	117.000	Pu_2O_3(cr) + 6 H^+ ⇄ 2 Pu^{3+} + 3 H_2O(l)	**50.655**	**-289.141**	**-385.095**	**-322.251**
	± 10.013	± 10.000	± 0.600	± 0.500		**± 1.992**	**± 11.369**	**± 10.748**	**± 12.325**
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]					
$PuOH^{2+}$	**-776.781**				Pu^{3+} + H_2O(l) ⇄ $PuOH^{2+}$ + H^+	-6.900	39.385		
	± 3.189					± 0.300	± 1.712		
						[2003GUI/FAN]	[2003GUI/FAN]		
$PuOH^{3+}$	**-715.171**				Pu^{4+} + OH^- ⇄ $PuOH^{3+}$	0.000	**0.000**		
	± 2.938					± 0.200	**± 1.142**		
						[2010FUJ/KIT]			
$Pu(OH)_2^+$	**-967.158**				Pu^{3+} + 2 H_2O(l) ⇄ $Pu(OH)_2^+$ + 2 H^+	-15.100	**86.191**		
	± 4.820					± 0.700	**± 3.996**		
						[2010KIT/FUJ2]			

Table A21 Selected thermodynamic data for plutonium (Pu) in JAEA-TDB-RN in 2020 (2/9)

Species / compound	$\Delta_f G^0_m$ (kJ.mol^{-1})	$\Delta_f H^0_m$ (kJ.mol^{-1})	S^0_m (J.K^{-1}.mol^{-1})	$C^0_{p,m}$ (J.K^{-1}.mol^{-1})	Reaction	$\log_{10} K°$	$\Delta_r G^0_m$ (kJ.mol^{-1})	$\Delta_r H^0_m$ (kJ.mol^{-1})	$\Delta_r S^0_m$ (J.K^{-1}.mol^{-1})
$Pu(OH)_2^{2+}$	**-945.504 ± 4.369**				$Pu^{4+} + 2\ H_2O(l) \rightleftarrows Pu(OH)_2^{2+} + 2\ H^+$	**-1.200 ± 0.600** [2010FUJ/KIT]	**6.850 ± 3.425**		
$Pu(OH)_3(cr)$	**-1200.345 ± 8.979**				$Pu^{3+} + 3\ H_2O(l) \rightleftarrows Pu(OH)_3(cr) + 3\ H^+$	-15.800 ± 1.500 [2003GUI/FAN]	90.187 ± 8.562 [2003GUI/FAN]		
$Pu(OH)_3(am)$	**-1194.066 ± 5.307**				$Pu^{3+} + 3\ H_2O(l) \rightleftarrows Pu(OH)_3(am) + 3\ H^+$	-16.900 ± 0.800 [2010KIT/FUJ2]	**96.466 ± 4.566**		
$Pu(OH)_3(aq)$	**-1140.981 ± 3.932**				$Pu^{3+} + 3\ H_2O(l) \rightleftarrows Pu(OH)_3(aq) + 3\ H^+$	-26.200 ± 0.500 [2010KIT/FUJ2]	**149.551 ± 2.854**		
$Pu(OH)_3^+$	**-1171.841 ± 5.814**				$Pu^{4+} + 3\ H_2O(l) \rightleftarrows Pu(OH)_3^+ + 3\ H^+$	**-3.100 ± 0.900**	**17.695 ± 5.137**		
$PuO_2OH(am)$	**-1061.288 ± 4.047**				$PuO_2^+ + H_2O(l) \rightleftarrows PuO_2OH(am) + H^+$	-5.000 ± 0.500 [2003GUI/FAN]	28.540 ± 2.854 [2003GUI/FAN]		
$PuO_2OH(aq)$	**≥-1034.289**				$PuO_2^+ + H_2O(l) \rightleftarrows PuO_2OH(aq) + H^+$	≤ -9.730 [2003GUI/FAN]	≥ 55.539 [2003GUI/FAN]		
PuO_2OH^+	**-968.141 ± 4.014**	**-1079.874 ± 16.379**	**-12.707 ± 55.786**		$PuO_2^{2+} + H_2O(l) \rightleftarrows PuO_2OH^+ + H^+$	-5.500 ± 0.500 [2003GUI/FAN]	31.394 ± 2.854 [2003GUI/FAN]	28.000 ± 15.000 [2003GUI/FAN]	-11.384 ± 51.213 [2003GUI/FAN]
$PuO_2(OH)_2(aq)$	**-1161.372 ± 9.017**				$PuO_2^{2+} + 2\ H_2O(l) \rightleftarrows PuO_2OH_2(aq) + 2\ H^+$	-13.200 ± 1.500 [2003GUI/FAN]	75.346 ± 8.562 [2003GUI/FAN]		
$Pu(OH)_4(aq)$	**-1378.200 ± 3.953**	−1632.809 ± 13.522 [2003GUI/FAN]			$Pu^{4+} + 4\ H_2O(l) \rightleftarrows Pu(OH)_4(aq) + 4\ H^+$	-8.500 ± 0.500 [2003GUI/FAN]	48.518 ± 2.854 [2003GUI/FAN]		
$PuO_2(OH)_2 \cdot H_2O(cr)$	**-1442.507 ± 6.374**	−1632.809 ± 13.522 [2003GUI/FAN]	190.000 ± 40.000 [2003GUI/FAN]	170.000 ± 20.000 [2003GUI/FAN]	$PuO_2^{2+} + 3\ H_2O(l) \rightleftarrows PuO_2(OH)_2 \cdot H_2O(cr) + 2\ H^+$	-5.500 ± 1.000 [2003GUI/FAN]	31.394 ± 5.708 [2003GUI/FAN]	**46.742 ± 15.040**	**51.477 ± 45.709**
$(PuO_2)_2(OH)_2^{2+}$	**-1956.261 ± 8.028**				$2\ PuO_2^{2+} + 2\ H_2O(l) \rightleftarrows (PuO_2)_2(OH)_2^{2+} + 2\ H^+$	-7.500 ± 1.000 [2003GUI/FAN]	42.810 ± 5.708 [2003GUI/FAN]		
$PuF(g)$	-140.967 ± 10.113 [2003GUI/FAN]	-112.600 ± 10.000 [2003GUI/FAN]	251.000 ± 5.000 [2003GUI/FAN]	33.500 ± 3.000 [2003GUI/FAN]	$PuF(g) \rightleftarrows Pu^{4+} + F^- + 3\ e^-$	**108.403 ± 1.838**	**-618.772 ± 10.490**	**-762.643 ± 10.492**	**-482.696 ± 11.366**
PuF^{2+}	**-880.142 ± 3.590**				$Pu^{3+} + F^- \rightleftarrows PuF^{2+}$	3.400 ± 0.400 [2010KIT/FUJ2]	**-19.407 ± 2.283**		

Table A21 Selected thermodynamic data for plutonium (Pu) in JAEA-TDB-RN in 2020 (3/9)

Species / compound	$\Delta_f G^0_m$ (kJ.mol^{-1})	$\Delta_f H^0_m$ (kJ.mol^{-1})	S^0_m (J.K^{-1}.mol^{-1})	$C^0_{p,m}$ (J.K^{-1}.mol^{-1})	Reaction	$\log_{10} K°$	$\Delta_r G^0_m$ (kJ.mol^{-1})	$\Delta_r H^0_m$ (kJ.mol^{-1})	$\Delta_r S^0_m$ (J.K^{-1}.mol^{-1})
PuF^{3+}	**-810.198**	**-866.143**	**-227.953**		$Pu^{4+} + F^- \rightleftarrows PuF^{3+}$	8.840	-50.459	9.100	199.762
	± 2.844	**± 3.862**	**± 12.739**			± 0.100	± 0.571	± 2.200	± 7.623
						[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]
$PuF_2(g)$	-626.151	-614.300	297.000	51.500	$PuF_2(g) \rightleftarrows Pu^{4+} + 2\ F^- + 2\ e^-$	**72.764**	**-415.338**	**-596.290**	**-607.215**
	± 6.704	± 6.000	± 10.000	± 5.000		**± 1.288**	**± 7.352**	**± 6.886**	**± 14.320**
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]					
PuF_2^+	**-1175.592**				$Pu^{3+} + 2\ F^- \rightleftarrows PuF_2^+$	5.800	**-33.107**		
	± 3.213					± 0.200	**± 1.142**		
						[2010KIT/FUJ2]			
PuF_2^{2+}	**-1131.105**	**-1199.590**	**-103.425**		$Pu^{4+} + 2\ F^- \rightleftarrows PuF_2^{2+}$	15.700	-89.616	11.000	337.469
	± 3.227	**± 6.035**	**± 20.024**			± 0.200	± 1.142	± 5.000	± 17.202
						[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]
$PuF_3(cr)$	-1517.369	-1586.700	126.110	92.640	$PuF_3(cr) \rightleftarrows Pu^{3+} + 3\ F^-$	**-16.316**	**93.133**	**-11.133**	**-350.159**
	± 3.709	± 3.700	± 0.360	± 0.280		**± 0.876**	**± 5.002**	**± 4.645**	**± 6.377**
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]					
$PuF_3(g)$	-1161.081	-1167.800	336.110	72.240	$PuF_3(g) \rightleftarrows Pu^{3+} + 3\ F^-$	**46.102**	**-263.155**	**-430.033**	**-560.159**
	± 4.758	± 3.700	± 10.000	± 5.000		**± 1.020**	**± 5.822**	**± 4.645**	**± 11.855**
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]					
$PuF_4(cr)$	-1756.741	-1850.000	147.250	116.190	$PuF_4(cr) \rightleftarrows Pu^{4+} + 4\ F^-$	**-26.585**	**151.751**	**-31.285**	**-614.503**
	± 20.002	± 20.000	± 0.370	± 0.290		**± 3.567**	**± 20.361**	**± 20.416**	**± 10.428**
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]					
$PuF_4(g)$	-1517.874	-1548.000	359.000	92.400	$PuF_4(g) \rightleftarrows Pu^{4+} + 4\ F^-$	**15.262**	**-87.116**	**-333.285**	**-826.253**
	± 22.202	± 22.000	± 10.000	± 5.000		**± 3.946**	**± 22.526**	**± 22.379**	**± 14.443**
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]					
$PuF_6(cr)$	-1729.856	-1861.350	221.800	168.100	$PuF_6(cr) + 2\ H_2O(l) \rightleftarrows PuO_2^{2+} + 6\ F^- + 4\ H^+$	**43.559**	**-248.635**	**-401.095**	**-511.970**
	± 20.174	± 20.170	± 1.100	± 2.000		**± 3.638**	**± 20.763**	**± 21.593**	**± 22.387**
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]					
$PuF_6(g)$	-1725.064	-1812.700	368.900	129.320	$PuF_6(g) + 2\ H_2O(l) \rightleftarrows PuO_2^{2+} + 6\ F^- + 4\ H^+$	**44.398**	**-253.427**	**-449.745**	**-659.070**
	± 20.104	± 20.100	± 1.000	± 1.000		**± 3.626**	**± 20.695**	**± 21.528**	**± 22.382**
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]					
PuOF(cr)	-1091.571	-1140.000	96.000	69.400	$PuOF(cr) + 2\ H^+ \rightleftarrows Pu^{3+} + F^- + H_2O(l)$	**1.112**	**-6.346**	**-72.976**	**-223.767**
	± 20.222	± 20.000	± 10.000	± 10.000		**± 3.576**	**± 20.411**	**± 20.108**	**± 11.755**
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]					
PuO_2F^+	**-1070.132**				$PuO_2^{2+} + F^- \rightleftarrows PuO_2F^+$	4.560	-26.029		
	± 3.116					± 0.200	± 1.142		
						[2003GUI/FAN]	[2003GUI/FAN]		
$PuO_2F_2(aq)$	**-1367.237**				$PuO_2^{2+} + 2\ F^- \rightleftarrows PuO_2F_2(aq)$	7.250	-41.383		
	± 4.043					± 0.450	± 2.569		
						[2003GUI/FAN]	[2003GUI/FAN]		
$PuCl^{2+}$	–717.051				$Pu^{3+} + Cl^- \rightleftarrows PuCl^{2+}$	**1.187**	**-6.777**		
	± 2.923					**± 0.696**	**± 3.972**		
	[2003GUI/FAN]								

Table A21 Selected thermodynamic data for plutonium (Pu) in JAEA-TDB-RN in 2020 (4/9)

Species / compound	$\Delta_f G^0_m$ (kJ.mol^{-1})	$\Delta_f H^0_m$ (kJ.mol^{-1})	S^0_m (J.K^{-1}.mol^{-1})	$C^0_{p,m}$ (J.K^{-1}.mol^{-1})	Reaction	$\log_{10} K°$	$\Delta_r G^0_m$ (kJ.mol^{-1})	$\Delta_r H^0_m$ (kJ.mol^{-1})	$\Delta_r S^0_m$ (J.K^{-1}.mol^{-1})
$PuCl^{3+}$	**-619.552**				$Pu^{4+} + Cl^- \rightleftarrows PuCl^{3+}$	1.800	-10.274		
	± 3.203					± 0.300	± 1.712		
						[2003GUI/FAN]	[2003GUI/FAN]		
$PuCl_2^+$	**-837.340**				$Pu^{3+} + 2\ Cl^- \rightleftarrows PuCl_2^+$	-0.740	**4.224**		
	± 2.711					± 0.050	**± 0.285**		
						[2010KIT/FUJ2]			
$PuCl_3$(cr)	-891.806	-959.600	161.700	101.200	$PuCl_3(cr) \rightleftarrows Pu^{3+} + 3\ Cl^-$	**14.199**	**-81.047**	**-133.429**	**-176.005**
	± 2.024	± 1.800	± 3.000	± 4.000		**± 0.592**	**± 3.378**	**± 2.677**	**± 6.865**
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]					
$PuCl_3$(g)	-641.299	-647.400	368.620	78.470	$PuCl_3(g) \rightleftarrows Pu^{3+} + 3\ Cl^-$	**58.085**	**-331.554**	**-445.629**	**-382.925**
	± 3.598	± 1.868	± 10.000	± 5.000		**± 0.789**	**± 4.501**	**± 2.723**	**± 11.753**
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]					
$PuCl_4$(cr)	-879.368	-968.700	201.000	121.400	$PuCl_4(cr) \rightleftarrows Pu^{4+} + 4\ Cl^-$	**21.685**	**-123.779**	**-239.514**	**-388.595**
	± 5.826	± 5.000	± 10.000	± 4.000		**± 1.128**	**± 6.436**	**± 5.895**	**± 14.294**
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]					
$PuCl_4$(g)	-764.683	-792.000	409.000	103.400	$PuCl_4(g) \rightleftarrows Pu^{4+} + 4\ Cl^-$	**41.777**	**-238.464**	**-416.214**	**-596.595**
	± 10.438	± 10.000	± 10.000	± 5.000		**± 1.890**	**± 10.790**	**± 10.476**	**± 14.294**
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]					
PuOCl(cr)	-882.409	-931.000	105.600	71.600	$PuOCl(cr) + 2\ H^+ \rightleftarrows Pu^{3+} + Cl^- + H_2O(l)$	**11.396**	**-65.047**	**-113.708**	**-163.452**
	± 1.936	± 1.700	± 3.000	± 4.000		**± 0.581**	**± 3.316**	**± 2.601**	**± 6.849**
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]					
PuO_2Cl^+	**-894.956**				$PuO_2^{2+} + Cl^- \rightleftarrows PuO_2Cl^+$	0.230	-1.313		
	± 2.828					± 0.030	± 0.171		
						[2003GUI/FAN]	[2003GUI/FAN]		
PuO_2Cl_2(aq)	**-1018.368**				$PuO_2^{2+} + 2\ Cl^- \rightleftarrows PuO_2Cl_2(aq)$	-1.150	6.564		
	± 3.306					± 0.300	± 1.712		
						[2003GUI/FAN]	[2003GUI/FAN]		
$PuCl_3 \cdot 6H_2O$(cr)	-2365.347	-2773.400	420.000		$PuCl_3 \cdot 6H_2O(cr) \rightleftarrows Pu^{3+} + 3\ Cl^- + 6\ H_2O(l)$	**5.361**	**-30.602**	**-34.659**	**-14.767**
	± 2.586	± 2.100	± 5.000			**± 0.664**	**± 3.790**	**± 2.955**	**± 7.961**
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]						
$PuBr^{3+}$	**-591.164**				$Pu^{4+} + Br^- \rightleftarrows PuBr^{3+}$	1.600	-9.133		
	± 3.206					± 0.300	± 1.712		
						[2003GUI/FAN]	[2003GUI/FAN]		
$PuBr_3$(cr)	-767.324	-792.600	198.000	101.800	$PuBr_3(cr) \rightleftarrows Pu^{3+} + 3\ Br^-$	**21.687**	**-123.791**	**-163.700**	**-133.980**
	± 2.697	± 2.000	± 6.000	± 6.000		**± 0.673**	**± 3.841**	**± 2.839**	**± 8.618**
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]					
$PuBr_3$(g)	-529.808	-488.000	423.000	81.600	$PuBr_3(g) \rightleftarrows Pu^{3+} + 3\ Br^-$	**63.298**	**-361.307**	**-468.300**	**-358.980**
	± 15.655	± 15.000	± 15.000	± 10.000		**± 2.784**	**± 15.892**	**± 15.135**	**± 16.225**
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]					
PuOBr(cr)	-838.354	-870.000	127.000	73.000	$PuOBr(cr) + 2\ H^+ \rightleftarrows Pu^{3+} + Br^- + H_2O(l)$	**14.340**	**-81.856**	**-129.132**	**-158.744**
	± 8.541	± 8.000	± 10.000	± 8.000		**± 1.569**	**± 8.956**	**± 8.240**	**± 11.744**
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]					

Table A21 Selected thermodynamic data for plutonium (Pu) in JAEA-TDB-RN in 2020 (5/9)

