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JAEA Thermodynamic Database for Performance Assessment of
Geological Disposal of High-level and TRU Wastes:
Refinement of Thermodynamic Data for Trivalent Actinoids and Samarium

Akira KITAMURA, Kenso FUJIWARA and Mikazu YUI

Geological Isolation Research Unit
Geological Isolation Research and Development Directorate

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独立行政法人日本原子力研究開発機構 研究技術情報部 研究技術情報課

〒319-1195 茨城県那珂郡東海村白方白根 2 番地 4

電話 029-282-6387, Fax 029-282-5920, E-mail:ird-support@jaea.go.jp

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Tel +81-29-282-6387, Fax +81-29-282-5901, E-mail:ird-support@jaea.go.jp

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Refinement of Thermodynamic Data for Trivalent Actinoids and Samarium

Akira KITAMURA, Kenso FUJIWARA and Mikazu YUI⁺

Geological Isolation Research Unit
Geological Isolation Research and Development Directorate
Japan Atomic Energy Agency
Tokai-mura, Naka-gun, Ibaraki-ken

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Within the scope of the JAEA thermodynamic database project for performance assessment of geological disposal of high-level radioactive and TRU wastes, the refinement of the thermodynamic data for the inorganic compounds and complexes of trivalent actinoids (actinium(III), plutonium(III), americium(III) and curium(III)) and samarium(III) was carried out. Refinement of thermodynamic data for these elements was based on the thermodynamic database for americium published by the Nuclear Energy Agency in the Organisation for Economic Co-operation and Development (OECD/NEA). Based on the similarity of chemical properties among trivalent actinoids and samarium, complementary thermodynamic data for their species expected under the geological disposal conditions were selected to complete the thermodynamic data set for the performance assessment of geological disposal of radioactive wastes.

Keywords: Thermodynamic Database, Performance Assessment, Geological Disposal, High-Level Radioactive Waste, TRU Waste, Data Selection, Actinium, Plutonium(III), Americium, Curium, Samarium

⁺ Geological Isolation Research and Development Directorate

高レベルおよび TRU 廃棄物地層処分の性能評価のための JAEA 熱力学データベース：
3 価アクチノイド元素およびサマリウムの熱力学データの再選定

日本原子力研究開発機構 地層処分研究開発部門

地層処分基盤研究開発ユニット

北村 暁, 藤原 健壮, 油井 三和⁺

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高レベル放射性廃棄物および TRU 廃棄物の地層処分の性能評価に用いるための熱力学データベースの整備の一環として、3 価アクチノイド元素（アクチニウム(III)、プルトニウム(III)、アメリシウム(III)およびキュリウム(III) およびサマリウム(III)の熱力学データ選定を実施した。熱力学データ選定は、経済協力開発機構原子力機関（OECD/NEA）が公開しているアメリシウム熱力学データベースの内容を基に行った。地層処分における地下水条件のもとで存在の可能性がある化学種でありながら、これらの調査でそのデータが欠落しているものについては、3 価アクチノイドおよびサマリウムの化学挙動が類似していると考えられることを利用して、熱力学データを推定してデータベースの補完を行った。

Contents

1. Introduction	1
2. Procedure for Refinement of Thermodynamic Data for JAEA-TDB.....	4
2.1 General Approach	4
2.2 Brief Procedure of Selection of Thermodynamic Data for Trivalent Actinoids and Samarium(III)	5
3. Detailed Procedure of Selection of Thermodynamic Data for Trivalent Actinoids and Samarium(III)	6
3.1 Americium(III) and Curium(III)	6
3.2 Plutonium(III)	7
3.3 Samarium(III).....	8
3.4 Actinium(III).....	9
4. Conclusions	11
Acknowledgement.....	11
References	12

目次

1. 緒言	1
2. JAEA-TDB 整備のための基本方針	4
2.1 全体概要	4
2.2 3 価アクチノイドおよびサマリウム(III)の熱力学データ選定の概要	5
3. 3 価アクチノイドおよびサマリウム(III)の熱力学データ選定の詳細	6
3.1 アメリシウム(III)およびキュリウム(III)	6
3.2 プルトニウム(III)	7
3.3 サマリウム(III)	8
3.4 アクチニウム(III)	9
4. 結言	11
謝辞	11
参考文献	12

List of Tables

Table 1	Part of selected thermodynamic data for americium(III) by the OECD/NEA.....	15
Table 2	Part of selected thermodynamic data for plutonium(III) by the OECD/NEA	17
Table 3	Crystal radius of trivalent actinoids and samarium(III)	18
Table 4	Thermodynamic data for americium(III) selected by the authors for the JAEA-TDB	19
Table 5	Selected Gibbs free energy of formation ($\Delta_f G_m^\circ$ (kJ·mol ⁻¹)) for actinoid(III) aqua ions by the OECD/NEA and the literature by Fuger and Oetting	20
Table 6	Thermodynamic data for curium(III) selected by the authors for the JAEA-TDB.....	21
Table 7	Thermodynamic data for plutonium(III) selected by the authors for the JAEA-TDB	22
Table 8	Solubility product and hydrolysis constants for samarium(III) and actinium(III) comparing with those for americium(III) and plutonium(III) selected by the OECD/NEA	23
Table 9	Thermodynamic data for samarium(III) selected by the authors for the JAEA-TDB	24
Table 10	Stability constants of the chloride and bromide complexes of some lanthanoids and actinoids with reaction of $M^{3+} + x L^- \rightleftharpoons ML_x^{3-x}$ (x: 1 and 2) at 3.0 mol·dm ⁻³ LiCl or LiBr solutions.....	25
Table 11	Thermodynamic data for actinium(III) selected for the JAEA-TDB.....	26

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1. Introduction

Many radionuclides are contained in high-level radioactive waste (HLW) and are part of TRU waste packages, and some of them have long half-lives (more than 10^4 year). It is necessary to estimate solubility of these radionuclides in ground and pore waters in natural and engineered barriers, respectively, for performance assessment of geological disposal of HLW and some TRU wastes (e.g. hulls and ends). Thermodynamic data, e.g. the solubility product of solubility limiting solids and equilibrium constants for aqueous complexes at standard state (i.e. ionic strength of 0), are needed to estimate the solubility and aqueous species in the ground waters and pore waters: these data are fundamental to estimating sorption and diffusion behaviors on/in engineered barriers and host rocks. The chemical properties of elements of interest have been investigated, and many thermodynamic values were obtained which are considered to be more reliable than those previously available. Therefore, the latest and the most reliable thermodynamic data with transparency and traceability will be published to carry out the reliable performance assessment by an implementer or a regulator.

Eighteen elements (actinoids, fission products, radiation products and their daughters, etc.) were selected in the second progress report on research and development of geological disposal of HLW in Japan (H12) ¹⁾ by the Japan Nuclear Cycle Development Institute (JNC), which was one of the predecessors of the Japan Atomic Energy Agency (JAEA). The JNC's thermodynamic database (JNC-TDB) was developed for the performance assessment of the geological disposal in 1999 ²⁾. To develop JAEA's thermodynamic database (JAEA-TDB), thermodynamic data for more than 20 elements (not only for the performance assessment of HLW but also for that of TRU waste in geological disposal) will be selected. Selection of thermodynamic data for americium(III) in the JNC-TDB was based on the first version of TDB by the OECD/NEA ⁴⁾ with a slight modification. Thermodynamic data on samarium(III), actinium(III) and curium(III) were assumed to be the same as those for americium(III) due to insufficient experimental data for these elements and because these elements have similar ionic radii and are known to form isostructural compounds and complexes that show, where reliable data are available, similarity in the values of equilibrium constants. We consider that reasonableness of the assumption should be further discussed to enhance reliability of the TDB.