Species / compound	$\Delta_f G^0_m$ (kJ.mol^{-1})	$\Delta_f H^0_m$ (kJ.mol^{-1})	S^0_m (J.K^{-1}.mol^{-1})	$C^0_{p,m}$ (J.K^{-1}.mol^{-1})	Reaction	$\log_{10} K°$	$\Delta_r G^0_m$ (kJ.mol^{-1})	$\Delta_r H^0_m$ (kJ.mol^{-1})	$\Delta_r S^0_m$ (J.K^{-1}.mol^{-1})
PuI^{2+}	**-637.186**				$Pu^{3+} + I^- \rightleftarrows PuI^{2+}$	1.100	-6.279		
	± 3.625					± 0.400	± 2.283		
						[2003GUI/FAN]	[2003GUI/FAN]		
PuI_3(cr)	-579.000	-579.200	228.000	110.000	$PuI_3(cr) \rightleftarrows Pu^{3+} + 3\ I^-$	**27.287**	**-155.754**	**-183.297**	**-92.434**
	± 4.551	± 2.800	± 12.000	± 8.000		**± 1.025**	**± 5.851**	**± 4.243**	**± 13.501**
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]					
PuI_3(g)	-366.517	-305.000	435.000	82.000	$PuI_3(g) \rightleftarrows Pu^{3+} + 3\ I^-$	**64.512**	**-368.237**	**-457.497**	**-299.434**
	± 15.655	± 15.000	± 15.000	± 5.000		**± 2.817**	**± 16.081**	**± 15.335**	**± 16.225**
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]					
PuOI(cr)	-776.626	-802.000	130.000	75.600	$PuOI(cr) + 2\ H^+ \rightleftarrows Pu^{3+} + I^- + H_2O(l)$	**16.024**	**-91.464**	**-132.531**	**-137.895**
	± 20.495	± 20.000	± 15.000	± 10.000		**± 3.624**	**± 20.688**	**± 20.114**	**± 16.215**
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]					
$PuSO_4^+$	**-1345.756**	**-1486.090**	**-39.481**		$Pu^{3+} + HSO_4^- \rightleftarrows PuSO_4^+ + H^+$	1.930	-11.017	-5.200	19.509
						± 0.610	± 3.482	± 2.000	± 13.468
						[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]
$PuSO_4^{2+}$	**-1261.770**				$Pu^{4+} + HSO_4^- \rightleftarrows PuSO_4^{2+} + H^+$	4.910	-28.026		
						± 0.220	± 1.256		
						[2003GUI/FAN]	[2003GUI/FAN]		
PuO_2SO_4(aq)	**-1526.105**	**-1715.538**	**66.291**		$PuO_2^{2+} + SO_4^{2-} \rightleftarrows PuO_2SO_4(aq)$	3.380	-19.293	16.100	118.709
	± 3.078	**± 6.618**	**± 22.545**			± 0.200	± 1.142	± 0.600	± 4.326
						[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]
$Pu(SO_4)_2$(aq)	**-2030.484**				$Pu^{4+} + 2\ HSO_4^- \rightleftarrows Pu(SO_4)_2(aq) + 2\ H^+$	7.180	-40.984		
						± 0.320	± 1.827		
						[2003GUI/FAN]	[2003GUI/FAN]		
$Pu(SO_4)_2^-$	**-2100.428**	**-2402.990**	**-10.840**		$Pu^{3+} + 2\ HSO_4^- \rightleftarrows Pu(SO_4)_2^- + 2\ H^+$	1.740	-9.932	-33.000	-77.370
						± 0.760	± 4.338	± 16.000	± 55.602
						[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]
$PuO_2(SO_4)_2^{2-}$	**-2276.387**	**-2598.239**	**194.870**		$PuO_2^{2+} + 2\ SO_4^{2-} \rightleftarrows PuO_2(SO_4)_2^{2-}$	4.400	-25.115	43.000	228.460
	± 3.179	**± 11.178**	**± 37.632**			± 0.200	± 1.142	± 9.000	± 30.428
						[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]
PuSe(cr)			92.100	59.700					
			± 1.800	± 1.200					
			[2003GUI/FAN]	[2003GUI/FAN]					
PuTe(cr)			107.900	73.100					
			± 4.300	± 2.900					
			[2003GUI/FAN]	[2003GUI/FAN]					
PuN(cr)	-273.719	-299.200	64.800	49.600	$PuN(cr) + 3\ H_2O(l) \rightleftarrows Pu^{4+} + NO_3^- + 6\ H^+ + 9\ e^-$	**-69.439**	**396.361**	**409.921**	**45.893**
	± 2.551	± 2.500	± 1.500	± 1.000		**± 0.788**	**± 4.496**	**± 4.019**	**± 10.340**
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]					
PuN_3^{2+}	**-240.316**				$Pu^{3+} + N_3^- \rightleftarrows PuN_3^{2+}$	1.670	**-9.532**		
	± 3.399					± 0.100	**± 0.571**		
						[2010KIT/FUJ2]			

Table A21 Selected thermodynamic data for plutonium (Pu) in JAEA-TDB-RN in 2020 (6/9)

Species / compound	$\Delta_f G^0_m$ (kJ.mol^{-1})	$\Delta_f H^0_m$ (kJ.mol^{-1})	S^0_m (J.K^{-1}.mol^{-1})	$C^0_{p,m}$ (J.K^{-1}.mol^{-1})	Reaction	$\log_{10} K°$	$\Delta_r G^0_m$ (kJ.mol^{-1})	$\Delta_r H^0_m$ (kJ.mol^{-1})	$\Delta_r S^0_m$ (J.K^{-1}.mol^{-1})
$PuNO_2^{2+}$	**-623.188**				$Pu^{3+} + NO_2^- \rightleftarrows PuNO_2^{2+}$	2.100	**-11.987**		
	± 8.863					± 0.200	**± 1.142**		
						[2010KIT/FUJ2]			
$PuNO_3^{2+}$	**-697.494**				$Pu^{3+} + NO_3^- \rightleftarrows PuNO_3^{2+}$	1.330	**-7.592**		
	± 3.851					± 0.200	**± 1.142**		
						[2010KIT/FUJ2]			
$PuNO_3^{3+}$	**-600.037**				$Pu^{4+} + NO_3^- \rightleftarrows PuNO_3^{3+}$	1.950	-11.131		
	± 3.788					± 0.150	± 0.856		
						[2003GUI/FAN]	[2003GUI/FAN]		
$PuO_2(NO_3)_2{\cdot}6H_2O$(cr)	-2393.300				$PuO_2(NO_3)_2{\cdot}6H_2O$(cr) $\rightleftarrows PuO_2^{2+} + 2\ NO_3^- + 6\ H_2O$(l)	**2.450**	**-13.984**		
	± 3.200					**± 1.159**	**± 6.616**		
	[2003GUI/FAN]								
PuP(cr)	-313.757	-318.000	81.320	50.200	PuP(cr) + 4 H_2O(l) $\rightleftarrows Pu^{4+} + PO_4^{3-} + 8\ H^+ + 9\ e^-$	**41.048**	**-234.305**	**-355.917**	**-409.244**
	± 21.078	± 21.000	± 6.000	± 4.000		**± 4.002**	**± 22.843**	**± 22.822**	**± 84.512**
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]					
$PuPO_4$(s, hyd)	**-1738.206**				$Pu^{3+} + PO_4^{3-} \rightleftarrows PuPO_4$(s, hyd)	24.600	-140.418		
	± 9.905					± 0.800	± 4.566		
						[2003GUI/FAN]	[2003GUI/FAN]		
$PuH_2PO_4^{2+}$	**-1726.374**				$Pu^{3+} + H_2PO_4^- \rightleftarrows PuH_2PO_4^{2+}$	3.000	**-17.124**		
	± 4.009					± 0.500	**± 2.854**		
						[2010KIT/FUJ2]			
$PuH_3PO_4^{4+}$	**-1634.338**				$Pu^{4+} + H_3PO_4$(aq) $\rightleftarrows PuH_3PO_4^{4+}$	2.400	-13.699		
	± 3.309					± 0.300	± 1.712		
						[2003GUI/FAN]	[2003GUI/FAN]		
$Pu(HPO_4)_2$(am,hyd)	**-2830.072**				$Pu^{4+} + 2\ HPO_4^{2-} \rightleftarrows Pu(HPO_4)_2$(am,hyd)	30.450	-173.810		
	± 4.312					± 0.510	± 2.911		
						[2003GUI/FAN]	[2003GUI/FAN]		
PuAs(cr)	-241.413	-240.000	94.300	51.600	PuAs(cr) + 4 H_2O(l) $\rightleftarrows Pu^{4+} + AsO_4^{3-} + 8\ H^+ + 9\ e^-$	**-11.176**	**63.795**	**-44.682**	**-363.272**
	± 20.111	± 20.000	± 7.000	± 4.000		**± 3.624**	**± 20.688**	**± 20.635**	**± 12.384**
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]					
PuSb(cr)	-152.063	-150.000	106.900	52.800	PuSb(cr) + 3 H_2O(l) $\rightleftarrows Pu^{4+} + Sb(OH)_3$(aq) $+ 3\ H^+ + 7\ e^-$	**45.109**	**-257.486**		
	± 20.126	± 20.000	± 7.500	± 3.500		**± 3.558**	**± 20.309**		
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]					
PuBi(cr)	-119.624	-117.000	120.000		PuBi(cr) $\rightleftarrows Pu^{4+} + Bi^{3+} + 7\ e^-$	**46.042**	**-262.811**		
	± 20.223	± 20.000	± 10.000			**± 3.574**	**± 20.403**		
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]						
$PuBi_2$(cr)	-124.527	-126.000	163.000		$PuBi_2$(cr) $\rightleftarrows Pu^{4+} + 2\ Bi^{3+} + 10\ e^-$	**28.443**	**-162.356**		
	± 22.395	± 22.000	± 14.000			**± 3.952**	**± 22.558**		
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]						
$PuC_{0.84}$(cr)	-49.827	-45.200	74.800	47.100	$PuC_{0.84}$(cr) + 2.52 H_2O(l) $\rightleftarrows Pu^{4+} + 0.84\ HCO_3^- + 4.2\ H^+ + 7.36$	**56.673**	**-323.490**	**-353.926**	**-101.945**
	± 8.028	± 8.000	± 2.100	± 1.000	e^-	**± 1.485**	**± 8.476**	**± 8.587**	**± 10.418**
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]					

Table A21 Selected thermodynamic data for plutonium (Pu) in JAEA-TDB-RN in 2020 (7/9)

Species / compound	$\Delta_f G^0_m$ (kJ.mol^{-1})	$\Delta_f H^0_m$ (kJ.mol^{-1})	S^0_m (J.K^{-1}.mol^{-1})	$C^0_{p,m}$ (J.K^{-1}.mol^{-1})	Reaction	$\log_{10} K°$	$\Delta_r G^0_m$ (kJ.mol^{-1})	$\Delta_r H^0_m$ (kJ.mol^{-1})	$\Delta_r S^0_m$ (J.K^{-1}.mol^{-1})
Pu_3C_2(cr)	-123.477 ± 30.046 [2003GUI/FAN]	-113.000 ± 30.000 [2003GUI/FAN]	210.000 ± 5.000 [2003GUI/FAN]	136.800 ± 2.500 [2003GUI/FAN]	Pu_3C_2(cr) + 6 H_2O(l) ⇄ 3 Pu^{4+} + 2 HCO_3^- + 10 H^+ + 20 e^-	**185.926 ± 5.454**	**-1061.271 ± 31.129**	**-1171.521 ± 31.420**	**-369.455 ± 31.004**
Pu_2C_3(cr)	-156.514 ± 16.729 [2003GUI/FAN]	-149.400 ± 16.700 [2003GUI/FAN]	150.000 ± 2.900 [2003GUI/FAN]	114.000 ± 0.400 [2003GUI/FAN]	Pu_2C_3(cr) + 9 H_2O(l) ⇄ 2 Pu^{4+} + 3 HCO_3^- + 15 H^+ + 20 e^-	**74.568 ± 3.085**	**-425.638 ± 17.609**	**-427.645 ± 17.852**	**-6.240 ± 20.661**
PuO_2CO_3(aq)	**-1344.563 ± 4.024**				PuO_2^{2+} + CO_3^{2-} ⇄ PuO_2CO_3(aq)	9.500 ± 0.500 [2003GUI/FAN]	-54.226 ± 2.854 [2003GUI/FAN]		
PuO_2CO_3(s)	**-1373.959 ± 3.904**				PuO_2^{2+} + CO_3^{2-} ⇄ PuO_2CO_3(s)	14.650 ± 0.470 [2003GUI/FAN]	-83.623 ± 2.683 [2003GUI/FAN]		
$PuCO_3^+$	**-1152.631 ± 3.539**				Pu^{3+} + CO_3^{2-} ⇄ $PuCO_3^+$	8.000 ± 0.400 [2010KIT/FUJ2]	**-45.664 ± 2.283**		
$PuO_2CO_3^-$	**-1409.854 ± 2.992**				PuO_2^+ + CO_3^{2-} ⇄ $PuO_2CO_3^-$	5.120 ± 0.140 [2003GUI/FAN]	-29.225 ± 0.799 [2003GUI/FAN]		
$Pu(CO_3)_2^-$	**-1708.584 ± 4.393**				Pu^{3+} + 2 CO_3^{2-} ⇄ $Pu(CO_3)_2^-$	12.900 ± 0.600 [2010KIT/FUJ2]	**-73.634 ± 3.425**		
$PuO_2(CO_3)_2^{2-}$	**-1902.228 ± 4.055**	**-2199.506 ± 7.751**	**19.627 ± 27.706**		PuO_2^{2+} + 2 CO_3^{2-} ⇄ $PuO_2(CO_3)_2^{2-}$	14.700 ± 0.500 [2003GUI/FAN]	-83.908 ± 2.854 [2003GUI/FAN]	-27.000 ± 4.000 [2003GUI/FAN]	190.871 ± 16.481 [2003GUI/FAN]
$Pu(CO_3)_3^{3-}$	**-2248.554 ± 6.370**				Pu^{3+} + 3 CO_3^{2-} ⇄ $Pu(CO_3)_3^{3-}$	15.000 ± 1.000 [2010KIT/FUJ2]	**-85.621 ± 5.708**		
$PuO_2(CO_3)_3^{4-}$	**-2449.047 ± 4.108**	**-2886.341 ± 7.007**	**-6.099 ± 25.319**		PuO_2^{2+} + 3 CO_3^{2-} ⇄ $PuO_2(CO_3)_3^{4-}$	18.000 ± 0.500 [2003GUI/FAN]	-102.745 ± 2.854 [2003GUI/FAN]	-38.600 ± 2.000 [2003GUI/FAN]	215.143 ± 11.689 [2003GUI/FAN]
$PuO_2(CO_3)_3^{5-}$	**-2465.278 ± 6.048**	**-2954.942 ± 12.396**	**-116.401 ± 45.153**		PuO_2^+ + 3 CO_3^{2-} ⇄ $PuO_2(CO_3)_3^{5-}$	5.025 ± 0.920 [2003GUI/FAN]	-28.683 ± 5.251 [2003GUI/FAN]	-19.110 ± 8.500 [2003GUI/FAN]	32.115 ± 33.509 [2003GUI/FAN]
$Pu(CO_3)_4^{4-}$	**-2801.118 ± 6.936**				Pu^{4+} + 4 CO_3^{2-} ⇄ $Pu(CO_3)_4^{4-}$	37.000 ± 1.100 [2003GUI/FAN]	-211.198 ± 6.279 [2003GUI/FAN]		
$Pu(CO_3)_5^{6-}$	**-3321.395 ± 7.146**				Pu^{4+} + 5 CO_3^{2-} ⇄ $Pu(CO_3)_5^{6-}$	35.650 ± 1.130 [2003GUI/FAN]	-203.492 ± 6.450 [2003GUI/FAN]		
$Pu_2(CO_3)_3$(am)	**-2932.566 ± 13.688**				2 Pu^{3+} + 3 CO_3^{2-} ⇄ $Pu_2(CO_3)_3$(am)	33.400 ± 2.200 [2010KIT/FUJ2]	**-190.649 ± 12.558**		

Table A21 Selected thermodynamic data for plutonium (Pu) in JAEA-TDB-RN in 2020 (8/9)

Species / compound	$\Delta_f G^0_m$ (kJ.mol^{-1})	$\Delta_f H^0_m$ (kJ.mol^{-1})	S^0_m (J.K^{-1}.mol^{-1})	$C^0_{p,m}$ (J.K^{-1}.mol^{-1})	Reaction	$\log_{10} K°$	$\Delta_r G^0_m$ (kJ.mol^{-1})	$\Delta_r H^0_m$ (kJ.mol^{-1})	$\Delta_r S^0_m$ (J.K^{-1}.mol^{-1})
$PuHCO_3^{2+}$	**-1183.619 ± 3.190**				$Pu^{3+} + HCO_3^- \rightleftarrows PuHCO_3^{2+}$	3.100 ± 0.300 [2010KIT/FUJ2]	**-17.695 ± 1.712**		
$PuCO_3OH{\cdot}0.5H_2O$(cr)	**-1510.716 ± 3.933**				$Pu^{3+} + CO_3^{2-} + OH^- + 0.5\ H_2O(l) \rightleftarrows PuCO_3OH{\bullet}0.5H_2O$(cr)	22.400 ± 0.500 [2010KIT/FUJ2]	**-127.860 ± 2.854**		
$PuCO_3OH$(am,hyd)	**-1379.567 ± 6.317**				$Pu^{3+} + CO_3^{2-} + OH^- \rightleftarrows PuCO_3OH$(am,hyd)	20.200 ± 1.000 [2010KIT/FUJ2]	**-115.302 ± 5.708**		
$Pu(CO_3)_2(OH)_2^{2-}$	**-2117.855 ± 2.863**				$Pu^{4+} + 2\ CO_3^{2-} + 2\ H_2O(l) \rightleftarrows Pu(CO_3)_2(OH)_2^{2-} + 2\ H^+$	47.180 ± 0.125 [2010FUJ/KIT]	**-269.305 ± 0.714**		
$PuSCN^{2+}$	**-493.520 ± 9.081**	**-515.223 ± 9.481**	**-15.274 ± 18.615**		$Pu^{3+} + SCN^- \rightleftarrows PuSCN^{2+}$	1.300 ± 0.400 [2003GUI/FAN]	-7.420 ± 2.283 [2003GUI/FAN]	0.000 ± 4.000 [2003GUI/FAN]	24.888 ± 15.448 [2003GUI/FAN]
$PuSiO(OH)_3^{2+}$	**-1877.167 ± 3.404**				$Pu^{3+} + Si(OH)_4(aq) \rightleftarrows PuSiO(OH)_3^{2+} + H^+$	-1.680 ± 0.180 [2010KIT/FUJ2]	**9.590 ± 1.027**		
Sr_3PuO_6(cr)		−3042.100 ± 7.900 [2003GUI/FAN]			$Sr_3PuO_6(cr) + 12\ H^+ + 2\ e^- \rightleftarrows Pu^{4+} + 3\ Sr^{2+} + 6\ H_2O(l)$			**-865.547 ± 8.643**	
$BaPuO_3$(cr)		−1654.200 ± 8.300 [2003GUI/FAN]			$BaPuO_3(cr) + 6\ H^+ \rightleftarrows Pu^{4+} + Ba^{2+} + 6\ H_2O(l)$			**-277.842 ± 9.023**	
Ba_3PuO_6(cr)		−2997.000 ± 10.000 [2003GUI/FAN]			$Ba_3PuO_6(cr) + 12\ H^+ + 2\ e^- \rightleftarrows Pu^{4+} + 3\ Ba^{2+} + 6\ H_2O(l)$			**-861.820 ± 11.629**	
Ba_2MgPuO_6(cr)		−2995.800 ± 8.800 [2003GUI/FAN]			$Ba_2MgPuO_6(cr) + 12\ H^+ + 2\ e^- \rightleftarrows Pu^{4+} + Mg^{2+} + 2\ Ba^{2+} + 6\ H_2O(l)$			**-794.348 ± 9.992**	
Ba_2CaPuO_6(cr)		−3067.500 ± 8.900 [2003GUI/FAN]			$Ba_2CaPuO_6(cr) + 12\ H^+ + 2\ e^- \rightleftarrows Pu^{4+} + Ca^{2+} + 2\ Ba^{2+} + 6\ H_2O(l)$			**-799.771 ± 10.053**	
Ba_2SrPuO_6(cr)		−3023.300 ± 9.000 [2003GUI/FAN]			$Ba_2SrPuO_6(cr) + 12\ H^+ + 2\ e^- \rightleftarrows Pu^{4+} + Sr^{2+} + 2\ Ba^{2+} + 6\ H_2O(l)$			**-851.795 ± 10.123**	
$NaPu(CO_3)_2{\cdot}5H_2O$(cr)	**-3202.613 ± 3.998**				$Pu^{3+} + Na^+ + 2\ CO_3^{2-} + 5\ H_2O(l) \rightleftarrows NaPu(CO_3)_2{\cdot}5H_2O(cr)$	21.000 ± 0.500 Am analogue	**-119.869 ± 2.854**		

Table A21 Selected thermodynamic data for plutonium (Pu) in JAEA-TDB-RN in 2020 (9/9)

Species / compound	$\Delta_f G^0_m$ (kJ.mol^{-1})	$\Delta_f H^0_m$ (kJ.mol^{-1})	S^0_m (J.K^{-1}.mol^{-1})	$C^0_{p,m}$ (J.K^{-1}.mol^{-1})	Reaction	$\log_{10} K°$	$\Delta_r G^0_m$ (kJ.mol^{-1})	$\Delta_r H^0_m$ (kJ.mol^{-1})	$\Delta_r S^0_m$ (J.K^{-1}.mol^{-1})
Cs_2PuCl_6(cr)	-1838.243	-1982.000	412.000		$Cs_2PuCl_6(cr) \rightleftarrows 2\ Cs^+ + Pu^{4+} + 6\ Cl^-$	**1.895**	**-10.817**	**-76.428**	**-220.441**
	± 6.717	± 5.000	± 15.000			**± 1.275**	**± 7.278**	**± 5.914**	**± 18.163**
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]						
Cs_3PuCl_6(cr)	-2208.045	-2364.415	454.925	258.600	$Cs_3PuCl_6(cr) \rightleftarrows 3\ Cs^+ + Pu^{3+} + 6\ Cl^-$	**5.900**	**-33.677**	**-3.935**	**99.501**
	± 9.491	± 9.040	± 10.959	± 10.000		**± 1.735**	**± 9.903**	**± 9.274**	**± 12.609**
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]					
$CsPu_2Cl_7$(cr)	-2235.119	-2399.380	424.000	254.900	$CsPu_2Cl_7(cr) \rightleftarrows Cs^+ + 2\ Pu^{3+} + 7\ Cl^-$	**23.396**	**-133.544**	**-211.785**	**-263.033**
	± 5.284	± 5.734	± 7.281	± 10.000		**± 1.327**	**± 7.574**	**± 6.979**	**± 14.348**
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]					
Cs_2PuBr_6(cr)	-1634.326	-1697.400	470.000		$Cs_2PuBr_6(cr) \rightleftarrows 2\ Cs^+ + Pu^{4+} + 6\ Br^-$	**8.980**	**-51.256**	**-87.570**	**-121.792**
	± 6.150	± 4.200	± 15.000			**± 1.192**	**± 6.806**	**± 5.306**	**± 18.179**
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]						
$Cs_2NaPuCl_6$(cr)	-2143.496	-2294.200	440.000		$Cs_2NaPuCl_6(cr) \rightleftarrows Na^+ + 2\ Cs^+ + Pu^{3+} + 6\ Cl^-$	**11.990**	**-68.440**	**-56.418**	**39.993**
	± 5.184	± 2.600	± 15.000			**± 1.031**	**± 5.887**	**± 3.311**	**± 16.246**
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]						

[2003GUI/FAN] Guillaumont et al.[A15A21)]
[2010FUJ/KIT] Fujiwara et al.[A33)]
[2010KIT/FUJ2] Kitamura et al.[A21)]

Table A22 Selected thermodynamic data for americium (Am) in JAEA-TDB-RN in 2020 (1/5)

Values indicated by **boldface** are calculated and selected in the present report.

Species / compound	$\Delta_f G^0_m$ (kJ.mol^{-1})	$\Delta_f H^0_m$ (kJ.mol^{-1})	S^0_m (J.K^{-1}.mol^{-1})	$C^0_{p,m}$ (J.K^{-1}.mol^{-1})	Reaction	$\log_{10} K°$	$\Delta_r G^0_m$ (kJ.mol^{-1})	$\Delta_r H^0_m$ (kJ.mol^{-1})	$\Delta_r S^0_m$ (J.K^{-1}.mol^{-1})
Am(cr)	0.000	0.000	55.400	25.500	$Am^{3+} + 3\ e^- \rightleftarrows Am(cr)$	**-104.887**	**598.698**	**616.700**	**60.382**
			± 2.000	± 1.500		**± 0.833**	**± 4.755**	**± 1.500**	**± 15.133**
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]					
Am(g)	242.312	283.800	194.550	20.786	$Am^{3+} + 3\ e^- \rightleftarrows Am(g)$	**-147.338**	**841.010**	**900.500**	**199.532**
	± 1.614	± 1.500	± 0.050	± 0.010		**± 0.880**	**± 5.021**	**± 2.121**	**± 15.000**
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]					
Am^{2+}	-376.780	-354.633	-1.000		$Am^{3+} + e^- \rightleftarrows Am^{2+}$	-38.878	221.917	**262.067**	**134.661**
	± 15.236	± 15.890	± 15.000			± 2.536	± 14.476	**± 15.961**	**± 21.213**
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]			[2003GUI/FAN]	[2003GUI/FAN]		
Am^{3+}	-598.698	-616.700	-201.000						
	± 4.755	± 1.500	± 15.000						
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]						
Am^{4+}	-346.358	-406.000	-406.000		$Am^{3+} \rightleftarrows Am^{4+} + e^-$	**-44.208**	**252.340**	**210.700**	**-139.661**
	± 8.692	± 6.000	± 21.000			**± 1.736**	**± 9.908**	**± 6.185**	**± 25.807**
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]						
$AmO_2(cr)$	-877.683	-932.200	77.700	66.170	$Am^{4+} + 2\ H_2O(l) \rightleftarrows AmO_2(cr) + 4\ H^+$	**9.979**	**-56.960**	**45.477**	**343.854**
	± 4.271	± 3.000	± 1.000	± 10.000		**± 1.697**	**± 9.687**	**± 6.711**	**± 21.024**
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]					
AmO_2^+	-739.796	-804.260	-21.000		$Am^{3+} + 2\ H_2O(l) \rightleftarrows AmO_2^+ + 4\ H^+ + 2\ e^-$	**-58.386**	**333.267**	384.100	**170.833**
	± 6.208	± 5.413	± 10.000			**± 1.370**	**± 7.822**	± 5.200	**± 18.029**
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]					[2003GUI/FAN]	
AmO_2^{2+}	-585.801	-650.760	-88.000		$Am^{3+} + 2\ H_2O(l) \rightleftarrows AmO_2^{2+} + 4\ H^+ + 3\ e^-$	**-85.364**	**487.262**	537.600	**169.172**
	± 5.715	± 4.839	± 10.000			**± 1.303**	**± 7.437**	± 4.600	**± 18.029**
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]					[2003GUI/FAN]	
$Am_2O_3(cr)$	-1605.449	-1690.400	133.600	117.500	$2\ Am^{3+} + 3\ H_2O(l) \rightleftarrows Am_2O_3(cr) + 6\ H^+$	**-53.170**	**303.495**	**400.515**	**325.831**
	± 8.284	± 8.000	± 6.000	± 15.000		**± 2.210**	**± 12.616**	**± 8.550**	**± 30.595**
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]					
$AmH_2(cr)$	-134.661	-175.800	48.100	38.200	$Am^{3+} + 2\ H^+ + 5\ e^- \rightleftarrows AmH_2(cr)$	**-81.295**	**464.037**	**440.900**	**-77.597**
	± 15.055	± 15.000	± 3.800	± 2.500		**± 2.766**	**± 15.788**	**± 15.075**	**± 15.474**
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]					
$AmOH^{2+}$	**-794.783**				$Am^{3+} + H_2O(l) \rightleftarrows AmOH^{2+} + H^+$	-7.200	41.098		
	± 5.547					± 0.500	± 2.854		
						[2003GUI/FAN]	[2003GUI/FAN]		
$Am(OH)_2^+$	**-986.872**				$Am^{3+} + 2\ H_2O(l) \rightleftarrows Am(OH)_2^+ + 2\ H^+$	-15.100	86.191		
	± 6.214					± 0.700	± 3.996		
						[2003GUI/FAN]	[2003GUI/FAN]		
$AmO_2OH(am)$	**-946.726**				$AmO_2^+ + H_2O(l) \rightleftarrows AmO_2OH(am) + H^+$	-5.300	30.253		
	± 6.833					± 0.500	± 2.854		
						[2003GUI/FAN]	[2003GUI/FAN]		

Table A22 Selected thermodynamic data for americium (Am) in JAEA-TDB-RN in 2020 (2/5)

Species / compound	$\Delta_f G^0_m$ (kJ.mol^{-1})	$\Delta_f H^0_m$ (kJ.mol^{-1})	S^0_m (J.K^{-1}.mol^{-1})	$C^0_{p,m}$ (J.K^{-1}.mol^{-1})	Reaction	$\log_{10} K°$	$\Delta_r G^0_m$ (kJ.mol^{-1})	$\Delta_r H^0_m$ (kJ.mol^{-1})	$\Delta_r S^0_m$ (J.K^{-1}.mol^{-1})
$Am(OH)_3$(cr)	**-1221.200**	-1353.198	116.000		$Am^{3+} + 3\ H_2O(l) \rightleftarrows Am(OH)_3(cr) + 3\ H^+$	-15.600	89.045		
	± 5.868	± 6.356	± 8.000			± 0.600	± 3.425		
		[2003GUI/FAN]	[2003GUI/FAN]			[2003GUI/FAN]	[2003GUI/FAN]		
$Am(OH)_3$(am)	**-1213.780**				$Am^{3+} + 3\ H_2O(l) \rightleftarrows Am(OH)_3(am) + 3\ H^+$	-16.900	96.466		
	± 6.599					± 0.800	± 4.566		
						[2003GUI/FAN]	[2003GUI/FAN]		
$Am(OH)_3$(aq)	**-1160.695**				$Am^{3+} + 3\ H_2O(l) \rightleftarrows Am(OH)_3(aq) + 3\ H^+$	-26.200	149.551		
	± 5.554					± 0.500	± 2.854		
						[2003GUI/FAN]	[2003GUI/FAN]		
AmF^{2+}	**-899.856**				$Am^{3+} + F^- \rightleftarrows AmF^{2+}$	3.400	-19.407		
	± 5.317					± 0.400	± 2.283		
						[2003GUI/FAN]	[2003GUI/FAN]		
AmF_2^+	**-1195.306**				$Am^{3+} + 2\ F^- \rightleftarrows AmF_2^+$	5.800	-33.107		
	± 5.070					± 0.200	± 1.142		
						[2003GUI/FAN]	[2003GUI/FAN]		
AmF_3(cr)	-1519.765	-1594.000	110.600		$Am^{3+} + 3\ F^- \rightleftarrows AmF_3(cr)$	**13.282**	**-75.815**	**28.743**	**351.139**
	± 14.126	± 14.000	± 6.000			**± 2.635**	**± 15.040**	**± 14.223**	**± 16.238**
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]						
AmF_3(g)	-1147.798	-1156.500	330.400	72.200	$Am^{3+} + 3\ F^- \rightleftarrows AmF_3(g)$	**-51.883**	**296.152**	**466.243**	**570.939**
	± 16.771	± 16.589	± 8.000	± 5.000		**± 3.074**	**± 17.547**	**± 16.777**	**± 17.078**
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]					
AmF_4(cr)	-1632.503	-1724.000	154.100		$Am^{4+} + 4\ F^- \rightleftarrows AmF_4(cr)$	**27.880**	**-159.143**	**23.390**	**612.818**
	± 17.177	± 17.000	± 8.000			**± 3.405**	**± 19.436**	**± 18.226**	**± 22.577**
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]						
$AmCl^{2+}$	**-731.358**				$Am^{3+} + Cl^- \rightleftarrows AmCl^{2+}$	0.240	-1.370		
	± 4.759					± 0.030	± 0.171		
						[2003GUI/FAN]	[2003GUI/FAN]		
$AmCl_2^+$	**-857.054**				$Am^{3+} + 2\ Cl^- \rightleftarrows AmCl_2^+$	-0.740	4.224		
	± 4.768					± 0.050	± 0.285		
						[2003GUI/FAN]	[2003GUI/FAN]		
$AmCl_3$(cr)	-905.105	-977.800	146.200	103.000	$Am^{3+} + 3\ Cl^- \rightleftarrows AmCl_3(cr)$	**-15.323**	**87.462**	**140.139**	**176.995**
	± 2.290	± 1.300	± 6.000	± 10.000		**± 0.926**	**± 5.286**	**± 2.002**	**± 16.163**
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]					
AmOCl(cr)	-897.052	-949.800	92.600	70.400	$Am^{3+} + Cl^- + H_2O(l) \rightleftarrows AmOCl(cr) + 2\ H^+$	**-12.284**	**70.118**	**119.818**	**166.942**
	± 6.726	± 6.000	± 10.000	± 10.000		**± 1.443**	**± 8.238**	**± 6.186**	**± 18.029**
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]					
$AmBr_3$(cr)	-773.674	-804.000	182.000		$Am^{3+} + 3\ Br^- \rightleftarrows AmBr_3(cr)$	**-24.028**	**137.155**	**177.210**	**134.470**
	± 6.728	± 6.000	± 10.000			**± 1.446**	**± 8.254**	**± 6.201**	**± 18.039**
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]						
AmOBr(cr)	-848.485	-887.000	104.900		$Am^{3+} + Br^{--} + H_2O(l) \rightleftarrows AmOBr(cr) + 2\ H^+$	**-16.019**	**91.439**	**137.042**	**153.134**
	± 9.794	± 9.000	± 12.800			**± 1.908**	**± 10.889**	**± 9.126**	**± 19.720**
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]						

Table A22 Selected thermodynamic data for americium (Am) in JAEA-TDB-RN in 2020 (3/5)

Species / compound	$\Delta_f G^0_m$ (kJ.mol^{-1})	$\Delta_f H^0_m$ (kJ.mol^{-1})	S^0_m (J.K^{-1}.mol^{-1})	$C^0_{p,m}$ (J.K^{-1}.mol^{-1})	Reaction	$\log_{10} K°$	$\Delta_r G^0_m$ (kJ.mol^{-1})	$\Delta_r H^0_m$ (kJ.mol^{-1})	$\Delta_r S^0_m$ (J.K^{-1}.mol^{-1})
AmI_3(cr)	-609.451 ± 10.068 [2003GUI/FAN]	-615.000 ± 9.000 [2003GUI/FAN]	211.000 ± 15.000 [2003GUI/FAN]		$Am^{3+} + 3\ I^- \rightleftarrows AmI_3$(cr)	**-25.406 ± 2.000**	**145.017 ± 11.414**	**172.407 ± 9.463**	**91.924 ± 21.222**
AmS(cr)			92.000 ± 12.000 [2003GUI/FAN]						
$AmSO_4^+$	**-1361.994 ± 4.853**				$Am^{3+} + SO_4^{2-} \rightleftarrows AmSO_4^+$	3.300 ± 0.150 [2003GUI/FAN]	-18.837 ± 0.856 [2003GUI/FAN]		
$Am(SO_4)_2^-$	**-2108.736 ± 4.918**				$Am^{3+} + 2\ SO_4^{2-} \rightleftarrows Am(SO_4)_2^-$	3.700 ± 0.150 [2003GUI/FAN]	-21.120 ± 0.856 [2003GUI/FAN]		
AmSe(cr)			109.000 ± 12.000 [2003GUI/FAN]						
AmTe(cr)			121.000 ± 12.000 [2003GUI/FAN]						
AmN_3^{2+}	**-260.030 ± 5.190**				$Am^{3+} + N_3^- \rightleftarrows AmN_3^{2+}$	1.670 ± 0.100 [2003GUI/FAN]	-9.532 ± 0.571 [2003GUI/FAN]		
$AmNO_2^{2+}$	**-642.902 ± 9.692**				$Am^{3+} + NO_2^- \rightleftarrows AmNO_2^{2+}$	2.100 ± 0.200 [2003GUI/FAN]	-11.987 ± 1.142 [2003GUI/FAN]		
$AmNO_3^{2+}$	**-717.208 ± 5.497**				$Am^{3+} + NO_3^- \rightleftarrows AmNO_3^{2+}$	1.330 ± 0.200 [2003GUI/FAN]	-7.592 ± 1.142 [2003GUI/FAN]		
$AmPO_4$(am,hyd)	**-1759.004 ± 10.216**				$Am^{3+} + PO_4^{3-} \rightleftarrows AmPO_4$(am,hydr)	24.790 ± 0.600 [2003GUI/FAN]	-141.502 ± 3.425 [2003GUI/FAN]		
$AmH_2PO_4^{2+}$	**-1746.088 ± 5.609**				$Am^{3+} + H_2PO_4^- \rightleftarrows AmH_2PO_4^{2+}$	3.000 ± 0.500 [2003GUI/FAN]	-17.124 ± 2.854 [2003GUI/FAN]		
Am_2C_3(cr)	-156.063 ± 42.438 [2003GUI/FAN]	-151.000 ± 42.000 [2003GUI/FAN]	145.000 ± 20.000 [2003GUI/FAN]		$2\ Am^{3+} + 15\ H^+ + 18\ e^- + 3\ HCO_3^- \rightleftarrows Am_2C_3$(cr) $+ 9\ H_2O$(l)	**-116.942 ± 7.621**	**667.509 ± 43.502**	**579.655 ± 42.122**	**-295.151 ± 36.096**
$AmCO_3^+$	**-1172.345 ± 5.283**				$Am^{3+} + CO_3^{2-} \rightleftarrows AmCO_3^+$	8.000 ± 0.400 [2003GUI/FAN]	-45.664 ± 2.283 [2003GUI/FAN]		
$AmO_2CO_3^-$	**-1296.890 ± 6.839**				$AmO_2^+ + CO_3^{2-} \rightleftarrows AmO_2CO_3^-$	5.100 ± 0.500 [2003GUI/FAN]	-29.111 ± 2.854 [2003GUI/FAN]		

Table A22 Selected thermodynamic data for americium (Am) in JAEA-TDB-RN in 2020 (4/5)