The Nuclear Energy Agency in the Organisation for Economic Co-operation and Development (OECD/NEA) has developed thermodynamic databases (NEA-TDBs) for some actinides (thorium, uranium, neptunium, plutonium and americium). All the published articles

containing experimentally determined thermodynamic values were carefully reviewed and discussed among experts gathered from all over the world. Procedure for the selection of thermodynamic data is based on the guideline “TDB-1” published by the OECD/NEA ³⁾. The first and the revised version of the TDB of americium were published in 1995 ⁴⁾ and 2003 ⁵⁾, respectively. The first and the revised version of the TDB of plutonium were published in 2001 ⁶⁾ and 2003 ⁵⁾, respectively. Although the revised version of TDB ⁵⁾ also contains some thermodynamic data for uranium(III) and neptunium(III), we will not select these data because these redox states are stable only under extremely reducing conditions and are unlikely to be stable in geological media. Selected thermodynamic data for americium(III) and plutonium(III) are listed in Table 1 and Table 2, respectively. The most enhanced thermodynamic data for trivalent actinoids are of americium(III), hence the refinement of thermodynamic data for the JAEA-TDB will be based on the thermodynamic data for americium(III) as mentioned below.

The National Cooperative for the Disposal of Radioactive Waste in Switzerland (Nagra) and the Paul Scherrer Institut (PSI) published their own TDB (Nagra/PSI-TDB) jointly in 2002 ⁷⁾. Their selection of thermodynamic data on americium(III) was based on the first version of the NEA-TDB ⁴⁾, modified with the literature data (e.g., Neck *et al.* ⁸⁾ that became available after the NEA-TDB review in 1995 and before they carried out their review in 2002. They also selected thermodynamic data for europium but their review did not address the selection of data for samarium and actinium. The update version of NEA-TDB was published later (2003), hence we did not review their selected data but referred only the Nagra/PSI-TDB.

The Swedish Nuclear Fuel and Waste Management Co. (SKB) also developed their own TDB (SKB-TDB) and published in 2006 ⁹⁾. Most of thermodynamic data were taken from the Nagra/PSI-TDB with some modifications, especially the selection of enthalpy. Selection of thermodynamic data for americium(III) and plutonium(III) was based on the Nagra/PSI-TDB, while thermodynamic data for curium(III) were assumed to be the same values as those for americium(III). It is interesting that they selected and reviewed the thermodynamic data for samarium and holmium as elements of interest in lanthanoids, but did not select actinium for review

Although the above TDBs except the JNC-TDB have not selected thermodynamic data for actinium, Ac-227, with a half-life of 21.8 y, is one of the important radionuclides as a daughter of the actinium decay series for the performance assessment of geological disposal in Japan. Therefore, we consider that thermodynamic data for actinium should be selected.

Based on the above circumstances, refinement of thermodynamic data for trivalent actinoids (actinium(III), plutonium(III), americium(III) and curium(III)) and samarium(III) (which is the only element of interest among lanthanoids in the H12 report ¹⁾) was carried out in the present report. In selecting the data for the JAEA-TDB, a great advantage was taken of the fact that these elements show analogous behavior in their thermodynamic properties and that a very comprehensive good quality data are available for Am(III), which forms the basis for filling in the data gaps for other elements in this group.

2. Procedure for Refinement of Thermodynamic Data for JAEA-TDB

2.1 General Approach

Selection of thermodynamic data for the JAEA-TDB is based on the fundamental plan ¹⁰⁾, the content of which is briefly described below.

Selection of standard Gibbs free energy of formation ($\Delta_f G_m^\circ$), equilibrium constant of reaction at standard state (K°) and standard Gibbs free energy of reaction ($\Delta_r G_m^\circ = -RT \ln K^\circ$, where R and T are gas constant and absolute temperature, respectively) is obligatory, and selection of other thermodynamic values on enthalpy, entropy and heat capacity is recommended.

Thermodynamic data for chemical compounds and species for radioelements with naturally occurring elements (e.g., halogen, oxygen, carbon, nitrogen, sulfur, phosphorus) should be selected. Thermodynamic data for elements with some organic ligands published by the OECD/NEA ¹¹⁾ may also be selected. Other thermodynamic data which are needed to select will be quoted from those called “Auxiliary Data” selected by the OECD/NEA ¹²⁾.

Review and selection of thermodynamic values obtained from experimental data should be based on the “TDB-1” guideline by the OECD/NEA ³⁾. Thermodynamic values or databases selected by the OECD/NEA ¹²⁾, the Nagra/PSI ⁷⁾ and Lothenbach *et al.* ¹³⁾, which are based on the “TDB-1” guideline ³⁾, could be selected to the JAEA-TDB after surveying the latest literature and checking consistency of the value in the database. Otherwise review and selection of thermodynamic values should be performed after surveying the literature to collect proposed thermodynamic data.

Application of chemical analogues and models should be considered to obtain thermodynamic values for some species for which there has been no published experimental data. Some unreliable thermodynamic values, which are important for the performance assessment of geological disposal of radioactive wastes, may be selected as tentative values while specifying their reliability and the needs for the values to be determined.

All thermodynamic values should be standardized at 298.15 K and at zero ionic strength, using the Brønsted-Guggenheim-Scatchard Model (usually called the “specific ion interaction theory (SIT)”) ¹²⁾ for correction of ionic strength.

2.2 Brief Procedure of Selection of Thermodynamic Data for Trivalent Actinoids and Samarium(III)

Selection of thermodynamic data for americium(III) is based on the revised version of the NEA-TDB ⁵⁾ with some slight modifications.

Thermodynamic data for curium(III) are taken from those for americium(III) without any modifications. In fact, some thermodynamic data for americium(III) are taken from (or together with) those for curium(III) in the NEA-TDB ⁵⁾. This shows that the OECD/NEA recommends applying thermodynamic data for americium(III) to curium(III).

Some thermodynamic data for samarium(III) are briefly reviewed by us. We will take thermodynamic data from those for americium(III) after discussing reasonableness of applying a chemical analogue.

Thermodynamic data for actinium(III) are tentatively selected by us based on the experimentally determined values, although the determined values are insufficient.

3. Detailed Procedure of Selection of Thermodynamic Data for Trivalent Actinoids and Samarium(III)

3.1 Americium(III) and Curium(III)

Lists of crystal ionic radius of M^{3+} (M: Sm, Ac, Pu, Am and Cm) are shown in Table 3¹⁴⁾. It is shown that the variation in ionic radius of Sm^{3+} , Pu^{3+} and Cm^{3+} against Am^{3+} is within 2 %. Assuming a Coulombic interaction as a mechanism of complexation of M^{3+} (e.g., the Hard Sphere Model¹⁵⁾), the difference in thermodynamic equilibrium constants for trivalent actinoids (except actinium due to lack of experimental data) and samarium is expected to be within the uncertainty (or error) reported in these values.. Therefore, except for actinium a chemical analogue approach should be applicable to these trivalent elements, where available reliable data for one of these elements may be subtitled for the missing data for the others..