Species / compound	$\Delta_f G^0_m$ (kJ.mol^{-1})	$\Delta_f H^0_m$ (kJ.mol^{-1})	S^0_m (J.K^{-1}.mol^{-1})	$C^0_{p,m}$ (J.K^{-1}.mol^{-1})	Reaction	$\log_{10} K°$	$\Delta_r G^0_m$ (kJ.mol^{-1})	$\Delta_r H^0_m$ (kJ.mol^{-1})	$\Delta_r S^0_m$ (J.K^{-1}.mol^{-1})
$Am(CO_3)_2^-$	**-1728.298 ± 5.889**				$Am^{3+} + 2\ CO_3^{2-} \rightleftarrows Am(CO_3)_2^-$	12.900 ± 0.600 [2003GUI/FAN]	-73.634 ± 3.425 [2003GUI/FAN]		
$AmO_2(CO_3)_2^{3-}$	**-1834.006 ± 7.729**				$AmO_2^+ + 2\ CO_3^{2-} \rightleftarrows AmO_2(CO_3)_2^{3-}$	6.700 ± 0.800 [2003GUI/FAN]	-38.244 ± 4.566 [2003GUI/FAN]		
$Am(CO_3)_3^{3-}$	**-2268.268 ± 7.481**				$Am^{3+} + 3\ CO_3^{2-} \rightleftarrows Am(CO_3)_3^{3-}$	15.000 ± 1.000 [2003GUI/FAN]	-85.621 ± 5.708 [2003GUI/FAN]		
$Am_2(CO_3)_3$(am)	**-2971.994 ± 15.777**				$2\ Am^{3+} + 3\ CO_3^{2-} \rightleftarrows Am_2(CO_3)_3$(am)	33.400 ± 2.200 [2003GUI/FAN]	-190.649 ± 12.558 [2003GUI/FAN]		
$AmO_2(CO_3)_3^{5-}$	**-2352.856 ± 8.479**				$AmO_2^+ + 3\ CO_3^{2-} \rightleftarrows AmO_2(CO_3)_3^{5-}$	5.100 ± 1.000 [2003GUI/FAN]	-29.111 ± 5.708 [2003GUI/FAN]		
$Am(CO_3)_5^{6-}$	**-3209.253 ± 9.127**				$Am(CO_3)_3^{3-} + 2\ CO_3^{2-} \rightleftarrows Am(CO_3)_5^{6-} + e^-$	-20.100 ± 0.900 [2003GUI/FAN]	114.732 ± 5.137 [2003GUI/FAN]		
$AmHCO_3^{2+}$	**-1203.333 ± 5.056**				$Am^{3+} + HCO_3^- \rightleftarrows AmHCO_3^{2+}$	3.100 ± 0.300 [2003GUI/FAN]	-17.695 ± 1.712 [2003GUI/FAN]		
$AmCO_3OH{\cdot}0.5H_2O$(cr)	**-1530.430 ± 5.554**	-1682.900 ± 2.600 [2003GUI/FAN]	141.413 ± 20.683 [2003GUI/FAN]		$Am^{3+} + CO_3^{2-} + 0.5\ H_2O$(l) + $OH^- \rightleftarrows AmCO_3OH{\cdot}0.5H_2O$(cr)	22.400 ± 0.500 [2003GUI/FAN]	-127.860 ± 2.854 [2003GUI/FAN]	**-18.022 ± 3.036**	**368.161 ± 25.583**
$AmCO_3OH$(am,hyd)	**-1399.281 ± 7.435**				$Am^{3+} + CO_3^{2-} + OH^- \rightleftarrows AmCO_3OH$(am,hyd)	20.200 ± 1.000 [2003GUI/FAN]	-115.302 ± 5.708 [2003GUI/FAN]		
$AmSiO(OH)_3^{2+}$	**-1896.881 ± 5.194**				$Am^{3+} + H_4SiO_4$(aq) $\rightleftarrows AmSiO(OH)_3^{2+} + H^+$	-1.680 ± 0.180 [2003GUI/FAN]	9.590 ± 1.027 [2003GUI/FAN]		
$AmSCN^{2+}$	**-513.234 ± 9.776**				$Am^{3+} + SCN^- \rightleftarrows AmSCN^{2+}$	1.300 ± 0.300 [2003GUI/FAN]	-7.420 ± 1.712 [2003GUI/FAN]		
$SrAmO_2$(cr)		-1539.000 ± 4.100 [2003GUI/FAN]			$Am^{2+} + Sr^{2+} + 2\ H_2O$(l) $\rightleftarrows SrAmO_2$(cr) + 4 H^+			**-61.783 ± 16.419**	
$BaAmO_2$(cr)		-1544.600 ± 3.400 [2003GUI/FAN]			$Am^{2+} + Ba^{2+} + 2\ H_2O$(l) $\rightleftarrows BaAmO_2$(cr) + 4 H^+			**-83.659 ± 16.337**	
$NaAmO_2CO_3$(s)	**-1591.878 ± 6.622**				$AmO_2^+ + CO_3^{2-} + Na^+ \rightleftarrows NaAmO_2CO_3$(s)	10.900 ± 0.400 [2003GUI/FAN]	-62.218 ± 2.283 [2003GUI/FAN]		

Table A22 Selected thermodynamic data for americium (Am) in JAEA-TDB-RN in 2020 (5/5)

Species / compound	$\Delta_f G^0_m$ (kJ.mol^{-1})	$\Delta_f H^0_m$ (kJ.mol^{-1})	S^0_m (J.K^{-1}.mol^{-1})	$C^0_{p,m}$ (J.K^{-1}.mol^{-1})	Reaction	$\log_{10} K°$	$\Delta_r G^0_m$ (kJ.mol^{-1})	$\Delta_r H^0_m$ (kJ.mol^{-1})	$\Delta_r S^0_m$ (J.K^{-1}.mol^{-1})
$NaAm(CO_3)_2 \cdot 5H_2O$(cr)	**-3222.327**				$AmO_2^+ + CO_3^{2-} + Na^+ + 5\ H_2O$(l) ⇄ $NaAm(CO_3)_2 \cdot 5H_2O$(cr)	21.000	-119.869		
	± 5.601					± 0.500	± 2.854		
						[2003GUI/FAN]	[2003GUI/FAN]		
$Cs_2NaAmCl_6$(cr)	-2159.151	-2315.800	421.000	260.000	$Am^{3+} + 6\ Cl^- + Na^+ + 2\ Cs^+$ ⇄ $Cs_2NaAmCl_6$(cr)	**-12.701**	**72.499**	**59.728**	**-42.503**
	± 4.864	± 1.800	± 15.000	± 15.000		**± 1.199**	**± 6.843**	**± 2.416**	**± 21.238**
	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]	[2003GUI/FAN]					

[2003GUI/FAN] Guillaumont et al. [A15)]

Table A23 Selected thermodynamic data for curium (Cm) in JAEA-TDB-RN in 2020 (1/2)

Values indicated by **boldface** are calculated and selected in the present report.

Species / compound	$\Delta_f G^0_m$ (kJ.mol^{-1})	$\Delta_f H^0_m$ (kJ.mol^{-1})	S^0_m (J.K^{-1}.mol^{-1})	$C^0_{p,m}$ (J.K^{-1}.mol^{-1})	Reaction	$\log_{10} K°$	$\Delta_r G^0_m$ (kJ.mol^{-1})	$\Delta_r H^0_m$ (kJ.mol^{-1})	$\Delta_r S^0_m$ (J.K^{-1}.mol^{-1})
Cm^{3+}	−595.802 ± 6.276 [1976FUG/OET]	−615.048 ± 5.021 [1976FUG/OET]	−188.280 ± 12.552 [1976FUG/OET]						
$CmOH^{2+}$	**-791.886 ± 6.895**				$Cm^{3+} + H_2O(l) \rightleftarrows CmOH^{2+} + H^+$	-7.200 ± 0.500 [2010KIT/FUJ2]	**41.098 ± 2.854**		
$Cm(OH)_2^+$	**-983.975 ± 7.443**				$Cm^{3+} + 2\ H_2O(l) \rightleftarrows Cm(OH)_2^+ + 2\ H^+$	-15.100 ± 0.700 [2010KIT/FUJ2]	**86.191 ± 3.996**		
$Cm(OH)_3$(am)	**-1210.883 ± 7.767**				$Cm^{3+} + 3\ H_2O(l) \rightleftarrows Cm(OH)_3(am) + 3\ H^+$	-16.900 ± 0.800 [2010KIT/FUJ2]	**96.466 ± 4.566**		
$Cm(OH)_3$(cr)	**-1218.304 ± 7.156**				$Cm^{3+} + 3\ H_2O(l) \rightleftarrows Cm(OH)_3(cr) + 3\ H^+$	-15.600 ± 0.600 [2010KIT/FUJ2]	**89.045 ± 3.425**		
$Cm(OH)_3$(aq)	**-1157.799 ± 6.901**				$Cm^{3+} + 3\ H_2O(l) \rightleftarrows Cm(OH)_3(aq) + 3\ H^+$	-26.200 ± 0.500 [2010KIT/FUJ2]	**149.551 ± 2.854**		
CmF^{2+}	**-896.960 ± 6.712**				$Cm^{3+} + F^- \rightleftarrows CmF^{2+}$	3.400 ± 0.400 [2010KIT/FUJ2]	**-19.407 ± 2.283**		
CmF_2^+	**-1192.409 ± 6.518**				$Cm^{3+} + 2\ F^- \rightleftarrows CmF_2^+$	5.800 ± 0.200 [2010KIT/FUJ2]	**-33.107 ± 1.142**		
$CmCl^{2+}$	**-728.461 ± 6.279**				$Cm^{3+} + Cl^- \rightleftarrows CmCl^{2+}$	0.240 ± 0.030 [2010KIT/FUJ2]	**-1.370 ± 0.171**		
$CmCl_2^+$	**-854.157 ± 6.286**				$Cm^{3+} + 2\ Cl^- \rightleftarrows CmCl_2^+$	-0.740 ± 0.050 [2010KIT/FUJ2]	**4.224 ± 0.285**		
$CmSO_4^+$	**-1359.097 ± 6.351**				$Cm^{3+} + SO_4^{2-} \rightleftarrows CmSO_4^+$	3.300 ± 0.150 [2010KIT/FUJ2]	**-18.837 ± 0.856**		
$Cm(SO_4)_2^-$	**-2105.840 ± 6.401**				$Cm^{3+} + 2\ SO_4^{2-} \rightleftarrows Cm(SO_4)_2^-$	3.700 ± 0.150 [2010KIT/FUJ2]	**-21.120 ± 0.856**		
CmN_3^{2+}	**-257.134 ± 6.612**				$Cm^{3+} + N_3^- \rightleftarrows CmN_3^{2+}$	1.670 ± 0.100 [2010KIT/FUJ2]	**-9.532 ± 0.571**		

Table A23 Selected thermodynamic data for curium (Cm) in JAEA-TDB-RN in 2020 (2/2)

Species / compound	$\Delta_f G^0_m$ (kJ.mol^{-1})	$\Delta_f H^0_m$ (kJ.mol^{-1})	S^0_m (J.K^{-1}.mol^{-1})	$C^0_{p,m}$ (J.K^{-1}.mol^{-1})	Reaction	$\log_{10} K°$	$\Delta_r G^0_m$ (kJ.mol^{-1})	$\Delta_r H^0_m$ (kJ.mol^{-1})	$\Delta_r S^0_m$ (J.K^{-1}.mol^{-1})
$CmNO_2^{2+}$	**-640.005**				$Cm^{3+} + NO_2^- \rightleftarrows CmNO_2^{2+}$	2.100	**-11.987**		
	± 10.522					± 0.200	**± 1.142**		
						[2010KIT/FUJ2]			
$CmNO_3^{2+}$	**-714.311**				$Cm^{3+} + NO_3^- \rightleftarrows CmNO_3^{2+}$	1.330	**-7.592**		
	± 6.855					± 0.200	**± 1.142**		
						[2010KIT/FUJ2]			
$CmH_2PO_4^{2+}$	**-1743.39**				$Cm^{3+} + 2\ H^+ + PO_4^{3-} \rightleftarrows CmH_2PO_4^{2+}$	22.562	**-128.785**		
	± 10.844					± 0.501	**± 2.860**		
						[2010KIT/FUJ2]			
$CmCO_3^+$	**-1169.447**				$Cm^{3+} + CO_3^{2-} \rightleftarrows CmCO_3^+$	8.000	**-45.664**		
	± 6.682					± 0.400	**± 2.283**		
						[2010KIT/FUJ2]			
$Cm(CO_3)_2^-$	**-1725.398**				$Cm^{3+} + 2\ CO_3^{2-} \rightleftarrows Cm(CO_3)_2^-$	12.900	**-73.634**		
	± 7.157					± 0.600	**± 3.425**		
						[2010KIT/FUJ2]			
$Cm(CO_3)_3^{3-}$	**-2265.367**				$Cm^{3+} + 3\ CO_3^{2-} \rightleftarrows Cm(CO_3)_3^{3-}$	15.000	**-85.621**		
	± 8.500					± 1.000	**± 5.708**		
						[2010KIT/FUJ2]			
$Cm_2(CO_3)_3$(am)	**-2966.196**				$2\ Cm^{3+} + 3\ CO_3^{2-} \rightleftarrows Cm_2(CO_3)_3$(am)	33.400	**-190.649**		
	± 14.045					± 1.100	**± 6.279**		
						[2010KIT/FUJ2]			
$CmHCO_3^{2+}$	**-1200.436**				$Cm^{3+} + H^+ + CO_3^{2-} \rightleftarrows CmHCO_3^{2+}$	13.429	**-76.653**		
	± 6.540					± 0.301	**± 1.718**		
						[2010KIT/FUJ2]			
$CmCO_3OH$(am)	**-1396.350**				$Cm^{3+} + CO_3^{2-} + H_2O(l) \rightleftarrows CmCO_3OH$(am) $+ H^+$	6.199	**-35.384**		
	± 8.485					± 1.000	**± 5.708**		
						[2010KIT/FUJ2]			
$CmCO_3OH•0.5H_2O$(cr)	**-1527.499**				$Cm^{3+} + CO_3^{2-} + 1.5\ H_2O(l) \rightleftarrows CmCO_3OH•0.5H_2O$(cr) $+ H^+$	8.399	**-47.942**		
	± 6.897					± 0.500	**± 2.854**		
						[2010KIT/FUJ2]			
$CmSiO(OH)_3^{2+}$	**-1893.984**				$Cm^{3+} + H_4SiO_4(aq) \rightleftarrows CmSiO(OH)_3^{2+} + H^+$	-1.680	**9.590**		
	± 6.615					± 0.180	**± 1.027**		
						[2010KIT/FUJ2]			
$CmSCN^{2+}$	**-510.337**				$Cm^{3+} + SCN^- \rightleftarrows CmSCN^{2+}$	1.300	**-7.420**		
	± 10.599					± 0.300	**± 1.712**		
						[2010KIT/FUJ2]			
$NaCm(CO_3)_2•5H_2O$(cr)	**-3219.427**				$Cm^{3+} + 2\ CO_3^{2-} + 5\ H_2O(l) + Na^+ \rightleftarrows NaCm(CO_3)_2•5H_2O$(cr)	21.000	**-119.869**		
	± 6.923					± 0.500	**± 2.854**		
						[2010KIT/FUJ2]			
$CmPO_4$(am,hydr)	**-1756.108**				$Cm^{3+} + PO_4^{3-} \rightleftarrows CmPO_4$(am,hydr)	24.790	**-141.502**		
	± 11.006					± 0.600	**± 3.425**		
						[2010KIT/FUJ2]			

[1976FUG/OET] Fuger and Oetting [A24)] with conversion using 1 cal = 4.184 J by the author.
[2010KIT/FUJ2] Kitamura et al. [A21)]

Table A24 Selected thermodynamic data for various elements with selected organics (oxalate (ox), citrate (cit), EDTA (edta) and ISA (isa)) in JAEA-TDB-RN in 2020 based on NEA Thermochemical Data Base Project [A35] (1/6)

Values indicated by **boldface** are calculated and selected in the present report.

Species / compound	$\Delta_f G^0_m$ (kJ.mol^{-1})	$\Delta_f H^0_m$ (kJ.mol^{-1})	S^0_m (J.K^{-1}.mol^{-1})	$C^0_{p,m}$ (J.K^{-1}.mol^{-1})	Reaction	$\log_{10} K°$	$\Delta_r G^0_m$ (kJ.mol^{-1})	$\Delta_r H^0_m$ (kJ.mol^{-1})	$\Delta_r S^0_m$ (J.K^{-1}.mol^{-1})
ox^{2-}	-680.134	-830.660	47.597		$Hox^- \rightleftarrows H^+ + (ox)^{2-}$	-4.250	24.259	-7.300	-105.850
	± 1.830	± 1.592	± 3.020			± 0.010	± 0.057	± 0.100	± 0.386
	[2005HUM/AND]	[2005HUM/AND]	[2005HUM/AND]			[2005HUM/AND]	[2005HUM/AND]	[2005HUM/AND]	[2005HUM/AND]
Hox^-	-704.393	-823.360	153.447		$H_2ox(aq) \rightleftarrows Hox^- + H^+$	-1.400	7.991	-3.300	-37.871
	± 1.831	± 1.588	± 3.045			± 0.030	± 0.171	± 0.500	± 1.773
	[2005HUM/AND]	[2005HUM/AND]	[2005HUM/AND]			[2005HUM/AND]	[2005HUM/AND]	[2005HUM/AND]	[2005HUM/AND]
α-H_2ox	-698.549	-828.800	115.600	105.900	$2\ H^+ + (ox)^{2-} \rightleftarrows$ α-H_2ox	**3.226**	**-18.415**	**1.860**	**68.003**
	± 1.502	± 1.500	± 0.200	± 0.200		**± 0.415**	**± 2.367**	**± 2.187**	**± 3.027**
	[2005HUM/AND]	[2005HUM/AND]	[2005HUM/AND]	[2005HUM/AND]					
$H_2ox(aq)$	-712.384	-820.060	191.318		$2\ H^+ + (ox)^{2-} \rightleftarrows H_2ox(aq)$	**5.650**	**-32.250**	**10.600**	**143.721**
	± 1.839	± 1.508	± 3.523			**± 0.455**	**± 2.594**	**± 2.193**	**± 4.640**
	[2005HUM/AND]	[2005HUM/AND]	[2005HUM/AND]						
β-H_2ox		-827.500			$2\ H^+ + (ox)^{2-} \rightleftarrows$ β-H_2ox			**3.160**	
		± 1.500						**± 2.187**	
		[2005HUM/AND]							
$H_2(ox)\cdot 2H_2O(cr)$		-1427.000			$2\ H^+ + (ox)^{2-} + 2\ H_2O(l) \rightleftarrows H_2(ox)\cdot 2H_2O(cr)$			**-24.663**	
		± 1.500						**± 2.197**	
		[2005HUM/AND]							
Ni(ox)(aq)	-755.531	-885.672	15.159		$Ni^{2+} + (ox)^{2-} \rightleftarrows Ni(ox)(aq)$	5.190	-29.625	0.000	99.362
	± 1.998	± 1.843	± 3.561			± 0.040	± 0.228	± 0.300	± 1.264
	[2005HUM/AND]	[2005HUM/AND]	[2005HUM/AND]			[2005HUM/AND]	[2005HUM/AND]	[2005HUM/AND]	[2005HUM/AND]
$Ni(ox)_2^{2-}$	-1449.650	-1724.132	83.499		$Ni^{2+} + 2\ (ox)^{2-} \rightleftarrows Ni(ox)_2^{2-}$	7.640	-43.609	-7.800	120.105
	± 3.761	± 3.317	± 6.423			± 0.070	± 0.400	± 0.300	± 1.676
	[2005HUM/AND]	[2005HUM/AND]	[2005HUM/AND]			[2005HUM/AND]	[2005HUM/AND]	[2005HUM/AND]	[2005HUM/AND]
$Am(ox)^+$	-1315.991				$Am^{3+} + (ox)^{2-} \rightleftarrows Am(ox)^+$	6.510	-37.159		
	± 5.166					± 0.150	± 0.856		
	[2005HUM/AND]					[2005HUM/AND]	[2005HUM/AND]		
$Am(ox)_2^-$	-2020.099				$Am^{3+} + 2(\ ox)^{2-} \rightleftarrows Am(ox)_2^-$	10.710	-61.133		
	± 6.107					± 0.200	± 1.142		
	[2005HUM/AND]					[2005HUM/AND]	[2005HUM/AND]		
$Am(ox)_3^{3-}$	-2713.304				$Am^{3+} + 3\ (ox)^{2-} \rightleftarrows Am(ox)_3^{3-}$	13.000	-74.205		
	± 9.237					± 1.000	± 5.708		
	[2005HUM/AND]					[2005HUM/AND]	[2005HUM/AND]		
$NpO_2(ox)^-$	-1610.160				$NpO_2^+ + (ox)^{2-} \rightleftarrows NpO_2(ox)^-$	3.900	-22.261		
	± 5.945					± 0.100	± 0.571		
	[2005HUM/AND]					[2005HUM/AND]	[2005HUM/AND]		
$NpO_2(ox)_2^{3-}$	-2301.140				$NpO_2^+ + 2\ (ox)^{2-} \rightleftarrows NpO_2(ox)_2^{3-}$	5.800	-33.107		
	± 6.809					± 0.200	± 1.142		
	[2005HUM/AND]					[2005HUM/AND]	[2005HUM/AND]		

Table A24 Selected thermodynamic data for various elements with selected organics (oxalate (ox), citrate (cit), EDTA (edta) and ISA (isa)) in JAEA-TDB-RN in 2020 based on NEA Thermochemical Data Base Project [A35] (2/6)

Species / compound	$\Delta_f G^0_m$ (kJ.mol^{-1})	$\Delta_f H^0_m$ (kJ.mol^{-1})	S^0_m (J.K^{-1}.mol^{-1})	$C^0_{p,m}$ (J.K^{-1}.mol^{-1})	Reaction	$\log_{10} K°$	$\Delta_r G^0_m$ (kJ.mol^{-1})	$\Delta_r H^0_m$ (kJ.mol^{-1})	$\Delta_r S^0_m$ (J.K^{-1}.mol^{-1})
$UO_2(ox)(aq)$	-1673.383 ± 2.690 [2005HUM/AND]	-1824.300 ± 18.300 [2005HUM/AND]	170.958 ± 62.039 [2005HUM/AND]		$UO_2^{2+} + (ox)^{2-} \rightleftarrows UO_2(ox)$ (aq)	7.130 ± 0.160 [2005HUM/AND]	-40.698 ± 0.913 [2005HUM/AND]		
$UO_2(ox)\cdot 3H_2O(cr)$	**-2395.205 ± 3.115**	**-2702.015 ± 18.634**	**347.437 ± 63.352**		$UO_2ox(aq) + 3\ H_2O(l) \rightleftarrows UO_2(ox)\cdot 3H_2O(cr)$	1.800 ± 0.270 [2005HUM/AND]	-10.274 ± 1.541 [2005HUM/AND]	-20.200 ± 3.500 [2005HUM/AND]	-33.290 ± 12.827 [2005HUM/AND]
$UO_2(ox)_2^{2-}$	-2379.317 ± 4.145 [2005HUM/AND]				$UO_2^{2+} + 2\ (ox)^{2-} \rightleftarrows UO_2(ox)_2^{2-}$	11.650 ± 0.150 [2005HUM/AND]	-66.499 ± 0.856 [2005HUM/AND]		
$UO_2(ox)_3^{4-}$	-3071.723 ± 10.320 [2005HUM/AND]				$UO_2^{2+} + 3\ (ox)^{2-} \rightleftarrows UO_2(ox)_3^{4-}$	13.800 ± 1.500 [2005HUM/AND]	-78.771 ± 8.562 [2005HUM/AND]		
Mg(ox)(aq)	**-1154.440 ± 2.141**				$Mg^{2+} + (ox)^{2-} \rightleftarrows Mg(ox)(aq)$	3.560 ± 0.040 [2005HUM/AND]	-20.321 ± 0.228 [2005HUM/AND]		
$Mg(ox)_2^{2-}$	**-1843.763 ± 3.845**				$Mg^{2+} + 2\ (ox)^{2-} \rightleftarrows Mg(ox)_2^{2-}$	5.170 ± 0.080 [2005HUM/AND]	-29.511 ± 0.457 [2005HUM/AND]		
$Ca(ox)\cdot H_2O(cr)$	**-1519.938 ± 2.027**	**-1681.082 ± 1.851**	**156.059 ± 3.665**	153.340 ± 2.000 [2005HUM/AND]	$Ca^{2+} + H_2O(l) + (ox)^{2-} \rightleftarrows Ca(ox)\cdot H_2O(cr)$	8.730 ± 0.060 [2005HUM/AND]	-49.831 ± 0.342 [2005HUM/AND]	-21.500 ± 0.500 [2005HUM/AND]	95.023 ± 2.033 [2005HUM/AND]
$Ca(ox)\cdot 2H_2O(cr)$	**-1754.666 ± 2.034**	**-1970.620 ± 2.102**	**205.340 ± 4.925**		$Ca^{2+} + 2\ H_2O(l) + (ox)^{2-} \rightleftarrows Ca(ox)\cdot 2H_2O(cr)$	8.300 ± 0.060 [2005HUM/AND]	-47.377 ± 0.342 [2005HUM/AND]	-25.200 ± 1.100 [2005HUM/AND]	74.381 ± 3.864 [2005HUM/AND]
$Ca(ox)\cdot 3H_2O(cr)$	**-1991.221 ± 2.031**	**-2260.958 ± 2.226**	**258.064 ± 5.381**		$Ca^{2+} + 3\ H_2O(l) + (ox)^{2-} \rightleftarrows Ca(ox)\cdot 3H_2O(cr)$	8.190 ± 0.040 [2005HUM/AND]	-46.749 ± 0.228 [2005HUM/AND]	-29.700 ± 1.300 [2005HUM/AND]	57.182 ± 4.427 [2005HUM/AND]
Ca(ox)(aq)	**-1251.133 ± 2.024**				$Ca^{2+} + (ox)^{2-} \rightleftarrows Ca(ox)(aq)$	3.190 ± 0.060 [2005HUM/AND]	-18.209 ± 0.342 [2005HUM/AND]		
$Ca(ox)_2^{2-}$	**-1917.796 ± 3.899**				$Ca(ox)(aq) + (ox)^{2-} \rightleftarrows Ca(ox)_2^{2-}$	0.830 ± 0.190 [2005HUM/AND]	-4.738 ± 1.085 [2005HUM/AND]		
$(cit)^{3-}$	-1162.258 ± 2.014 [2005HUM/AND]	-1519.920 ± 2.070 [2005HUM/AND]	75.587 ± 1.855 [2005HUM/AND]						
$H(cit)^{2-}$	-1198.561 ± 2.011 [2005HUM/AND]	-1516.620 ± 2.048 [2005HUM/AND]	208.417 ± 1.510 [2005HUM/AND]		$(cit)^{3-} + H^+ \rightleftarrows H(cit)^{2-}$	6.360 ± 0.020 [2005HUM/AND]	36.303 ± 0.114 [2005HUM/AND]	3.300 ± 0.300 [2005HUM/AND]	132.830 ± 1.077 [2005HUM/AND]
$H_2(cit)^-$	-1225.845 ± 2.010 [2005HUM/AND]	-1519.020 ± 2.026 [2005HUM/AND]	291.879 ± 1.110 [2005HUM/AND]		$H(cit)^{2-} + H^+ \rightleftarrows H_2(cit)^-$	4.780 ± 0.010 [2005HUM/AND]	27.284 ± 0.057 [2005HUM/AND]	-2.400 ± 0.300 [2005HUM/AND]	83.463 ± 1.024 [2005HUM/AND]

Table A24 Selected thermodynamic data for various elements with selected organics (oxalate (ox), citrate (cit), EDTA (edta) and ISA (isa)) in JAEA-TDB-RN in 2020 based on NEA Thermochemical Data Base Project [A35] (3/6)

Species / compound	$\Delta_f G^0_m$ (kJ.mol^{-1})	$\Delta_f H^0_m$ (kJ.mol^{-1})	S^0_m (J.K^{-1}.mol^{-1})	$C^0_{p,m}$ (J.K^{-1}.mol^{-1})	Reaction	$\log_{10} K°$	$\Delta_r G^0_m$ (kJ.mol^{-1})	$\Delta_r H^0_m$ (kJ.mol^{-1})	$\Delta_r S^0_m$ (J.K^{-1}.mol^{-1})
H_3(cit)(cr)	-1236.695	-1541.730	252.100	225.400	$(cit)^{3-} + 3\ H^+ \rightleftarrows H_3$(cit)(cr)	**13.041**	**-74.437**	**-21.810**	**176.513**
	± 2.019	± 2.010	± 0.200	± 0.200		**± 0.500**	**± 2.852**	**± 2.885**	**± 1.866**
	[2005HUM/AND]	[2005HUM/AND]	[2005HUM/AND]	[2005HUM/AND]					
H_3(cit)(aq)	-1243.712	-1523.520	336.710		$H_2(cit)^- + H^+ \rightleftarrows H_3$(cit)(aq)	3.130	17.866	-4.500	44.830
	± 2.009	± 2.003	± 0.428			± 0.010	± 0.057	± 0.300	± 1.024
	[2005HUM/AND]	[2005HUM/AND]	[2005HUM/AND]			[2005HUM/AND]	[2005HUM/AND]	[2005HUM/AND]	[2005HUM/AND]
H_3(cit)·H_2O(cr)	**-1488.475**	**-1838.468**	**283.573**	268.050	H_3(cit)(aq) + H_2O(l) ⇄ H_3(cit)·H_2O(cr)	-1.328	-7.580	-29.110	-123.060
	± 2.012	**± 2.009**	**± 0.576**	± 0.100		± 0.004	± 0.023	± 0.110	± 0.377
				[2005HUM/AND]		[2005HUM/AND]	[2005HUM/AND]	[2005HUM/AND]	[2005HUM/AND]
Ni(cit)$^-$	-1246.617				$Ni^{2+} + (cit)^{3-} \rightleftarrows$ Ni(cit)$^-$	6.760	-38.586		
	± 2.207					± 0.080	± 0.457		
	[2005HUM/AND]					[2005HUM/AND]	[2005HUM/AND]		
Ni(cit)$_2^{4-}$	-2418.807				$Ni^{2+} + 2\ (cit)^{3-} \rightleftarrows Ni(cit)_2^{4-}$	8.500	-48.518		
	± 4.694					± 0.400	± 2.283		
	[2005HUM/AND]					[2005HUM/AND]	[2005HUM/AND]		
Ni(Hcit)(aq)	-1268.079				$Ni^{2+} + H(cit)^{2-} \rightleftarrows$ NiH(cit)(aq)	4.160	-23.745		
	± 2.228					± 0.100	± 0.571		
	[2005HUM/AND]					[2005HUM/AND]	[2005HUM/AND]		
Ni(H_2cit)$^+$	-1283.320				$Ni^{2+} + H_2(cit)^- \rightleftarrows$ Ni(H_2cit)$^+$	2.050	-11.701		
	± 2.583					± 0.250	± 1.427		
	[2005HUM/AND]					[2005HUM/AND]	[2005HUM/AND]		
Am(cit)(aq)	-1809.759				$Am^{3+} + (cit)^{3-} \rightleftarrows$ Am(cit)(aq)	8.550	-48.804		
	± 5.288					± 0.200	± 1.142		
	[2005HUM/AND]					[2005HUM/AND]	[2005HUM/AND]		
Am(cit)$_2^{3-}$	-3002.555				$Am^{3+} + 2\ (cit)^{3-} \rightleftarrows Am(cit)_2^{3-}$	13.900	-79.342		
	± 8.451					± 1.000	± 5.708		
	[2005HUM/AND]					[2005HUM/AND]	[2005HUM/AND]		
Am(Hcit)$^+$	-1834.361				$Am^{3+} + H(cit)^{2-} \rightleftarrows$ AmH(cit)$^+$	6.500	-37.102		
	± 7.696					± 1.000	± 5.708		
	[2005HUM/AND]					[2005HUM/AND]	[2005HUM/AND]		
Am(Hcit)$_2^-$	-3057.466				$Am^{3+} + 2\ H(cit)^{2-} \rightleftarrows AmH_2(cit)_2^-$	10.800	-61.647		
	± 8.448					± 1.000	± 5.708		
	[2005HUM/AND]					[2005HUM/AND]	[2005HUM/AND]		
NpO_2(cit)$^{2-}$	-2091.029				$NpO_2^+ + (cit)^{3-} \rightleftarrows NpO_2(cit)^{2-}$	3.680	-21.006		
	± 5.984					± 0.050	± 0.285		
	[2005HUM/AND]					[2005HUM/AND]	[2005HUM/AND]		
UO_2(cit)$^-$	-2165.953				$UO_2^{2+} + (cit)^{3-} \rightleftarrows UO_2(cit)^-$	8.960	-51.144		
	± 2.838					± 0.170	± 0.970		
	[2005HUM/AND]					[2005HUM/AND]	[2005HUM/AND]		
$(UO_2)_2(cit)_2^{2-}$	-4351.198				$2\ UO_2^{2+} + 2\ (cit)^{3-} \rightleftarrows (UO_2)_2(cit)_2^{2-}$	21.300	-121.581		
	± 6.049					± 0.500	± 2.854		
	[2005HUM/AND]					[2005HUM/AND]	[2005HUM/AND]		

Table A24 Selected thermodynamic data for various elements with selected organics (oxalate (ox), citrate (cit), EDTA (edta) and ISA (isa)) in JAEA-TDB-RN in 2020 based on NEA Thermochemical Data Base Project [A35] (4/6)

Species / compound	$\Delta_f G^0_m$ (kJ.mol^{-1})	$\Delta_f H^0_m$ (kJ.mol^{-1})	S^0_m (J.K^{-1}.mol^{-1})	$C^0_{p,m}$ (J.K^{-1}.mol^{-1})	Reaction	$\log_{10} K°$	$\Delta_r G^0_m$ (kJ.mol^{-1})	$\Delta_r H^0_m$ (kJ.mol^{-1})	$\Delta_r S^0_m$ (J.K^{-1}.mol^{-1})
UO_2(Hcit)(aq)	-2179.652 ± 6.299 [2005HUM/AND]				UO_2^{2+} + H(cit)$^{2-}$ ⇄ UO_2H(cit)(aq)	5.000 ± 1.000 [2005HUM/AND]	-28.540 ± 5.708 [2005HUM/AND]		
Mg(cit)$^-$	**-1643.699 ± 2.295**				Mg^{2+} + (cit)$^{3-}$ ⇄ Mg(cit)$^-$	4.810 ± 0.030 [2005HUM/AND]	-27.456 ± 0.171 [2005HUM/AND]		
Mg(Hcit)(aq)	**-1667.387 ± 2.321**				Mg^{2+} + H(cit)$^{2-}$ ⇄ MgH(cit)(aq)	2.600 ± 0.070 [2005HUM/AND]	-14.841 ± 0.400 [2005HUM/AND]		
Mg(H_2cit)$^+$	**-1687.307 ± 2.461**				Mg^{2+} + H_2(cit)$^-$ ⇄ MgH_2(cit)$^+$	1.310 ± 0.160 [2005HUM/AND]	-7.478 ± 0.913 [2005HUM/AND]		
Ca(cit)$^-$	**-1742.447 ± 2.172**	**-2063.003 ± 6.397**	**110.998 ± 20.222**		Ca^{2+} + (cit)$^{3-}$ ⇄ Ca(cit)$^-$	4.800 ± 0.030 [2005HUM/AND]	-27.399 ± 0.171 [2005HUM/AND]	0.000 ± 6.000 [2005HUM/AND]	91.895 ± 20.132 [2005HUM/AND]
Ca(Hcit)(aq)	**-1768.019 ± 2.199**				Ca^{2+} + H(cit)$^{2-}$ ⇄ CaH(cit)(aq)	2.920 ± 0.070 [2005HUM/AND]	-16.667 ± 0.400 [2005HUM/AND]		
Ca(H_2cit)$^+$	**-1787.368 ± 2.347**				Ca^{2+} + H_2(cit)$^-$ ⇄ CaH_2(cit)$^+$	1.530 ± 0.160 [2005HUM/AND]	-8.733 ± 0.913 [2005HUM/AND]		
Ca_3(cit)$_2$·4H_2O(cr)	**-5033.791 ± 4.733**				3 Ca^{2+} 4 H_2O(l) + 2 (cit)$^{3-}$ ⇄ Ca_3(cit)$_2$·4H_2O(cr)	17.900 ± 0.100 [2005HUM/AND]	-102.174 ± 0.571 [2005HUM/AND]		
(edta)$^{4-}$		-1704.800 ± 3.751 [2005HUM/AND]							
H(edta)$^{3-}$		-1724.600 ± 3.718 [2005HUM/AND]			(edta)$^{4-}$ + H^+ ⇄ H(edta)$^{3-}$	11.240 ± 0.030 [2005HUM/AND]	-64.158 ± 0.171 [2005HUM/AND]	-19.800 ± 0.500 [2005HUM/AND]	148.779 ± 1.773 [2005HUM/AND]
H_2(edta)$^{2-}$		-1739.800 ± 3.696 [2005HUM/AND]			H(edta)$^{3-}$ + H^+ ⇄ H_2(edta)$^{2-}$	6.800 ± 0.020 [2005HUM/AND]	-38.815 ± 0.114 [2005HUM/AND]	-15.200 ± 0.400 [2005HUM/AND]	79.204 ± 1.395 [2005HUM/AND]
H_3(edta)$^-$		-1732.700 ± 3.674 [2005HUM/AND]			H_2(edta)$^{2-}$ + H^+ ⇄ H_3(edta)$^-$	3.150 ± 0.020 [2005HUM/AND]	-17.980 ± 0.114 [2005HUM/AND]	7.100 ± 0.400 [2005HUM/AND]	84.120 ± 1.395 [2005HUM/AND]
H_4(edta)(cr)		-1759.800 ± 1.500 [2005HUM/AND]			H_4(edta)(aq) ⇄ H_4(edta)(cr)	3.800 ± 0.190 [2005HUM/AND]	-21.691 ± 1.085 [2005HUM/AND]	-29.000 ± 3.000 [2005HUM/AND]	-24.516 ± 10.699 [2005HUM/AND]
H_4edta(aq)		-1730.800 ± 3.354 [2005HUM/AND]			H_3(edta)$^-$ + H^+ ⇄ H_4(edta)(aq)	2.230 ± 0.050 [2005HUM/AND]	-12.729 ± 0.285 [2005HUM/AND]	1.900 ± 1.500 [2005HUM/AND]	49.066 ± 5.121 [2005HUM/AND]