Selection of thermodynamic data for americium(III) is based on those selected in the NEA-TDB shown in Table 1. We accepted thermodynamic data only for trivalent americium because americium would exist only in the trivalent oxidation state in the geological disposal system. Species and compounds for which the equilibrium constants ($\log_{10} K^\circ$) were not selected were excluded because they were unlikely to be useful in applying thermodynamic data to geochemical calculations. Even if the $\log_{10} K^\circ$ values are provided in the NEA-TDB, we excluded the $\log_{10} K^\circ$ values for some reactions which are not expected in geologic environments (e.g., Eq. 1 involving gaseous HCl and H₂O);



Some $\Delta_f G^\circ_m$ values were estimated by us. The $\Delta_f G^\circ_m$ for NO_2^- of $-32.200 \pm 0.100 \text{ kJ}\cdot\text{mol}^{-1}$ was derived from the NBS Table¹⁶⁾ with approximate errors added by us. Selected thermodynamic data on americium(III) for the JAEA-TDB are summarized in Table 4.

As mentioned above, some thermodynamic data for americium(III) are taken from (or together with) those for curium(III) in the NEA-TDB⁵⁾. This shows that the OECD/NEA recommends applying thermodynamic data for americium(III) to curium(III), although there are no solubility data for curium(III). Therefore, equilibrium constants for curium(III) are taken from those for americium(III) without any modifications in the JAEA-TDB.

On the other hand, Gibbs free energy of formation ($\Delta_f G^\circ_m$) for Cm^{3+} should be taken from elsewhere because it has not been selected by the OECD/NEA. We have found that

Fuger and Oetting¹⁷⁾ have thoroughly reviewed and selected thermodynamic data for actinoid (from actinium through lawrencium) elements and compounds. Some of molar enthalpies and entropies of formation for curium(III) selected by Fuger and Oetting¹⁷⁾ were accepted by the OECD/NEA. Although the $\Delta_r G_m^\circ$ values for actinoid(III) aqua ions were reevaluated in the NEA-TDB, selected values by the OECD/NEA were quite similar to those by Fuger and Oetting as shown in Table 5. Therefore, for consistency the $\Delta_r G_m^\circ$ value of Cm^{3+} ((-595.802 ± 6.276) $\text{kJ}\cdot\text{mol}^{-1}$) was taken from Fuger and Oetting¹⁷⁾. Gibbs free energies of formation for other curium(III) aqueous complexes and solid phases were determined from $\log K^\circ$ values of reactions involving these species, and Gibbs free energies of formation of Cm^{3+} and other non-curium species involved in the reactions.

Selected thermodynamic data for curium(III) for the JAEA-TDB are summarized in Table 6. Thermodynamic data of enthalpy, entropy and heat capacity were not selected in the JAEA-TDB due to insufficiency of data and models used.

3.2 Plutonium(III)

Thermodynamic data on plutonium(III) were selected by the OECD/NEA⁵⁾ as shown in Table 2. However, it is found that the selected thermodynamic data for plutonium(III) is much more limited than that for americium (compare Table 2 and Table 1). The reason for the difference is a basic policy to select thermodynamic data by the OECD/NEA, which focuses on experimental data, careful review of literature, and exclusion of unreliable data and/or conclusions. Hence selected thermodynamic data are considered to be very reliable. However, only using the selected data for plutonium(III) from the NEA-TDB may sometimes because of incompleteness of the data lead to wrong conclusions from the point of view of performance assessment.

Comparing selected equilibrium constants for plutonium(III) species and compounds to those for americium(III), it is found that the values of equilibrium constants are similar. Furthermore, the ionic radius of Pu^{3+} is quite similar to that of Am^{3+} as shown in Table 3, therefore interaction between a central ion (i.e. Am^{3+} or Pu^{3+}) and ligands is expected to be quite similar, as the comparisons of the values of equilibrium constants show. Thus equilibrium constants for americium(III) species and compounds, where the data for corresponding reactions for Pu(III) are lacking, are considered to be applicable to use for plutonium(III) reactions.

Plutonium(III) easily oxidizes to the tetravalent state. Even in the reducing conditions, oxidation state of plutonium tends to become tetravalent in basic solutions, and no

thermodynamic data for plutonium(III) carbonates and carbonate complexes ⁶⁾ are recommended by the OECD/NEA. We basically agree with the recommendation, but we select thermodynamic data for carbonate complexes and solids of plutonium(III) from the comprehensive point of view.

Gibbs free energy of formation for Pu^{3+} (-578.984 ± 2.688) $\text{kJ}\cdot\text{mol}^{-1}$) is taken from the NEA-TDB ⁵⁾. Gibbs free energies of formation of other plutonium(III) species were estimated from Gibbs free energies of formation of Pu^{3+} and other species involved in the reaction including the given species, and from $\log K^\circ$ values of the reaction.

Selected thermodynamic data on plutonium(III) for the JAEA-TDB are summarized in Table 7. Thermodynamic data of enthalpy, entropy and heat capacity were not selected in the JAEA-TDB due to insufficiency of data and models used.

3.3 Samarium(III)

The OECD/NEA has no current plans to review data for samarium(III). Some experimentally determined thermodynamic data for Sm(III) are available but the total amount of data available data for Sm(III) is far less than that for americium(III). Equilibrium constants for samarium(III) hydroxides and hydrolyses species which have been experimentally determined are shown in Table 8 as an example. Although there were some studies to determine the solubility product of $\text{Sm}(\text{OH})_3(\text{s})$ as shown in Table 8, most of the experiments were performed in a short time periods (such as half an hour) ¹⁸⁾. The short contacting time may be the reason that most of the obtained equilibrium constants for $\text{Sm}(\text{OH})_3(\text{s})$ are much lower than those for $\text{Am}(\text{OH})_3(\text{am})$.

We believe that the most reliable thermodynamic data for samarium(III) hydroxide and hydrolyses species is by Shibutani ¹⁹⁾. She conducted solubility experiments not only for $\text{Sm}(\text{OH})_3(\text{s})$ but also for $\text{SmCO}_3\text{OH}(\text{s})$ and approached the solubility from both over- and under-saturation directions. Contact time was up to 106 days. She determined solubility products and hydrolyses constants for samarium(III) as shown in Table 8, and the hydrolysis constant of $\text{Sm}(\text{OH})_2^+$ was revised afterwards due to large uncertainty ²⁰⁾. The obtained equilibrium constants were quite similar to those for americium(III) as shown in Table 4. As with plutonium(III), the ionic radius of Sm^{3+} is quite similar to that of Am^{3+} as shown in Table 3, hence interaction between a central ion (i.e. Am^{3+} or Pu^{3+}) and ligands is considered to be quite similar. Thus, equilibrium constants for americium(III) species and compounds were considered to be applicable to use for samarium(III).

Gibbs free energy of formation for Sm^{3+} ($-666.6 \text{ kJ}\cdot\text{mol}^{-1}$) was taken from the NBS Tables ¹⁶⁾ with addition of an uncertainty of the value ($1 \text{ kJ}\cdot\text{mol}^{-1}$) because neither the OECD/NEA nor the literature by Fuger and Oetting ¹⁷⁾ has selected this value.

Gibbs free energies of formation for other samarium(III) species were estimated from Gibbs free energies of formation of Sm^{3+} and other species involved in the reaction including the given species, and from $\log K^\circ$ values of the reaction.

Gibbs free energies of reaction which were easily determined from $\log K^\circ$ values.

Selected thermodynamic data on samarium(III) for the JAEA-TDB are summarized in Table 9. Thermodynamic data of enthalpy, entropy and heat capacity were not selected in the JAEA-TDB due to insufficiency of data and models used.

3.4 Actinium(III)

The OECD/NEA has no current plans to review data for actinium(III). We found only one article about the solubility of actinium(III). Ziv and Shestakova conducted solubility experiments on actinium(III) hydroxide from the oversaturation direction in $0.001 \text{ M NH}_4\text{NO}_3$ solution, and obtained a solubility product of fresh and old $\text{Ac}(\text{OH})_3(\text{s})$ (with contacting time of one hour and one week, respectively) as shown in Table 8 ²¹⁾. They found that the obtained solubility product for $\text{Ac}(\text{OH})_3(\text{s})$ is more than 4 orders of magnitude larger than that for $\text{Am}(\text{OH})_3(\text{am})$. One of the reasons may be radiation effect of α -emitters (i.e. actinium itself), but a major reason is considered to be the difference in the crystal ionic radius between Ac^{3+} (shown in Table 3) and other trivalent lanthanoid and actinoid ions. Large ionic radius may weaken Coulomb interactions between a central ion and ligands and thus destabilize solid phases. We are uncertain whether the differences in observed solubility products are a result of the experimental difficulties or truly due to the inherent differences in the chemistry of these elements. However, the study by Ziv and Shestakova ²¹⁾ was the only one for solubility of actinium(III); therefore we refer the solubility data by Ziv and Shestakova ²¹⁾ to estimate solubility product of $\text{Ac}(\text{OH})_3(\text{am})$.

On the other hand, formation constants for actinium(III) complexes may be similar to those of other trivalent lanthanoid and actinoid ions. Stability constants for actinium(III) with chloride and bromide ions were determined by Fukasawa *et al.* ²²⁾ together with some trivalent lanthanoids and actinoids by solvent extraction method as shown in Table 10 ²²⁾. It was found that differences in the values of stability constants between actinium(III) and other trivalent lanthanoids/actinoids were quite small (within 0.2). This result suggests that the effect of

crystal ionic radius is negligible in the aqueous species.

Based on above experimental observations, we decided refinement of thermodynamic data for actinium(III) as follows:

- Refinement of thermodynamic data for actinium(III) was based on those for americium(III),
- Solubility products for amorphous actinium(III) compounds ($\text{Ac}(\text{OH})_3(\text{am})$, $\text{AcPO}_4(\text{am,hydr})$, $\text{Ac}_2(\text{CO}_3)_3(\text{am})$ and $\text{AcCO}_3\text{OH}(\text{am})$) were set to the values as those for americium(III), with addition of larger uncertainties (4 order of magnitude),
- Solubility products for crystalline actinium(III) compounds were not selected due to destabilization by self α -radiation effect of actinium,
- Stability constants for actinium(III) complexes were taken from those of americium(III) with addition of larger uncertainties (0.2 order of magnitude).

Gibbs free energy of formation for Ac^{3+} ($-640.152 \pm 25.104 \text{ kJ}\cdot\text{mol}^{-1}$) was taken from Fuger and Oetting ¹⁷⁾ on the same basis as that of Cm^{3+} . Gibbs free energies of formation of complex actinium(III) species were estimated from the Gibbs free energies of formation of Ac^{3+} and of other species involved in the given reaction and from $\log K^\circ$ values of the reaction.

Selected thermodynamic data for actinium(III) for JAEA-TDB are summarized in Table 11. Thermodynamic data of enthalpy, entropy and heat capacity were not selected in the JAEA-TDB due to insufficiency of data and models used. All the obtained thermodynamic data for actinium(III) should be treated as tentative values, because the correction of values and addition of uncertainties are not quantitative.

4. Conclusions

Thermodynamic data for samarium(III), actinium(III), plutonium(III), americium(III) and curium(III) were refined on the basis of those of americium(III) from the OECD/NEA. It was found that equilibrium constants for samarium(III), plutonium(III) and curium(III) were almost the same as those for americium(III). Solubility products and stability constants for actinium(III) were set to the same mean values as those for americium(III) with addition of much larger uncertainties based on experimental observations noted in the literature. Selected thermodynamic data will be included in the JAEA-TDB, and revision of thermodynamic data will enhance reliability of thermodynamic database comparing with previous ones.

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Table 1 Part of selected thermodynamic data for americium(III) by the OECD/NEA⁵⁾