Table A24 Selected thermodynamic data for various elements with selected organics (oxalate (ox), citrate (cit), EDTA (edta) and ISA (isa)) in JAEA-TDB-RN in 2020 based on NEA Thermochemical Data Base Project [A35] (5/6)

Species / compound	$\Delta_f G^0_m$ (kJ.mol^{-1})	$\Delta_f H^0_m$ (kJ.mol^{-1})	S^0_m (J.K^{-1}.mol^{-1})	$C^0_{p,m}$ (J.K^{-1}.mol^{-1})	Reaction	$\log_{10} K°$	$\Delta_r G^0_m$ (kJ.mol^{-1})	$\Delta_r H^0_m$ (kJ.mol^{-1})	$\Delta_r S^0_m$ (J.K^{-1}.mol^{-1})
H_5edta^+					$H_4(edta)(aq) + H^+ \rightleftarrows H_5(edta)^+$	1.300 ± 0.100 [2005HUM/AND]	-7.420 ± 0.571 [2005HUM/AND]		
H_6edta^{2+}					$H_5(edta)^+ + H^+ \rightleftarrows H_6(edta)^{2+}$	-0.500 ± 0.200 [2005HUM/AND]	2.854 ± 1.142 [2005HUM/AND]		
$Ni(edta)^{2-}$		-1785.912 ± 3.873 [2005HUM/AND]			$Ni^{2+} + (edta)^{4-} \rightleftarrows Ni(edta)^{2-}$	20.540 ± 0.130 [2005HUM/AND]	-117.243 ± 0.742 [2005HUM/AND]	-26.100 ± 0.400 [2005HUM/AND]	305.696 ± 2.827 [2005HUM/AND]
$Ni(Hedta)^-$					$Ni(edta)^{2-} + H^+ \rightleftarrows NiH(edta)^-$	3.660 ± 0.160 [2005HUM/AND]	-20.891 ± 0.913 [2005HUM/AND]		
$Am(edta)^-$		-2332.100 ± 4.508 [2005HUM/AND]			$Am^{3+} + (edta)^{4-} \rightleftarrows Am(edta)^-$	19.670 ± 0.110 [2005HUM/AND]	-112.277 ± 0.628 [2005HUM/AND]	-10.600 ± 2.000 [2005HUM/AND]	341.027 ± 7.031 [2005HUM/AND]
Am(Hedta)(aq)					$Am(edta)^- + H^+ \rightleftarrows AmH(edta)(aq)$	2.170 ± 0.250 [2005HUM/AND]	-12.386 ± 1.427 [2005HUM/AND]		
$Pu(edta)^-$		-2305.290 ± 4.401 [2005HUM/AND]			$Pu^{3+} + (edta)^{4-} \rightleftarrows Pu(edta)^-$	20.180 ± 0.370 [2005HUM/AND]	-115.188 ± 2.112 [2005HUM/AND]	-8.700 ± 1.200 [2005HUM/AND]	357.163 ± 8.147 [2005HUM/AND]
Pu(Hedta)(aq)					$Pu(edta)^- + H^+ \rightleftarrows PuH(edta)(aq)$	1.840 ± 0.260 [2005HUM/AND]	-10.503 ± 1.484 [2005HUM/AND]		
Np(edta)(aq)					$Np^{4+} + (edta)^{4-} \rightleftarrows Np(edta)(aq)$	31.200 ± 0.600 [2005HUM/AND]	-178.091 ± 3.425 [2005HUM/AND]		
NpO_2edta^{3-}					$NpO_2^+ + (edta)^{4-} \rightleftarrows NpO_2(edta)^{3-}$	9.230 ± 0.130 [2005HUM/AND]	-52.685 ± 0.742 [2005HUM/AND]		
$NpO_2(Hedta)^{2-}$					$NpO_2^+ + H(edta)^3 \rightleftarrows NpO_2H(edta)^{2-}$	5.820 ± 0.110 [2005HUM/AND]	-33.221 ± 0.628 [2005HUM/AND]		
$NpO_2(H_2edta)^-$					$NpO_2^+ + H_2(edta)^{2-} \rightleftarrows NpO_2H_2(edta)^-$	4.470 ± 0.140 [2005HUM/AND]	-25.515 ± 0.799 [2005HUM/AND]		
Uedta(aq)					$U^{4+} + (edta)^{4-} \rightleftarrows U(edta)(aq)$	29.500 ± 0.200 [2005HUM/AND]	-168.387 ± 1.142 [2005HUM/AND]		
UO_2edta^{2-}					$UO_2^{2+} + (edta)^{4-} \rightleftarrows UO_2(edta)^{2-}$	13.700 ± 0.200 [2005HUM/AND]	-78.200 ± 1.142 [2005HUM/AND]		

Table A24 Selected thermodynamic data for various elements with selected organics (oxalate (ox), citrate (cit), EDTA (edta) and ISA (isa)) in JAEA-TDB-RN in 2020 based on NEA Thermochemical Data Base Project [A35] (6/6)

Species / compound	$\Delta_f G^0_m$ (kJ.mol^{-1})	$\Delta_f H^0_m$ (kJ.mol^{-1})	S^0_m (J.K^{-1}.mol^{-1})	$C^0_{p,m}$ (J.K^{-1}.mol^{-1})	Reaction	$\log_{10} K°$	$\Delta_r G^0_m$ (kJ.mol^{-1})	$\Delta_r H^0_m$ (kJ.mol^{-1})	$\Delta_r S^0_m$ (J.K^{-1}.mol^{-1})
$(UO_2)_2$edta(aq)					$2\ UO_2^{2+} + (edta)^{4-} \rightleftarrows (UO_2)_2(edta)(aq)$	20.600 ± 0.400 [2005HUM/AND]	-117.586 ± 2.283 [2005HUM/AND]		
UO_2(Hedta)$^-$					$UO_2^{2+} + H(edta)^{3-} \rightleftarrows UO_2H(edta)^-$	8.370 ± 0.100 [2005HUM/AND]	-47.776 ± 0.571 [2005HUM/AND]		
Mg(edta)$^{2-}$		-2152.000 ± 3.820 [2005HUM/AND]			$Mg^{2+} + (edta)^{4-} \rightleftarrows Mg(edta)^{2-}$	10.900 ± 0.100 [2005HUM/AND]	-62.218 ± 0.571 [2005HUM/AND]	19.800 ± 0.400 [2005HUM/AND]	275.089 ± 2.338 [2005HUM/AND]
Mg(Hedta)$^-$					$Mg(edta)^{2-} + H^+ \rightleftarrows MgH(edta)^-$	4.500 ± 0.200 [2005HUM/AND]	-25.686 ± 1.142 [2005HUM/AND]		
Ca(edta)$^{2-}$		-2270.000 ± 3.903 [2005HUM/AND]			$Ca^{2+} + (edta)^{4-} \rightleftarrows Ca(edta)^{2-}$	12.690 ± 0.060 [2005HUM/AND]	-72.435 ± 0.342 [2005HUM/AND]	-22.200 ± 0.400 [2005HUM/AND]	168.489 ± 1.766 [2005HUM/AND]
Ca(Hedta)$^-$					$Ca(edta)^{2-} + H^+ \rightleftarrows CaH(edta)^-$	3.540 ± 0.090 [2005HUM/AND]	-20.206 ± 0.514 [2005HUM/AND]		
Na(edta)$^{3-}$		-1949.140 ± 4.803 [2005HUM/AND]			$Na^+ + (edta)^{4-} \rightleftarrows Na(edta)^{3-}$	2.800 ± 0.200 [2005HUM/AND]	-15.983 ± 1.142 [2005HUM/AND]	-4.000 ± 3.000 [2005HUM/AND]	40.190 ± 10.766 [2005HUM/AND]
K(edta)$^{3-}$					$K^+ + (edta)^{4-} \rightleftarrows Na(edta)^{3-}$	1.800 ± 0.300 [2005HUM/AND]	-10.274 ± 1.712 [2005HUM/AND]		
Ca(isa)$^+$					$Ca^{2+} + (isa)^- \rightleftarrows Ca(isa)^+$	1.700 ± 0.300 [2005HUM/AND]	-9.704 ± 1.712 [2005HUM/AND]		
Ca(isa$_{-H}$)(aq)					$Ca^{2+} + (isa)^- \rightleftarrows Ca(isa_{-H})(aq) + H^+$	-10.400 ± 0.500 [2005HUM/AND]	59.364 ± 2.854 [2005HUM/AND]		

[2005HUM/AND] Hummel et al. [A35]

Table A25 Selected thermodynamic data for various elements with selected organics (oxalate (ox), citrate (cit), EDTA (edta) and ISA (isa)) in JAEA-TDB-RN in 2020 based on JAEA's project (1/8)

Values indicated by **boldface** are calculated and selected in the present report.

Species / compound	$\Delta_f G^0_m$ (kJ.mol^{-1})	$\Delta_f H^0_m$ (kJ.mol^{-1})	S^0_m (J.K^{-1}.mol^{-1})	$C^0_{p,m}$ (J.K^{-1}.mol^{-1})	Reaction	$\log_{10} K°$	$\Delta_r G^0_m$ (kJ.mol^{-1})	$\Delta_r H^0_m$ (kJ.mol^{-1})	$\Delta_r S^0_m$ (J.K^{-1}.mol^{-1})
$Na(ox)^-$	**-947.723**				$Na^+ + (ox)^{2-} \rightleftarrows Na(ox)^-$	1.000 [2010MIH]	**-5.708**		
$K(ox)^-$	**-967.733**				$K^+ + (ox)^{2-} \rightleftarrows K(ox)^-$	0.900 [2010MIH]	**-5.137**		
Sr(ox)(aq)	**-1257.270**				$Sr^{2+} + (ox)^{2-} \rightleftarrows Sr(ox)(aq)$	2.330 [2010MIH]	**-13.300**		
$Sr(ox)_2^{2-}$	**-1941.114**				$Sr^{2+} + 2\ (ox)^{2-} \rightleftarrows Sr(ox)_2^{2-}$	2.980 [2010MIH]	**-17.010**		
Ra(ox)(aq)	**-1251.584**				$Ra^{2+} + (ox)^{2-} \rightleftarrows Ra(ox)(aq)$	2.780 [2010MIH]	**-15.868**		
$Ra(ox)_2^{2-}$	**-1935.485**				$Ra^{2+} + 2\ (ox)^{2-} \rightleftarrows Ra(ox)_2^{2-}$	3.440 [2010MIH]	**-19.636**		
Fe(ox)(aq)	**-794.427**				$Fe^{2+} + (ox)^{2-} \rightleftarrows Fe(ox)(aq)$	4.130 [2010MIH]	**-23.574**		
$Fe(ox)_2^{2-}$	**-1486.548**				$Fe^{2+} + 2\ (ox)^{2-} \rightleftarrows Fe(ox)_2^{2-}$	6.230 [2010MIH]	**-35.561**		
Co(ox)(aq)	**-761.474**				$Co^{2+} + (ox)^{2-} \rightleftarrows Co(ox)(aq)$	4.720 [2010MIH]	**-26.942**		
$Co(ox)_2^{2-}$	**-1454.622**				$Co^{2+} + 2\ (ox)^{2-} \rightleftarrows Co(ox)_2^{2-}$	7.000 [2010MIH]	**-39.956**		
Pb(ox)(aq)	**-732.093**				$Pb^{2+} + 2\ (ox)^{2-} \rightleftarrows Pb(ox)(aq)$	4.910 [2010MIH]	**-28.026**		
$Pb(ox)_2^{2-}$	**-1422.787**				$Pb^{2+} + 2\ (ox)^{2-} \rightleftarrows Pb(ox)_2^{2-}$	6.760 [2010MIH]	**-38.586**		
$Al(ox)^+$	**-1211.816**				$Al^{3+} + (ox)^{2-} \rightleftarrows Al(ox)^+$	7.720 [2010MIH]	**-44.066**		
$Al(ox)_2^-$	**-1923.230**				$Al^{3+} + 2\ (ox)^{2-} \rightleftarrows Al(ox)_2^-$	13.200 [2010MIH]	**-75.346**		
$Al(ox)_3^{3-}$	**-2623.571**				$Al^{3+} + 3\ (ox)^{2-} \rightleftarrows Al(ox)_3^{3-}$	16.740 [2010MIH]	**-95.553**		
$Zr(ox)^{2+}$	**-1251.259**				$Zr^{4+} + (ox)^{2-} \rightleftarrows Zr(ox)^{2+}$	7.466 [2010MIH]	**-42.616**		
$Zr(ox)_2$(aq)	**-1974.946**				$Zr^{4+} + 2\ (ox)^{2-} \rightleftarrows Zr(ox)_2(aq)$	15.096 [2010MIH]	**-86.169**		
TcO(ox)(aq)	**-851.049**				$TcO(OH)_2(aq) + 2\ H^+ + (ox)^{2-} \rightleftarrows TcO(ox)(aq) + 2\ H_2O(l)$	13.500 [2010MIH]	**-77.059**		
$TcOH(ox)_2^{2-}$	**-1569.484**				$TcO(OH)_2(aq) + 2\ H^+ + 2\ (ox)^{2-} \rightleftarrows TcOH(ox)_2^{2-} + 2\ H_2O(l)$	20.210 [2010MIH]	**-115.360**		
$Sm(ox)^+$	**-1382.695**				$Sm^{3+} + (ox)^{2-} \rightleftarrows Sm(ox)^+$	6.300 [2010MIH]	**-35.961**		

Table A25 Selected thermodynamic data for various elements with selected organics (oxalate (ox), citrate (cit), EDTA (edta) and ISA (isa)) in JAEA-TDB-RN in 2020 based on JAEA's project (2/8)

Species / compound	$\Delta_f G^0_m$ (kJ.mol^{-1})	$\Delta_f H^0_m$ (kJ.mol^{-1})	S^0_m (J.K^{-1}.mol^{-1})	$C^0_{p,m}$ (J.K^{-1}.mol^{-1})	Reaction	$\log_{10} K°$	$\Delta_r G^0_m$ (kJ.mol^{-1})	$\Delta_r H^0_m$ (kJ.mol^{-1})	$\Delta_r S^0_m$ (J.K^{-1}.mol^{-1})
$Sm(ox)_2^-$	**-2084.690**				$Sm^{3+} + 2\ (ox)^{2-} \rightleftarrows Sm(ox)_2^-$	10.130 [2010MIH]	**-57.822**		
$Ac(ox)^+$	**-1352.536**				$Ac^{3+} + (ox)^{2-} \rightleftarrows Ac(ox)^+$	5.650 [2010MIH]	**-32.250**		
$Ac(ox)_2^-$	**-2050.651**				$Ac^{3+} + 2\ (ox)^{2-} \rightleftarrows Ac(ox)_2^-$	8.800 [2010MIH]	**-50.231**		
$Th(ox)^{2+}$	**-1445.422**				$Th^{4+} + (ox)^{2-} \rightleftarrows Th(ox)^{2+}$	10.600 [2010MIH]	**-60.505**		
$Th(ox)_2(aq)$	**-2180.353**				$Th^{4+} + 2\ (ox)^{2-} \rightleftarrows Th(ox)_2(aq)$	20.200 [2010MIH]	**-115.302**		
$Th(ox)_3^{2-}$	**-2895.877**				$Th^{4+} + 3\ (ox)^{2-} \rightleftarrows Th(ox)_3^{2-}$	26.400 [2010MIH]	**-150.692**		
$Pu(ox)^{2+}$	**-1217.143**				$Pu^{4+} + (ox)^{2-} \rightleftarrows Pu(ox)^{2+}$	10.340 [2010MIH]	**-59.021**		
$Pu(ox)_2(aq)$	**-1939.859**				$Pu^{4+} + 2\ (ox)^{2-} \rightleftarrows Pu(ox)_2(aq)$	17.800 [2010MIH]	**-101.603**		
$U(ox)^{2+}$	**-1268.102**				$U^{4+} + (ox)^{2-} \rightleftarrows U(ox)^{2+}$	10.180 [2010MIH]	**-58.108**		
$U(ox)_2(aq)$	**-1990.019**				$U^{4+} + 2\ (ox)^{2-} \rightleftarrows U(ox)_2(aq)$	17.500 [2010MIH]	**-99.891**		
$Np(ox)^{2+}$	**-1230.644**				$Np^{4+} + (ox)^{2-} \rightleftarrows Np(ox)^{2+}$	10.290 [2010MIH]	**-58.736**		
$Np(ox)_2(aq)$	**-1953.131**				$Np^{4+} + 2\ (ox)^{2-} \rightleftarrows Np(ox)_2(aq)$	17.710 [2010MIH]	**-101.089**		
$PuO_2(ox)(aq)$	**-1483.870**				$PuO_2^{2+} + (ox)^{2-} \rightleftarrows PuO_2(ox)(aq)$	7.250 [2010MIH]	**-41.383**		
$PuO_2(ox)_2^{2-}$	**-2190.775**				$PuO_2^{2+} + 2\ (ox)^{2-} \rightleftarrows PuO_2(ox)_2^{2-}$	11.940 [2010MIH]	**-68.154**		
$Cm(ox)^+$	**-1313.266**				$Cm^{3+} + (ox)^{2-} \rightleftarrows Cm(ox)^+$	6.540 [2010MIH]	**-37.331**		
$Cm(ox)_2^-$	**-2016.404**				$Cm^{3+} + 2\ (ox)^{2-} \rightleftarrows Cm(ox)_2^-$	10.570 [2010MIH]	**-60.334**		
$Na(cit)^{2-}$	**-1431.788**				$Na^+ + (cit)^{3-} \rightleftarrows Na(cit)^{2-}$	1.340 [2010MIH]	**-7.649**		
$K(cit)^{2-}$	**-1451.741**				$K^+ + (cit)^{3-} \rightleftarrows K(cit)^{2-}$	1.230 [2010MIH]	**-7.021**		
$Sr(cit)^-$	**-1749.554**				$Sr^{2+} + (cit)^{3-} \rightleftarrows Sr(cit)^-$	4.110 [2010MIH]	**-23.460**		
$SrH(cit)(aq)$	**-1777.923**				$Sr^{2+} + H^+ + (cit)^{3-} \rightleftarrows SrH(cit)(aq)$	9.080 [2010MIH]	**-51.829**		
$Ra(cit)^-$	**-1738.331**				$Ra^{2+} + (cit)^{3-} \rightleftarrows Ra(cit)^-$	3.590 [2010MIH]	**-20.492**		
RaH(cit) (aq)	**-1769.212**				$Ra^{2+} + H^+ + (cit)^{3-} \rightleftarrows Ra(H(cit)(aq)$	9.000 [2010MIH]	**-51.372**		

Table A25 Selected thermodynamic data for various elements with selected organics (oxalate (ox), citrate (cit), EDTA (edta) and ISA (isa)) in JAEA-TDB-RN in 2020 based on JAEA's project (3/8)

Species / compound	$\Delta_f G^0_m$ (kJ.mol^{-1})	$\Delta_f H^0_m$ (kJ.mol^{-1})	S^0_m (J.K^{-1}.mol^{-1})	$C^0_{p,m}$ (J.K^{-1}.mol^{-1})	Reaction	$\log_{10} K°$	$\Delta_r G^0_m$ (kJ.mol^{-1})	$\Delta_r H^0_m$ (kJ.mol^{-1})	$\Delta_r S^0_m$ (J.K^{-1}.mol^{-1})
$Fe(cit)^-$	**-1285.456**				$Fe^{2+} + (cit)^{3-} \rightleftarrows Fe(cit)^-$	5.690 [2010MIH]	**-32.479**		
FeH(cit)(aq)	**-1309.315**				$Fe^{2+} + H^+ + (cit)^{3-} \rightleftarrows FeH(cit)(aq)$	9.870 [2010MIH]	**-56.338**		
$Co(cit)^-$	**-1252.559**				$Co^{2+} + (cit)^{3-} \rightleftarrows Co(cit)^-$	6.290 [2010MIH]	**-35.904**		
CoH(cit)(aq)	**-1275.277**				$Co^{2+} + H^+ + (cit)^{3-} \rightleftarrows CoH(cit)(aq)$	10.270 [2010MIH]	**-58.622**		
$Pb(cit)^-$	**-1218.726**				$Pb^{2+} + (cit)^{3-} \rightleftarrows Pb(cit)^-$	5.700 [2010MIH]	**-32.536**		
$Pb(cit)_2^{4-}$	**-2405.015**				$Pb^{2+} + 2\ (cit)^{3-} \rightleftarrows Pb(cit)_2^{4-}$	9.910 [2010MIH]	**-56.567**		
$Pb(cit)_3^{7-}$	**-3536.678**				$Pb^{2+} + 3\ (cit)^{3-} \rightleftarrows Pb(cit)_3^{7-}$	4.550 [2010MIH]	**-25.972**		
PbH(cit)(aq)	**-1245.611**				$Pb^{2+} + H^+ + (cit)^{3-} \rightleftarrows PbH(cit)(aq)$	10.410 [2010MIH]	**-59.421**		
Al(cit)(aq)	**-1706.441**				$Al^{3+} + (cit)^{3-} \rightleftarrows Al(cit)(aq)$	9.910 [2010MIH]	**-56.567**		
$Al(cit)_2^{3-}$	**-2892.729**				$Al^{3+} + 2\ (cit)^{3-} \rightleftarrows Al(cit)_2^{3-}$	14.120 [2010MIH]	**-80.598**		
$AlH(cit)^+$	**-1723.279**				$Al^{3+} + H^+ + (cit)^{3-} \rightleftarrows AlH(cit)^+$	12.860 [2010MIH]	**-73.405**		
$Zr(cit)^+$	**-1749.080**				$Zr^{4+} + (cit)^{3-} \rightleftarrows Zr(cit)^+$	10.216 [2010MIH]	**-58.313**		
$ZrH(cit)^{2+}$	**-1758.270**				$Zr^{4+} + H^+ + (cit)^{3-} \rightleftarrows ZrH(cit)^{2+}$	11.826 [2010MIH]	**-67.503**		
$TcO(cit)^-$	**-1347.438**				$TcO(OH)_2(aq) + 2\ H^+ + (cit)^{3-} \rightleftarrows TcO(cit)^- + 2\ H_2O(l)$	15.999 [2010MIH]	**-91.323**		
TcOH(cit)(aq)	**-1359.487**				$TcO(OH)_2(aq) + 3\ H^+ + (cit)^{3-} \rightleftarrows TcOH(cit)(aq) + 2\ H_2O(l)$	18.110 [2010MIH]	**-103.373**		
Sm(cit)(aq)	**-1874.465**				$Sm^{3+} + (cit)^{3-} \rightleftarrows Sm(cit)(aq)$	7.990 [2010MIH]	**-45.607**		
$SmH(cit)^+$	**-1895.471**				$Sm^{3+} + H^+ + (cit)^{3-} \rightleftarrows SmH(cit)^+$	11.670 [2010MIH]	**-66.613**		
Ac(cit)(aq)	**-1848.017**				$Ac^{3+} + (cit)^{3-} \rightleftarrows Ac(cit)(aq)$	7.990 [2010MIH]	**-45.607**		
$AcH(cit)^+$	**-1869.023**				$Ac^{3+} + H^+ + (cit)^{3-} \rightleftarrows AcH(cit)^+$	11.670 [2010MIH]	**-66.613**		
$Th(cit)^+$	**-1931.485**				$Th^{4+} + (cit)^{3-} \rightleftarrows Th(cit)^+$	11.290 [2010MIH]	**-64.444**		
$ThH(cit)^{2+}$	**-1945.127**				$Th^{4+} + H^+ + (cit)^{3-} \rightleftarrows ThH(cit)^{2+}$	13.680 [2010MIH]	**-78.086**		
$U(cit)^+$	**-1765.409**				$U^{4+} + (cit)^{3-} \rightleftarrows U(cit)^+$	12.840 [2010MIH]	**-73.291**		

Table A25 Selected thermodynamic data for various elements with selected organics (oxalate (ox), citrate (cit), EDTA (edta) and ISA (isa)) in JAEA-TDB-RN in 2020 based on JAEA's project (4/8)

Species / compound	$\Delta_f G^0_m$ (kJ.mol^{-1})	$\Delta_f H^0_m$ (kJ.mol^{-1})	S^0_m (J.K^{-1}.mol^{-1})	$C^0_{p,m}$ (J.K^{-1}.mol^{-1})	Reaction	$\log_{10} K°$	$\Delta_r G^0_m$ (kJ.mol^{-1})	$\Delta_r H^0_m$ (kJ.mol^{-1})	$\Delta_r S^0_m$ (J.K^{-1}.mol^{-1})
$UH(cit)^{2+}$	**-1775.570**				$U^{4+} + H^+ + (cit)^{3-} \rightleftarrows UH(cit)^{2+}$	14.620 [2010MIH]	**-83.452**		
$Np(cit)^+$	**-1728.122**				$Np^{4+} + (cit)^{3-} \rightleftarrows Np(cit)^+$	12.980 [2010MIH]	**-74.090**		
$NpH(cit)^{2+}$	**-1737.997**				$Np^{4+} + H^+ + (cit)^{3-} \rightleftarrows NpH(cit)^{2+}$	14.710 [2010MIH]	**-83.965**		
$NpO_2H(cit)^-$	**-2126.647**				$NpO_2^+ + H^+ + (cit)^{3-} \rightleftarrows NpO_2H(cit)^-$	9.920 [2010MIH]	**-56.624**		
$Pu(cit)^+$	**-1714.679**				$Pu^{4+} + (cit)^{3-} \rightleftarrows Pu(cit)^+$	13.040 [2010MIH]	**-74.433**		
$PuH(cit)^{2+}$	**-1724.440**				$Pu^{4+} + H^+ + (cit)^{3-} \rightleftarrows PuH(cit)^{2+}$	14.750 [2010MIH]	**-84.194**		
Pu(cit)(aq)	**-1786.849**				$Pu^{3+} + (cit)^{3-} \rightleftarrows Pu(cit)(aq)$	7.990 [2010MIH]	**-45.607**		
$PuH(cit)^+$	**-1807.855**				$Pu^{3+} + H^+ + (cit)^{3-} \rightleftarrows PuH(cit)^+$	11.670 [2010MIH]	**-66.613**		
$PuO_2(cit)^-$	**-1977.011**				$PuO_2^{2+} + (cit)^{3-} \rightleftarrows PuO_2(cit)^-$	9.180 [2010MIH]	**-52.400**		
$PuO_2H(cit)(aq)$	**-1995.391**				$PuO_2^{2+} + H^+ + (cit)^{3-} \rightleftarrows PuO_2H(cit)(aq)$	12.400 [2010MIH]	**-70.780**		
Cm(cit)(aq)	**-1803.667**				$Cm^{3+} + (cit)^{3-} \rightleftarrows Cm(cit)(aq)$	7.990 [2010MIH]	**-45.607**		
$CmH(cit)^+$	**-1824.672**				$Cm^{3+} + H^+ + (cit)^{3-} \rightleftarrows CmH(cit)^+$	11.670 [2010MIH]	**-66.613**		
$Sr(edta)^{2-}$					$Sr^{2+} + (edta)^{4-} \rightleftarrows Sr(edta)^{2-}$	10.460 [2010MIH]	**-59.706**		
$SrH(edta)^-$					$Sr^{2+} + H^+ + (edta)^{4-} \rightleftarrows SrH(edta)^-$	14.820 [2010MIH]	**-84.593**		
$Fe(edta)^{2-}$					$Fe^{2+} + (edta)^{4-} \rightleftarrows Fe(edta)^{2-}$	16.020 [2010MIH]	**-91.443**		
$FeH(edta)^-$					$Fe^{2+} + H^+ + (edta)^{4-} \rightleftarrows FeH(edta)^-$	19.250 [2010MIH]	**-109.880**		
$Co(edta)^{2-}$					$Co^{2+} + (edta)^{4-} \rightleftarrows Co(edta)^{2-}$	18.170 [2010MIH]	**-103.715**		
$CoH(edta)^-$					$Co^{2+} + H^+ + (edta)^{4-} \rightleftarrows CoH(edta)^-$	21.600 [2010MIH]	**-123.294**		
$CoH_2(edta)(aq)$					$Co^{2+} + 2\,H^+ + (edta)^{4-} \rightleftarrows CoH_2(edta)(aq)$	23.570 [2010MIH]	**-134.539**		
$Pb(edta)^{2-}$					$Pb^{2+} + (edta)^{4-} \rightleftarrows Pb(edta)^{2-}$	19.680 [2010MIH]	**-112.334**		
$PbH(edta)^-$					$Pb^{2+} + H^+ + (edta)^{4-} \rightleftarrows PbH(edta)^-$	22.610 [2010MIH]	**-129.059**		

Table A25 Selected thermodynamic data for various elements with selected organics (oxalate (ox), citrate (cit), EDTA (edta) and ISA (isa)) in JAEA-TDB-RN in 2020 based on JAEA's project (5/8)

Species / compound	$\Delta_f G^0_m$ (kJ.mol^{-1})	$\Delta_f H^0_m$ (kJ.mol^{-1})	S^0_m (J.K^{-1}.mol^{-1})	$C^0_{p,m}$ (J.K^{-1}.mol^{-1})	Reaction	$\log_{10} K°$	$\Delta_r G^0_m$ (kJ.mol^{-1})	$\Delta_r H^0_m$ (kJ.mol^{-1})	$\Delta_r S^0_m$ (J.K^{-1}.mol^{-1})
$PbH_2(edta)(aq)$					$Pb^{2+} + 2\ H^+ + (edta)^{4-} \rightleftarrows PbH_2(edta)(aq)$	24.570 [2010MIH]	**-140.247**		
$PbH_3(edta)^+$					$Pb^{2+} + 3\ H^+ + (edta)^{4-} \rightleftarrows PbH_3(edta)^+$	25.770 [2010MIH]	**-147.096**		
$Th(edta)(aq)$					$Th^{4+} + (edta)^{4-} \rightleftarrows Th(edta)(aq)$	26.630 [2010MIH]	**-152.005**		
$ThH(edta)^+$					$Th^{4+} + H^+ + (edta)^{4-} \rightleftarrows ThH(edta)^+$	28.610 [2010MIH]	**-163.307**		
$PuOH(edta)^-$					$Pu^{4+} + (edta)^{4-} + H_2O \rightleftarrows PuOH(edta)^- + H^+$	24.200 [2010MIH]	**-138.135**		
$Pu(OH)_2(edta)^{2-}$					$Pu^{4+} + (edta)^{4-} + 2\ H_2O \rightleftarrows Pu(OH)_2(edta)^{2-} + 2\ H^+$	19.220 [2010MIH]	**-109.709**		
$Pu(OH)_3(edta)^{3-}$					$Pu^{4+} + (edta)^{4-} + 3\ H_2O \rightleftarrows Pu(OH)_3(edta)^{3-} + 3\ H^+$	9.710 [2010MIH]	**-55.425**		
$H(isa)(aq)$					$H^+ + (isa)^- \rightleftarrows H(isa)(aq)$	3.270 ± 0.010 [2016RAI/KIT]	**-18.665** **± 0.057**		
$(isl)(aq)$					$H(isa)(aq)^- \rightleftarrows (isl)(aq) + H_2O(l)$	0.490 ± 0.090 [2016RAI/KIT]	**-2.797** **± 0.514**		
$(isa)^-$					$(isl)(aq) + H_2O(l) \rightleftarrows (isa)^- + H^+$	-3.760 ± 0.090 [2016RAI/KIT]	**21.462** **± 0.514**		
$Ca(isa)_2(cr)$					$Ca^{2+} + 2\ (isa)^- \rightleftarrows Ca(isa)_2(cr)$	6.400 ± 0.090 [2016RAI/KIT]	**-36.531** **± 0.514**		
$Fe(isa)^+$					$Fe^{2+} + (isa)^- \rightleftarrows Fe(isa)^+$	6.200 [2017RAI/KIT]	**-35.390**		
$Fe(isa)_2^+$					$Fe^{3+} + 2\ (isa)^- \rightleftarrows Fe(isa)_2^+$	10.410 [2017RAI/KIT]	**-59.421**		
$Fe(isa)_3(aq)$					$Fe^{3+} + 3\ (isa)^- \rightleftarrows Fe(isa)_3(aq)$	13.100 [2017RAI/KIT]	**-74.775**		
$Fe(isa)_4^-$					$Fe^{3+} + 4\ (isa)^- \rightleftarrows Fe(isa)_4^-$	15.090 [2017RAI/KIT]	**-86.134**		
$Fe(OH)_2(isa)(aq)$					$Fe^{3+} + (isa)^- + 2\ H_2O(l) \rightleftarrows Fe(OH)_2(isa)(aq) + 2\ H^+$	1.900 ± 0.900 [2017RAI/KIT]	**-10.845** **± 5.137**		
$Fe(OH)_3(isa)_2^{2-}$					$Fe^{3+} + 2\ (isa)^- + 3\ H_2O(l) \rightleftarrows Fe(OH)_3(isa)_2^{2-} + 3\ H^+$	-3.270 ± 0.320 [2017RAI/KIT]	**18.665** **± 1.827**		
$NiOH(isa)(aq)$					$Ni^{2+} + H_2O(l) + (isa)^- \rightleftarrows NiOH(isa)(aq) + H^+$	-6.500 ± 0.300 [2018GON/GAO]	**37.102** **± 1.712**		

Table A25 Selected thermodynamic data for various elements with selected organics (oxalate (ox), citrate (cit), EDTA (edta) and ISA (isa)) in JAEA-TDB-RN in 2020 based on JAEA's project (6/8)

Species / compound	$\Delta_f G^0_m$ (kJ.mol^{-1})	$\Delta_f H^0_m$ (kJ.mol^{-1})	S^0_m (J.K^{-1}.mol^{-1})	$C^0_{p,m}$ (J.K^{-1}.mol^{-1})	Reaction	$\log_{10} K°$	$\Delta_r G^0_m$ (kJ.mol^{-1})	$\Delta_r H^0_m$ (kJ.mol^{-1})	$\Delta_r S^0_m$ (J.K^{-1}.mol^{-1})
$Ni(OH)_2(isa)^-$					$Ni^{2+} + 2\ H_2O(l) + (isa)^- \rightleftarrows Ni(OH)_2(isa)^- + 2\ H^+$	-17.600	**100.462**		
						± 0.500	**± 2.854**		
						[2018GON/GAO]			
$Ni(OH)_3(isa)^{2-}$					$Ni^{2+} + 3\ H_2O(l) + (isa)^- \rightleftarrows Ni(OH)_3(isa)^{2-} + 3\ H^+$	-31.000	**176.949**		
						± 0.700	**± 3.996**		
						[2018GON/GAO]			
$Zr(OH)_4(isa)_2^{2-}$					$Zr^{4+} + 4\ H_2O(l) + 2\ (isa)^- \rightleftarrows Zr(OH)_4(isa)_2^{2-} + 4\ H^+$	-2.554	**14.578**		
						± 0.135	**± 0.771**		
						[2017KOB/SAS]			
$Zr(OH)_4(isa)(isa_{-H})^{3-}$					$Zr^{4+} + 5\ H_2O(l) + 2\ (isa)^- \rightleftarrows Zr(OH)_4(isa)(isa_{-H})^{3-} + 5\ H^+$	-15.155	**86.505**		
						± 0.142	**± 0.811**		
						[2017KOB/SAS]			
$Sm(OH)_3(isa)^-$					$Sm^{3+} + 3\ H_2O(l) + (isa)^- \rightleftarrows Sm(OH)_3(isa)^- + 3\ H^+$	-21.400	**122.152**		
						± 2.000	**± 11.416**		
						[2019KIT]			
$Sm(isa)^{2+}$					$Sm^{3+} + (isa)^- \rightleftarrows Sm(isa)^{2+}$	4.030	**-23.003**		
						± 0.560	**± 3.197**		
						[2019KIT]			
$Sm(isa)_2^+$					$Sm^{3+} + 2\ (isa)^- \rightleftarrows Sm(isa)_2^+$	7.640	**-43.609**		
						± 0.260	**± 1.484**		
						[2019KIT]			
$ThOH(isa)^{2+}$					$Th^{4+} + H_2O(l) + (isa)^- \rightleftarrows ThOH(isa)^{2+} + H^+$	3.200	**-18.266**		
						± 0.500	**± 2.854**		
						[2017RAI/KIT]			
$Th(OH)_3(isa)_2^-$					$Th^{4+} + 3\ H_2O(l) + 2\ (isa)^- \rightleftarrows Th(OH)_3(isa)_2^- + 3\ H^+$	-4.900	**27.969**		
						± 0.500	**± 2.854**		
						[2017RAI/KIT]			
$Th(OH)_4(isa)_2^{2-}$					$Th^{4+} + 4\ H_2O(l) + 2\ (isa)^- \rightleftarrows Th(OH)_4(isa)_2^{2-} + 4\ H^+$	-12.500	**71.351**		
						± 0.500	**± 2.854**		
						[2017RAI/KIT]			
$U(OH)_4(isa)^-$					$U^{4+} + 4\ H_2O(l) + (isa)^- \rightleftarrows U(OH)_4(isa)^- + 4\ H^+$	-7.581	**43.271**		
						± 0.490	**± 2.796**		
						[2019KOB/SAS]			
$U(OH)_4(isa)_2^{2-}$					$U^{4+} + 4\ H_2O(l) + 2\ (isa)^- \rightleftarrows U(OH)_4(isa)_2^{2-} + 4\ H^+$	-5.381	**30.714**		
						± 0.190	**± 1.083**		
						[2019KOB/SAS]			
$UO_2(isa)^+$					$UO_2^{2+} + ISA^- \rightleftarrows UO_2(isa)^+$	3.670	**-20.949**		
						± 0.190	**± 1.085**		
						[2017RAI/KIT]			