Species	$\Delta_f G_m^\circ$ (kJ·mol ⁻¹)	$\Delta_f H_m^\circ$ (kJ·mol ⁻¹)	Reaction	$\log_{10} K^\circ$	$\Delta_f G_m^\circ$ (kJ·mol ⁻¹)	$\Delta_f H_m^\circ$ (kJ·mol ⁻¹)
Am(cr)	0.000	0.000				
Am ³⁺	-598.698 ± 4.755	-616.700 ± 1.500				
Am ₂ O ₃ (cr)	-1605.449 ± 8.284	-1690.400 ± 8.000				
AmOH ²⁺	-794.740 ± 5.546		Am ³⁺ + H ₂ O(l) ⇌ AmOH ²⁺ + H ⁺	-7.200 ± 0.500	41.098 ± 2.854	
Am(OH) ₂ ⁺	-986.787 ± 6.211		Am ³⁺ + 2 H ₂ O(l) ⇌ Am(OH) ₂ ⁺ + 2 H ⁺	-15.100 ± 0.700	86.191 ± 3.996	
Am(OH) ₃ (aq)	-1160.568 ± 5.547		Am ³⁺ + 3 H ₂ O(l) ⇌ Am(OH) ₃ (aq) + 3 H ⁺	-26.200 ± 0.500	149.551 ± 2.854	
Am(OH) ₃ (am)	--		Am ³⁺ + 3 H ₂ O(l) ⇌ Am(OH) ₃ (am) + 3 H ⁺	-16.900 ± 0.800	96.466 ± 4.566	
Am(OH) ₃ (cr)	-1221.073 ± 5.861	-1353.198 ± 6.356	Am ³⁺ + 3 H ₂ O(l) ⇌ Am(OH) ₃ (cr) + 3 H ⁺	-15.600 ± 0.600	89.045 ± 3.425	
AmF ₂ ⁺	-899.628 ± 5.320		Am ³⁺ + F ⁻ ⇌ AmF ₂ ⁺	3.400 ± 0.400	-19.407 ± 2.283	
AmF ₂ ⁺	-1194.851 ± 5.082		Am ³⁺ + 2 F ⁻ ⇌ AmF ₂ ⁺	5.800 ± 0.200	-33.107 ± 1.142	
AmF ₃ (cr)	-1519.765 ± 14.126	-1594.000 ± 14.000				
AmF ₃ (g)	-1147.798 ± 16.771	-1156.500 ± 16.589	AmF ₃ (cr) ⇌ AmF ₃ (g)	--	--	437.500 ± 8.900
AmCl ²⁺	-731.285 ± 4.759		Am ³⁺ + Cl ⁻ ⇌ AmCl ²⁺	0.240 ± 0.030	-1.370 ± 0.171	
AmCl ₂ ⁺	-856.908 ± 4.769		Am ³⁺ + 2 Cl ⁻ ⇌ AmCl ₂ ⁺	-0.740 ± 0.050	4.224 ± 0.285	
AmCl ₃ (cr)	-905.105 ± 2.290	-977.800 ± 1.300				
AmOCl(cr)	-897.052 ± 6.726	-949.800 ± 6.000	AmCl ₃ (cr) + H ₂ O(g) ⇌ AmOCl(cr) + 2 HCl(g)	-8.066 ± 1.115	46.042 ± 6.364	85.213 ± 5.900
AmBr ₃ (cr)	-773.674 ± 6.728	-804.000 ± 6.000				
AmOBr(cr)	-848.485 ± 9.794	-887.000 ± 9.000	AmBr ₃ (cr) + H ₂ O(g) ⇌ AmOBr(cr) + 2 HBr(g)	-8.246 ± 2.661	47.070 ± 15.188	86.256 ± 15.000
AmI ₃ (cr)	-609.451 ± 10.068	-615.000 ± 9.000				
AmSO ₄ ⁺	-1361.538 ± 4.849		Am ³⁺ + SO ₄ ²⁻ ⇌ AmSO ₄ ⁺	3.300 ± 0.150	-18.837 ± 0.856	
Am(SO ₄) ₂ ⁻	-2107.826 ± 4.903		Am ³⁺ + 2 SO ₄ ²⁻ ⇌ Am(SO ₄) ₂ ⁻	3.700 ± 0.150	-21.120 ± 0.856	
AmN ₃ ²⁺	-260.030 ± 5.190		Am ³⁺ + N ₃ ⁻ ⇌ AmN ₃ ²⁺	1.670 ± 0.100	-9.532 ± 0.571	
AmNO ₂ ²⁺	--		Am ³⁺ + NO ₂ ⁻ ⇌ AmNO ₂ ²⁺	2.100 ± 0.200	-11.987 ± 1.142	
AmNO ₃ ²⁺	-717.083 ± 4.908		Am ³⁺ + NO ₃ ⁻ ⇌ AmNO ₃ ²⁺	1.330 ± 0.200	-7.592 ± 1.142	
AmPO ₄ (am,hydr)	--		Am ³⁺ + PO ₄ ³⁻ ⇌ AmPO ₄ (am,hydr)	24.790 ± 0.600	-141.500 ± 3.425	
AmH ₂ PO ₄ ²⁺	-1752.974 ± 5.763		Am ³⁺ + H ₂ PO ₄ ⁻ ⇌ AmH ₂ PO ₄ ²⁺	3.000 ± 0.500	-17.124 ± 2.854	

Table 1 (Continued)

Species	$\Delta_f G_m^\circ$ (kJ·mol ⁻¹)	$\Delta_f H_m^\circ$ (kJ·mol ⁻¹)	Reaction	$\log_{10} K^\circ$	$\Delta_r G_m^\circ$ (kJ·mol ⁻¹)	$\Delta_r H_m^\circ$ (kJ·mol ⁻¹)
AmCO ₃ ⁺	-1172.262 ± 5.289		Am ³⁺ + CO ₃ ²⁻ ⇌ AmCO ₃ ⁺	8.000 ± 0.400	-45.664 ± 2.283	
Am(CO ₃) ₂ ⁻	-1728.131 ± 5.911		Am ³⁺ + 2 CO ₃ ²⁻ ⇌ Am(CO ₃) ₂ ⁻	12.900 ± 0.600	-73.634 ± 3.425	
Am(CO ₃) ₃ ³⁻	-2268.018 ± 7.521		Am ³⁺ + 3 CO ₃ ²⁻ ⇌ Am(CO ₃) ₃ ³⁻	15.000 ± 1.000	-85.621 ± 5.708	
Am(CO ₃) ₅ ⁶⁻	-3210.227 ± 7.919		Am(CO ₃) ₃ ³⁻ + 2 CO ₃ ²⁻ ⇌ Am(CO ₃) ₅ ⁶⁻ + e ⁻	-20.100 ± 0.900	114.732 ± 5.137	
AmHCO ₃ ²⁺	-1203.238 ± 5.060		Am ³⁺ + HCO ₃ ⁻ ⇌ AmHCO ₃ ²⁺	3.100 ± 0.300	-17.695 ± 1.712	
Am ₂ (CO ₃) ₃ (am)	--		2 Am ³⁺ + 3 CO ₃ ²⁻ ⇌ Am ₂ (CO ₃) ₃ (am)	16.700 ± 1.100	-95.324 ± 6.279	
AmCO ₃ OH(am)	--		Am ³⁺ + CO ₃ ²⁻ + OH ⁻ ⇌ AmCO ₃ OH(am)	20.200 ± 1.000	-115.302 ± 5.708	
AmCO ₃ OH•0.5H ₂ O(cr)	-1530.248 ± 5.560	-1682.900 ± 2.600	Am ³⁺ + CO ₃ ²⁻ + 0.5 H ₂ O(l) + OH ⁻ ⇌ AmCO ₃ OH•0.5H ₂ O(cr)	22.400 ± 0.500	-127.860 ± 2.854	
AmSiO(OH) ₃ ²⁺	-1896.844 ± 5.000		Am ³⁺ + Si(OH) ₄ (aq) ⇌ AmSiO(OH) ₃ ²⁺ + H ⁺	-1.680 ± 0.180	9.590 ± 1.027	
AmSCN ²⁺	-513.418 ± 6.445		Am ³⁺ + SCN ⁻ ⇌ AmSCN ²⁺	1.300 ± 0.300	-7.420 ± 1.712	
NaAm(CO ₃) ₂ •5H ₂ O(cr)	-3222.021 ± 5.605		Am ³⁺ + 2 CO ₃ ²⁻ + 5 H ₂ O(l) + Na ⁺ ⇌ NaAm(CO ₃) ₂ •5H ₂ O(cr)	21.000 ± 0.500	-119.869 ± 2.854	
Cs ₂ NaAmCl ₆ (cr)	-2159.151 ± 4.864	-2315.800 ± 1.800				