Table A25 Selected thermodynamic data for various elements with selected organics (oxalate (ox), citrate (cit), EDTA (edta) and ISA (isa)) in JAEA-TDB-RN in 2020 based on JAEA's project (7/8)

Species / compound	$\Delta_f G^0_m$ (kJ.mol^{-1})	$\Delta_f H^0_m$ (kJ.mol^{-1})	S^0_m (J.K^{-1}.mol^{-1})	$C^0_{p,m}$ (J.K^{-1}.mol^{-1})	Reaction	$\log_{10} K°$	$\Delta_r G^0_m$ (kJ.mol^{-1})	$\Delta_r H^0_m$ (kJ.mol^{-1})	$\Delta_r S^0_m$ (J.K^{-1}.mol^{-1})
$UO_2(isa)_2(aq)$					$UO_2^{2+} + 2\ ISA^- \rightleftarrows UO_2(isa)_2(aq)$	6.400	**-36.531**		
						± 0.080	**± 0.457**		
						[2017RAI/KIT]			
$UO_2(isa)_3^-$					$UO_2^{2+} + 3\ ISA^- \rightleftarrows UO_2(isa)_3^-$	8.280	**-47.263**		
						± 0.200	**± 1.142**		
						[2017RAI/KIT]			
$UO_2(OH)_3(isa)_2^{3-}$					$UO_2^{2+} + 3\ H_2O(l) + 2\ (isa)^- \rightleftarrows UO_2(OH)_3(isa)_2^{3-} + 3\ H^+$	-14.486	**82.684**		
						± 0.167	**± 0.955**		
						[2019KOB/SAS]			
$Np(OH)_3(isa)(aq)$					$Np^{4+} + 3\ H_2O(l) + (isa)^- \rightleftarrows Np(OH)_3(isa)(aq) + 3\ H^+$	3.270	**-18.665**		
						± 0.620	**± 3.539**		
						[2017RAI/KIT]			
$Np(OH)_3(isa)_2^-$					$Np^{4+} + 3\ H_2O(l) + 2\ (isa)^- \rightleftarrows Np(OH)_3(isa)_2^- + 3\ H^+$	5.380	**-30.709**		
						± 0.620	**± 3.539**		
						[2017RAI/KIT]			
$Np(OH)_4(isa)^-$					$Np^{4+} + 4\ H_2O(l) + (isa)^- \rightleftarrows Np(OH)_4(isa)^- + 4\ H^+$	-4.060	**23.175**		
						± 0.620	**± 3.539**		
						[2017RAI/KIT]			
$Np(OH)_4(isa)_2^{2-}$					$Np^{4+} + 4\ H_2O(l) + 2\ (isa)^- \rightleftarrows Np(OH)_4(isa)_2^{2-} + 4\ H^+$	-2.200	**12.558**		
						± 0.620	**± 3.539**		
						[2017RAI/KIT]			
$Pu(OH)_3(isa)^-$					$Pu^{3+} + 3\ H_2O(l) + (isa)^- \rightleftarrows Pu(OH)_3(isa)^- + 3\ H^+$	-21.400	**122.152**		
						± 2.000	**± 11.416**		
						[2019KIT]			
$Pu(isa)^{2+}$					$Pu^{3+} + (isa)^- \rightleftarrows Pu(isa)^{2+}$	4.030	**-23.003**		
						± 0.560	**± 3.197**		
						[2019KIT]			
$Pu(isa)_2^+$					$Pu^{3+} + 2\ (isa)^- \rightleftarrows Pu(isa)_2^+$	7.640	**-43.609**		
						± 0.260	**± 1.484**		
						[2019KIT]			
$Pu(OH)_4(isa)^-$					$Pu^{4+} + 4\ H_2O(l) + (isa)^- \rightleftarrows Pu(OH)_4(isa)^- + 4\ H^+$	-0.690	**3.939**		
						± 0.430	**± 2.454**		
						[2017RAI/KIT]			
$Pu(OH)_4(isa)_2^{2-}$					$Pu^{4+} + 4\ H_2O(l) + 2\ (isa)^- \rightleftarrows Pu(OH)_4(isa)_2^{2-} + 4\ H^+$	3.150	**-17.980**		
						± 0.430	**± 2.454**		
						[2017RAI/KIT]			
$Am(OH)_3(isa)^-$					$Am^{3+} + 3\ H_2O(l) + (isa)^- \rightleftarrows Am(OH)_3(isa)^- + 3\ H^+$	-21.400	**122.152**		
						± 2.000	**± 11.416**		
						[2017RAI/KIT]			

Table A25 Selected thermodynamic data for various elements with selected organics (oxalate (ox), citrate (cit), EDTA (edta) and ISA (isa)) in JAEA-TDB-RN in 2020 based on JAEA's project (8/8)

Species / compound	$\Delta_f G^0_m$ (kJ.mol^{-1})	$\Delta_f H^0_m$ (kJ.mol^{-1})	S^0_m (J.K^{-1}.mol^{-1})	$C^0_{p,m}$ (J.K^{-1}.mol^{-1})	Reaction	$\log_{10} K°$	$\Delta_r G^0_m$ (kJ.mol^{-1})	$\Delta_r H^0_m$ (kJ.mol^{-1})	$\Delta_r S^0_m$ (J.K^{-1}.mol^{-1})
$Am(isa)^{2+}$					$Am^{3+} + (isa)^- \rightleftarrows Am(isa)^{2+}$	4.030	**-23.003**		
						± 0.560	**± 3.197**		
						[2017RAI/KIT]			
$Am(isa)_2^+$					$Am^{3+} + 2\ (isa)^- \rightleftarrows Am(isa)_2^+$	7.640	**-43.609**		
						± 0.260	**± 1.484**		
						[2017RAI/KIT]			
$Cm(OH)_3(isa)^-$					$Cm^{3+} + 3\ H_2O(l) + (isa)^- \rightleftarrows Cm(OH)_3(isa)^- + 3\ H^+$	-21.400	**122.152**		
						± 2.000	**± 11.416**		
						[2019KIT]			
$Cm(isa)^{2+}$					$Cm^{3+} + (isa)^- \rightleftarrows Cm(isa)^{2+}$	4.030	**-23.003**		
						± 0.560	**± 3.197**		
						[2019KIT]			
$Cm(isa)_2^+$					$Cm^{3+} + 2\ (isa)^- \rightleftarrows Cm(isa)_2^+$	7.640	**-43.609**		
						± 0.260	**± 1.484**		
						[2019KIT]			

[2010MIH] Mihara [A37)]
[2017KOB/SAS] Kobayashi et al. [A38)]
[2017RAI/KIT] Rai and Kitamura [A39)]
[2018GON/GAO] González-Siso et al. [A40)]
[2019KIT] Kitamura [A41)]
[2019KOB/SAS] Kobayashi et al. [A42)]

国際単位系（SI）

表１．SI 基本単位

基本量	SI 基本単位	
	名称	記号
長さ	メートル	m
質量	キログラム	kg
時間	秒	s
電流	アンペア	A
熱力学温度	ケルビン	K
物質量	モル	mol
光度	カンデラ	cd

表２．基本単位を用いて表されるSI組立単位の例

組立量	SI 組立単位	
	名称	記号
面積	平方メートル	m^2
体積	立方メートル	m^3
速さ，速度	メートル毎秒	m/s
加速度	メートル毎秒毎秒	m/s^2
波数	毎メートル	m^{-1}
密度，質量密度	キログラム毎立方メートル	kg/m^3
面積密度	キログラム毎平方メートル	kg/m^2
比体積	立方メートル毎キログラム	m^3/kg
電流密度	アンペア毎平方メートル	A/m^2
磁界の強さ	アンペア毎メートル	A/m
量濃度(a)，濃度	モル毎立方メートル	mol/m^3
質量濃度	キログラム毎立方メートル	kg/m^3
輝度	カンデラ毎平方メートル	cd/m^2
屈折率(b)	（数字の） 1	1
比透磁率(b)	（数字の） 1	1

(a) 量濃度（amount concentration）は臨床化学の分野では物質濃度（substance concentration）ともよばれる。
(b) これらは無次元量あるいは次元１をもつ量であるが、そのことを表す単位記号である数字の１は通常は表記しない。

表３．固有の名称と記号で表されるSI組立単位

組立量	SI 組立単位			
	名称	記号	他のSI単位による表し方	SI基本単位による表し方
平面角	ラジアン(b)	rad	1 (b)	m/m
立体角	ステラジアン(b)	sr(c)	1 (b)	m^2/m^2
周波数	ヘルツ(d)	Hz		s^{-1}
力	ニュートン	N		$m\ kg\ s^{-2}$
圧力，応力	パスカル	Pa	N/m^2	$m^{-1}\ kg\ s^{-2}$
エネルギー，仕事，熱量	ジュール	J	N m	$m^2\ kg\ s^{-2}$
仕事率，工率，放射束	ワット	W	J/s	$m^2\ kg\ s^{-3}$
電荷，電気量	クーロン	C		s A
電位差（電圧），起電力	ボルト	V	W/A	$m^2\ kg\ s^{-3}\ A^{-1}$
静電容量	ファラド	F	C/V	$m^{-2}\ kg^{-1}\ s^4\ A^2$
電気抵抗	オーム	Ω	V/A	$m^2\ kg\ s^{-3}\ A^{-2}$
コンダクタンス	ジーメンス	S	A/V	$m^{-2}\ kg^{-1}\ s^3\ A^2$
磁束	ウエーバ	Wb	Vs	$m^2\ kg\ s^{-2}\ A^{-1}$
磁束密度	テスラ	T	Wb/m^2	$kg\ s^{-2}\ A^{-1}$
インダクタンス	ヘンリー	H	Wb/A	$m^2\ kg\ s^{-2}\ A^{-2}$
セルシウス温度	セルシウス度(e)	℃		K
光束	ルーメン	lm	cd sr(c)	cd
照度	ルクス	lx	lm/m^2	m^{-2} cd
放射性核種の放射能(f)	ベクレル(d)	Bq		s^{-1}
吸収線量，比エネルギー分与，カーマ	グレイ	Gy	J/kg	$m^2\ s^{-2}$
線量当量，周辺線量当量，方向性線量当量，個人線量当量	シーベルト(g)	Sv	J/kg	$m^2\ s^{-2}$
酸素活性	カタール	kat		s^{-1} mol

(a)SI接頭語は固有の名称と記号を持つ組立単位と組み合わせても使用できる。しかし接頭語を付した単位はもはやコヒーレントではない。
(b)ラジアンとステラジアンは数字の１に対する単位の特別な名称で、量についての情報をつたえるために使われる。実際には、使用する時には記号radおよびsrが用いられるが、習慣として組立単位としての記号である数字の１は明示されない。
(c)測光学ではステラジアンという名称と記号srを単位の表し方の中に、そのまま維持している。
(d)ヘルツは周期現象についてのみ、ベクレルは放射性核種の統計的過程についてのみ使用される。
(e)セルシウス度はケルビンの特別な名称で、セルシウス温度を表すために使用される。セルシウス度とケルビンの単位の大きさは同一である。したがって、温度差や温度間隔を表す数値はどちらの単位で表しても同じである。
(f)放射性核種の放射能（activity referred to a radionuclide）は、しばしば誤った用語で"radioactivity"と記される。
(g)単位シーベルト（PV,2002,70,205）についてはCIPM勧告2（CI-2002）を参照。

表４．単位の中に固有の名称と記号を含むSI組立単位の例

組立量	SI 組立単位		
	名称	記号	SI 基本単位による表し方
粘度	パスカル秒	Pa s	$m^{-1}\ kg\ s^{-1}$
力のモーメント	ニュートンメートル	N m	$m^2\ kg\ s^{-2}$
表面張力	ニュートン毎メートル	N/m	$kg\ s^{-2}$
角速度	ラジアン毎秒	rad/s	$m\ m^{-1}\ s^{-1}=s^{-1}$
角加速度	ラジアン毎秒毎秒	rad/s^2	$m\ m^{-1}\ s^{-2}=s^{-2}$
熱流密度，放射照度	ワット毎平方メートル	W/m^2	$kg\ s^{-3}$
熱容量，エントロピー	ジュール毎ケルビン	J/K	$m^2\ kg\ s^{-2}\ K^{-1}$
比熱容量，比エントロピー	ジュール毎キログラム毎ケルビン	J/(kg K)	$m^2\ s^{-2}\ K^{-1}$
比エネルギー	ジュール毎キログラム	J/kg	$m^2\ s^{-2}$
熱伝導率	ワット毎メートル毎ケルビン	W/(m K)	$m\ kg\ s^{-3}\ K^{-1}$
体積エネルギー	ジュール毎立方メートル	J/m^3	$m^{-1}\ kg\ s^{-2}$
電界の強さ	ボルト毎メートル	V/m	$m\ kg\ s^{-3}\ A^{-1}$
電荷密度	クーロン毎立方メートル	C/m^3	m^{-3} s A
表面電荷	クーロン毎平方メートル	C/m^2	m^{-2} s A
電束密度，電気変位	クーロン毎平方メートル	C/m^2	m^{-2} s A
誘電率	ファラド毎メートル	F/m	$m^{-3}\ kg^{-1}\ s^4\ A^2$
透磁率	ヘンリー毎メートル	H/m	$m\ kg\ s^{-2}\ A^{-2}$
モルエネルギー	ジュール毎モル	J/mol	$m^2\ kg\ s^{-2}\ mol^{-1}$
モルエントロピー，モル熱容量	ジュール毎モル毎ケルビン	J/(mol K)	$m^2\ kg\ s^{-2}\ K^{-1}\ mol^{-1}$
照射線量（X線及びγ線）	クーロン毎キログラム	C/kg	kg^{-1} s A
吸収線量率	グレイ毎秒	Gy/s	$m^2\ s^{-3}$
放射強度	ワット毎ステラジアン	W/sr	$m^4\ m^{-2}\ kg\ s^{-3}=m^2\ kg\ s^{-3}$
放射輝度	ワット毎平方メートル毎ステラジアン	$W/(m^2\ sr)$	$m^2\ m^{-2}\ kg\ s^{-3}=kg\ s^{-3}$
酵素活性濃度	カタール毎立方メートル	kat/m^3	$m^{-3}\ s^{-1}$ mol

表５．SI 接頭語

乗数	名称	記号	乗数	名称	記号
10^{24}	ヨタ	Y	10^{-1}	デシ	d
10^{21}	ゼタ	Z	10^{-2}	センチ	c
10^{18}	エクサ	E	10^{-3}	ミリ	m
10^{15}	ペタ	P	10^{-6}	マイクロ	μ
10^{12}	テラ	T	10^{-9}	ナノ	n
10^9	ギガ	G	10^{-12}	ピコ	p
10^6	メガ	M	10^{-15}	フェムト	f
10^3	キロ	k	10^{-18}	アト	a
10^2	ヘクト	h	10^{-21}	ゼプト	z
10^1	デカ	da	10^{-24}	ヨクト	y

表６．SIに属さないが、SIと併用される単位

名称	記号	SI 単位による値
分	min	1 min=60 s
時	h	1 h =60 min=3600 s
日	d	1 d=24 h=86 400 s
度	°	1°=(π/180) rad
分	’	1’=(1/60)°=(π/10 800) rad
秒	”	1”=(1/60)’=(π/648 000) rad
ヘクタール	ha	1 ha=1 $hm^2=10^4m^2$
リットル	L, l	1 L=1 l=1 $dm^3=10^3cm^3=10^{-3}m^3$
トン	t	1 t=10^3 kg

表７．SIに属さないが、SIと併用される単位で、SI単位で表される数値が実験的に得られるもの

名称	記号	SI 単位で表される数値
電子ボルト	eV	1 eV=1.602 176 53(14)×10^{-19}J
ダルトン	Da	1 Da=1.660 538 86(28)×10^{-27}kg
統一原子質量単位	u	1 u=1 Da
天文単位	ua	1 ua=1.495 978 706 91(6)×10^{11}m

表８．SIに属さないが、SIと併用されるその他の単位

名称	記号	SI 単位で表される数値
バール	bar	1 bar=0.1MPa=100 kPa=10^5Pa
水銀柱ミリメートル	mmHg	1 mmHg≈133.322Pa
オングストローム	Å	1 Å=0.1nm=100pm=10^{-10}m
海里	M	1 M=1852m
バーン	b	1 b=100fm^2=$(10^{-12}cm)^2$=$10^{-28}m^2$
ノット	kn	1 kn=(1852/3600)m/s
ネーパ	Np	SI単位との数値的な関係は、対数量の定義に依存。
ベル	B	
デシベル	dB	

表９．固有の名称をもつCGS組立単位

名称	記号	SI 単位で表される数値
エルグ	erg	1 erg=10^{-7} J
ダイン	dyn	1 dyn=10^{-5}N
ポアズ	P	1 P=1 dyn s cm^{-2}=0.1Pa s
ストークス	St	1 St =1$cm^2\ s^{-1}$=$10^{-4}m^2\ s^{-1}$
スチルブ	sb	1 sb =1cd cm^{-2}=10^4cd m^{-2}
フォト	ph	1 ph=1cd sr cm^{-2} =10^4lx
ガル	Gal	1 Gal =1cm s^{-2}=$10^{-2}ms^{-2}$
マクスウエル	Mx	1 Mx = 1G cm^2=10^{-8}Wb
ガウス	G	1 G =1Mx cm^{-2} =10^{-4}T
エルステッド(a)	Oe	1 Oe ≙ $(10^3/4\pi)$A m^{-1}

(a) ３元系のCGS単位系とSIでは直接比較できないため、等号「 ≙ 」は対応関係を示すものである。

表10．SIに属さないその他の単位の例

名称	記号	SI 単位で表される数値
キュリー	Ci	1 Ci=3.7×10^{10}Bq
レントゲン	R	1 R = 2.58×10^{-4}C/kg
ラド	rad	1 rad=1cGy=10^{-2}Gy
レム	rem	1 rem=1 cSv=10^{-2}Sv
ガンマ	γ	1 γ=1 nT=10^{-9}T
フェルミ		1 フェルミ=1 fm=10^{-15}m
メートル系カラット		1 メートル系カラット= 0.2 g = 2×10^{-4}kg
トル	Torr	1 Torr = (101 325/760) Pa
標準大気圧	atm	1 atm = 101 325 Pa
カロリー	cal	1 cal=4.1858J（「15℃」カロリー），4.1868J（「IT」カロリー），4.184J（「熱化学」カロリー）
ミクロン	μ	1 μ =1μm=10^{-6}m

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