Table 2 Part of selected thermodynamic data for plutonium(III) by the OECD/NEA⁵⁾

Species	$\Delta_f G_m^\circ$ (kJ·mol ⁻¹)	$\Delta_f H_m^\circ$ (kJ·mol ⁻¹)	Reaction	log ₁₀ K°	$\Delta_f G_m^\circ$ (kJ·mol ⁻¹)	$\Delta_f H_m^\circ$ (kJ·mol ⁻¹)
Pu(cr)	0.000	0.000				
Pu ³⁺	-578.984 ± 2.688	-591.790 ± 1.964				
Pu ₂ O ₃ (cr)	-1580.375 ± 10.013	-1656.000 ± 10.000				
PuOH ²⁺	-776.739 ± 3.187		Pu ³⁺ + H ₂ O(l) ⇌ PuOH ²⁺ + H ⁺	-6.900 ± 0.300	39.385 ± 1.712	
Pu(OH) ₃ (cr)	-1200.218 ± 8.975		Pu ³⁺ + 3 H ₂ O(l) ⇌ Pu(OH) ₃ (cr) + 3 H ⁺	-15.800 ± 1.500	90.187 ± 8.562	
PuF ₃ (cr)	-1517.369 ± 3.709	-1586.700 ± 3.700		--	--	418.900 ± 0.500
PuF ₃ (g)	-1161.081 ± 4.758	-1167.800 ± 3.700				
PuCl ²⁺	-717.051 ± 2.923		PuF ₃ (cr) ⇌ PuF ₃ (g)			
PuCl ₃ (cr)	-891.806 ± 2.024	-959.600 ± 1.800				
PuCl ₃ ·6H ₂ O(cr)	-2365.347 ± 2.586	-2773.400 ± 2.100				
PuCl ₃ (g)	-641.299 ± 3.598	-647.400 ± 1.868	PuCl ₃ (cr) ⇌ PuCl ₃ (g)			312.200 ± 0.500
PuOCl(cr)	-882.409 ± 1.936	-931.000 ± 1.700				
PuBr ₃ (cr)	-767.324 ± 2.697	-792.600 ± 2.000				
PuBr ₃ (g)	-529.808 ± 15.655	-488.000 ± 15.000	PuBr ₃ (cr) ⇌ PuBr ₃ (g)	-41.565 ± 2.728	237.257 ± 15.570	304.400 ± 15.000
PuOBr(cr)	-838.354 ± 8.541	-870.000 ± 8.000	PuBr ₃ (cr) + H ₂ O(g) ⇌ PuOBr(cr) + 2 HBr(l)(g)	-8.893 ± 0.914	50.764 ± 5.218	91.700 ± 5.000
PuI ²⁺	-636.987 ± 3.529		Pu ³⁺ + I ⁻ ⇌ PuI ²⁺	1.100 ± 0.400	-6.279 ± 2.283	
PuI ₃ (cr)	-579.000 ± 4.551	-579.200 ± 2.800				
PuI ₃ (g)	-366.517 ± 15.655	-305.000 ± 15.000				
PuOI(cr)	-776.626 ± 20.495	-802.000 ± 20.000				
PuSO ₄ ⁺	-1261.329 ± 3.270		Pu ³⁺ + HSO ₄ ⁻ ⇌ PuSO ₄ ⁺ + H ⁺	1.930 ± 0.610	-11.017 ± 3.482	-5.200 ± 2.000
Pu(SO ₄) ₂ ⁻	-2099.545 ± 5.766	-2398.590 ± 16.244	Pu ³⁺ + 2 HSO ₄ ⁻ ⇌ Pu(SO ₄) ₂ ⁻ + 2 H ⁺	1.740 ± 0.760	-9.932 ± 4.338	-33.000 ± 16.000
PuPO ₄ (s,hydr)	-1744.893 ± 5.528		Pu ³⁺ + PO ₄ ³⁻ ⇌ PuPO ₄ (s,hydr)	24.600 ± 0.800	-140.418 ± 4.566	
PuSCN ²⁺	-493.704 ± 5.333	-515.390 ± 5.988	Pu ³⁺ + SCN ⁻ ⇌ PuSCN ²⁺	1.300 ± 0.400	-7.420 ± 2.283	0.000 ± 4.000
Cs ₃ PuCl ₆ (cr)	-2208.045 ± 9.491	-2364.415 ± 9.040				
Cs ₂ NaPuCl ₆ (cr)	-2143.496 ± 5.184	-2294.200 ± 2.600	CsCl(cr) + 0.2 CsPu ₂ Cl ₇ (cr) ⇌ 0.4 Cs ₃ PuCl ₆ (cr)	3.922 ± 0.658	-22.387 ± 3.640	-23.580 ± 3.426

Table 3 Crystal radius of trivalent actinoids and samarium(III) ¹⁴⁾

ion	electrical configuration	crystal radius (Å)	
		CN* = 6	CN* = 8
Ac ³⁺	[Rn] (6p ⁶)	1.12	1.26
Pu ³⁺	[Rn]5f ⁵	0.995	1.123
Am ³⁺	[Rn]5f ⁶	0.980	1.106
Cm ³⁺	[Rn]5f ⁷	0.970	1.094
Sm ³⁺	[Xe]4f ⁵	0.958	1.079

* CN: coordination number

Table 4 Thermodynamic data for americium(III) selected by the authors for the JAEA-TDB

Species	$\Delta_f G^\circ_m$ (kJ·mol ⁻¹)	Reaction	log ₁₀ K°	$\Delta_f G^\circ_m$ (kJ·mol ⁻¹)
Am(cr)	0.000			
Am ³⁺	-598.698 ± 4.755	Am ³⁺ + H ₂ O(l) ⇌ AmOH ²⁺ + H ⁺	-7.200 ± 0.500	41.098 ± 2.854
AmOH ²⁺	-794.740 ± 5.546	Am ³⁺ + 2 H ₂ O(l) ⇌ Am(OH) ₂ ⁺ + 2 H ⁺	-15.100 ± 0.700	86.191 ± 3.996
Am(OH) ₂ ⁺	-986.787 ± 6.211	Am ³⁺ + 3 H ₂ O(l) ⇌ Am(OH) ₃ (aq) + 3 H ⁺	-26.200 ± 0.500	149.551 ± 2.854
Am(OH) ₃ (aq)	-1160.568 ± 5.547	Am ³⁺ + 3 H ₂ O(l) ⇌ Am(OH) ₃ (am) + 3 H ⁺	-16.900 ± 0.800	96.466 ± 4.566
Am(OH) ₃ (am)	-1213.652 ± 6.594 *	Am ³⁺ + 3 H ₂ O(l) ⇌ Am(OH) ₃ (cr) + 3 H ⁺	-15.600 ± 0.600	89.045 ± 3.425
Am(OH) ₃ (cr)	-1221.073 ± 5.861	Am ³⁺ + F ⁻ ⇌ AmF ²⁺	3.400 ± 0.400	-19.407 ± 2.283
AmF ²⁺	-899.628 ± 5.320	Am ³⁺ + 2 F ⁻ ⇌ AmF ₂ ⁺	5.800 ± 0.200	-33.107 ± 1.142
AmF ₂ ⁺	-1194.851 ± 5.082	Am ³⁺ + Cl ⁻ ⇌ AmCl ²⁺	0.240 ± 0.030	-1.370 ± 0.171
AmCl ²⁺	-731.285 ± 4.759	Am ³⁺ + 2 Cl ⁻ ⇌ AmCl ₂ ⁺	-0.740 ± 0.050	4.224 ± 0.285
AmCl ₂ ⁺	-856.908 ± 4.769	Am ³⁺ + SO ₄ ²⁻ ⇌ AmSO ₄ ⁺	3.300 ± 0.150	-18.837 ± 0.856
AmSO ₄ ⁺	-1361.538 ± 4.849	Am ³⁺ + 2 SO ₄ ²⁻ ⇌ Am(SO ₄) ₂ ⁻	3.700 ± 0.150	-21.120 ± 0.856
Am(SO ₄) ₂ ⁻	-2107.826 ± 4.903	Am ³⁺ + N ₃ ⁻ ⇌ AmN ₃ ²⁺	1.670 ± 0.100	-9.532 ± 0.571
AmN ₃ ²⁺	-260.030 ± 5.190	Am ³⁺ + NO ₂ ⁻ ⇌ AmNO ₂ ²⁺	2.100 ± 0.200	-11.987 ± 1.142
AmNO ₂ ²⁺	-642.885 ± 4.991	Am ³⁺ + NO ₃ ⁻ ⇌ AmNO ₃ ²⁺	1.330 ± 0.200	-7.592 ± 1.142
AmNO ₃ ²⁺	-717.083 ± 4.908	Am ³⁺ + PO ₄ ³⁻ ⇌ AmPO ₄ (am,hydr)	24.790 ± 0.600	-141.500 ± 3.425
AmPO ₄ (am,hydr)	-1765.689 ± 6.068 *	Am ³⁺ + H ₂ PO ₄ ⁻ ⇌ AmH ₂ PO ₄ ²⁺	3.000 ± 0.500	-17.124 ± 2.854
AmH ₂ PO ₄ ²⁺	-1752.974 ± 5.763	Am ³⁺ + CO ₃ ²⁻ ⇌ AmCO ₃ ⁺	8.000 ± 0.400	-45.664 ± 2.283
AmCO ₃ ⁺	-1172.262 ± 5.289	Am ³⁺ + 2 CO ₃ ²⁻ ⇌ Am(CO ₃) ₂ ⁻	12.900 ± 0.600	-73.634 ± 3.425
Am(CO ₃) ₂ ⁻	-1728.131 ± 5.911	Am ³⁺ + 3 CO ₃ ²⁻ ⇌ Am(CO ₃) ₃ ³⁻	15.000 ± 1.000	-85.621 ± 5.708
Am(CO ₃) ₃ ³⁻	-2268.018 ± 7.521	Am ³⁺ + HCO ₃ ⁻ ⇌ AmHCO ₃ ²⁺	3.100 ± 0.300	-17.695 ± 1.712
AmHCO ₃ ²⁺	-1203.238 ± 5.060	2 Am ³⁺ + 3 CO ₃ ²⁻ ⇌ Am ₂ (CO ₃) ₃ (am)	16.700 ± 1.100	-95.324 ± 6.279
Am ₂ (CO ₃) ₃ (am)	-2876.420 ± 11.456 *	Am ³⁺ + CO ₃ ²⁻ + OH ⁻ ⇌ AmCO ₃ OH(am)	20.200 ± 1.000	-115.302 ± 5.708
AmCO ₃ OH(am)	-1399.120 ± 7.440 *	Am ³⁺ + CO ₃ ²⁻ + 0.5 H ₂ O(l) + OH ⁻ ⇌ AmCO ₃ OH•0.5H ₂ O(cr)	22.400 ± 0.500	-127.860 ± 2.854
AmCO ₃ OH•0.5H ₂ O(cr)	-1530.248 ± 5.560	Am ³⁺ + Si(OH) ₄ (aq) ⇌ AmSi(OH) ₃ ²⁺ + H ⁺	-1.680 ± 0.180	9.590 ± 1.027
AmSi(OH) ₃ ²⁺	-1896.844 ± 5.000	Am ³⁺ + SCN ⁻ ⇌ AmSCN ²⁺	1.300 ± 0.300	-7.420 ± 1.712
AmSCN ²⁺	-513.418 ± 6.445	Am ³⁺ + 2 CO ₃ ²⁻ + 5 H ₂ O(l) + Na ⁺ ⇌ NaAm(CO ₃) ₂ •5H ₂ O(cr)	21.000 ± 0.500	-119.869 ± 2.854
NaAm(CO ₃) ₂ •5H ₂ O(cr)	-3222.021 ± 5.605			

* Determined or modified by the authors

Table 5 Selected Gibbs free energy of formation ($\Delta_f G_m^\circ$ ($\text{kJ}\cdot\text{mol}^{-1}$)) for actinoid(III) aqua ions by the OECD/NEA and the literature by Fuger and Oetting

ion	OECD/NEA ⁵⁾	Fuger and Oetting ¹⁷⁾ *
Ac ³⁺	—	-640.152 ± 25.104
U ³⁺	-476.473 ± 1.810	—
Np ³⁺	-512.866 ± 5.669	—
Pu ³⁺	-578.984 ± 2.688	-578.647 ± 3.347
Am ³⁺	-598.698 ± 4.755	-599.149 ± 1.255
Cm ³⁺	—	-595.802 ± 6.276

* The $\Delta_f G_m^\circ$ values by Fuger and Oetting were converted from a unit of $\text{kcal}\cdot\text{mol}^{-1}$ to $\text{kJ}\cdot\text{mol}^{-1}$ by the authors using $1 \text{ cal} = 4.184 \text{ J}$.

Table 6 Thermodynamic data for curium(III) selected by the authors for the JAEA-TDB

Species	$\Delta_f G_m^\circ$ (kJ·mol ⁻¹)	Reaction	$\log_{10} K^\circ$	$\Delta_f G_m^\circ$ (kJ·mol ⁻¹)
Cm(cr)	0.000			
Cm ³⁺	-595.802 ± 6.276 *			
CmOH ²⁺	-791.844 ± 6.895 **	Cm ³⁺ + H ₂ O(l) ⇌ CmOH ²⁺ + H ⁺	-7.200 ± 0.500	41.098 ± 2.854
Cm(OH) ₂ ⁺	-983.890 ± 7.440 **	Cm ³⁺ + 2 H ₂ O(l) ⇌ Cm(OH) ₂ ⁺ + 2 H ⁺	-15.100 ± 0.700	86.191 ± 3.996
Cm(OH) ₃ (aq)	-1210.756 ± 7.762 **	Cm ³⁺ + 3 H ₂ O(l) ⇌ Cm(OH) ₃ (aq) + 3 H ⁺	-26.200 ± 0.500	149.551 ± 2.854
Cm(OH) ₃ (am)	-1157.671 ± 6.896 **	Cm ³⁺ + 3 H ₂ O(l) ⇌ Cm(OH) ₃ (am) + 3 H ⁺	-16.900 ± 0.800	96.466 ± 4.566
Cm(OH) ₃ (cr)	-1218.176 ± 7.151 **	Cm ³⁺ + 3 H ₂ O(l) ⇌ Cm(OH) ₃ (cr) + 3 H ⁺	-15.600 ± 0.600	89.045 ± 3.425
CmF ²⁺	-896.732 ± 6.714 **	Cm ³⁺ + F ⁻ ⇌ CmF ²⁺	3.400 ± 0.400	-19.407 ± 2.283
CmF ₂ ⁺	-1191.954 ± 6.527 **	Cm ³⁺ + 2 F ⁻ ⇌ CmF ₂ ⁺	5.800 ± 0.200	-33.107 ± 1.142
CmCl ²⁺	-728.389 ± 6.279 **	Cm ³⁺ + Cl ⁻ ⇌ CmCl ²⁺	0.240 ± 0.030	-1.370 ± 0.171
CmCl ₂ ⁺	-854.012 ± 6.287 **	Cm ³⁺ + 2 Cl ⁻ ⇌ CmCl ₂ ⁺	-0.740 ± 0.050	4.224 ± 0.285
CmSO ₄ ⁺	-1358.642 ± 6.348 **	Cm ³⁺ + SO ₄ ²⁻ ⇌ CmSO ₄ ⁺	3.300 ± 0.150	-18.837 ± 0.856
Cm(SO ₄) ₂ ⁻	-2104.929 ± 6.389 **	Cm ³⁺ + 2 SO ₄ ²⁻ ⇌ Cm(SO ₄) ₂ ⁻	3.700 ± 0.150	-21.120 ± 0.856
CmN ₃ ²⁺	-257.134 ± 6.612 **	Cm ³⁺ + N ₃ ⁻ ⇌ CmN ₃ ²⁺	1.670 ± 0.100	-9.532 ± 0.571
CmNO ₂ ²⁺	-639.988 ± 6.457 **	Cm ³⁺ + NO ₂ ⁻ ⇌ CmNO ₂ ²⁺	2.100 ± 0.200	-11.987 ± 1.142
CmNO ₃ ²⁺	-714.187 ± 6.393 **	Cm ³⁺ + NO ₃ ⁻ ⇌ CmNO ₃ ²⁺	1.330 ± 0.200	-7.592 ± 1.142
CmPO ₄ (am,hydr)	-1762.793 ± 7.321 **	Cm ³⁺ + PO ₄ ³⁻ ⇌ CmPO ₄ (am,hydr)	24.790 ± 0.600	-141.500 ± 3.425
CmH ₂ PO ₄ ²⁺	-1750.078 ± 7.070 **	Cm ³⁺ + H ₂ PO ₄ ⁻ ⇌ CmH ₂ PO ₄ ²⁺	3.000 ± 0.500	-17.124 ± 2.854
CmCO ₃ ⁺	-1169.366 ± 6.690 **	Cm ³⁺ + CO ₃ ²⁻ ⇌ CmCO ₃ ⁺	8.000 ± 0.400	-45.664 ± 2.283
Cm(CO ₃) ₂ ⁻	-1725.235 ± 7.192 **	Cm ³⁺ + 2 CO ₃ ²⁻ ⇌ Cm(CO ₃) ₂ ⁻	12.900 ± 0.600	-73.634 ± 3.425
Cm(CO ₃) ₃ ³⁻	-2265.122 ± 8.564 **	Cm ³⁺ + 3 CO ₃ ²⁻ ⇌ Cm(CO ₃) ₃ ³⁻	15.000 ± 1.000	-85.621 ± 5.708
CmHCO ₃ ²⁺	-1200.342 ± 6.510 **	Cm ³⁺ + HCO ₃ ⁻ ⇌ CmHCO ₃ ²⁺	3.100 ± 0.300	-17.695 ± 1.712
Cm ₂ (CO ₃) ₃ (am)	-2870.628 ± 14.084 **	2 Cm ³⁺ + 3 CO ₃ ²⁻ ⇌ Cm ₂ (CO ₃) ₃ (am)	16.700 ± 1.100	-95.324 ± 6.279
CmCO ₃ OH(am)	-1396.224 ± 8.493 **	Cm ³⁺ + CO ₃ ²⁻ + OH ⁻ ⇌ CmCO ₃ OH(am)	20.200 ± 1.000	-115.302 ± 5.708
CmCO ₃ OH•0.5H ₂ O(cr)	-1527.352 ± 6.906 **	Cm ³⁺ + CO ₃ ²⁻ + 0.5 H ₂ O(l) + OH ⁻ ⇌ CmCO ₃ OH•0.5H ₂ O(cr)	22.400 ± 0.500	-127.860 ± 2.854
CmSiO(OH) ₃ ²⁺	-1893.947 ± 6.464 **	Cm ³⁺ + Si(OH) ₄ (aq) ⇌ CmSiO(OH) ₃ ²⁺ + H ⁺	-1.680 ± 0.180	9.590 ± 1.027
CmSCN ²⁺	-510.522 ± 7.637 **	Cm ³⁺ + SCN ⁻ ⇌ CmSCN ²⁺	1.300 ± 0.300	-7.420 ± 1.712
NaCm(CO ₃) ₂ •5H ₂ O(cr)	-3219.123 ± 6.942 **	Cm ³⁺ + 2 CO ₃ ²⁻ + 5 H ₂ O(l) + Na ⁺ ⇌ NaCm(CO ₃) ₂ •5H ₂ O(cr)	21.000 ± 0.500	-119.869 ± 2.854

* Taken from the literature ¹⁷⁾

** Determined by the authors

Table 7 Thermodynamic data for plutonium(III) selected by the authors for the JAEA-TDB

Species	$\Delta_f G_m^\circ$ (kJ·mol ⁻¹)	Reaction	log ₁₀ K ^o	$\Delta_f G_m^\circ$ (kJ·mol ⁻¹)
Pu(cr)	0.000			
Pu ³⁺	-578.984 ± 2.688			
PuOH ²⁺	-775.026 ± 3.921 *	Pu ³⁺ + H ₂ O(l) ⇌ PuOH ²⁺ + H ⁺	-7.200 ± 0.500	41.098 ± 2.854
Pu(OH) ₂ ⁺	-967.073 ± 4.816 *	Pu ³⁺ + 2 H ₂ O(l) ⇌ Pu(OH) ₂ ⁺ + 2 H ⁺	-15.100 ± 0.700	86.191 ± 3.996
Pu(OH) ₃ (aq)	-1193.938 ± 5.300 *	Pu ³⁺ + 3 H ₂ O(l) ⇌ Pu(OH) ₃ (aq) + 3 H ⁺	-26.200 ± 0.500	149.551 ± 2.854
Pu(OH) ₃ (am)	-1140.853 ± 3.922 *	Pu ³⁺ + 3 H ₂ O(l) ⇌ Pu(OH) ₃ (am) + 3 H ⁺	-16.900 ± 0.800	96.466 ± 4.566
Pu(OH) ₃ (cr)	-1201.359 ± 4.355 *	Pu ³⁺ + 3 H ₂ O(l) ⇌ Pu(OH) ₃ (cr) + 3 H ⁺	-15.600 ± 0.600	89.045 ± 3.425
PuF ²⁺	-879.914 ± 3.594 *	Pu ³⁺ + F ⁻ ⇌ PuF ²⁺	3.400 ± 0.400	-19.407 ± 2.283
PuF ₂ ⁺	-1175.137 ± 3.232 *	Pu ³⁺ + 2 F ⁻ ⇌ PuF ₂ ⁺	5.800 ± 0.200	-33.107 ± 1.142
PuCl ²⁺	-711.571 ± 2.696 *	Pu ³⁺ + Cl ⁻ ⇌ PuCl ²⁺	0.240 ± 0.030	-1.370 ± 0.171
PuCl ₂ ⁺	-837.194 ± 2.713 *	Pu ³⁺ + 2 Cl ⁻ ⇌ PuCl ₂ ⁺	-0.740 ± 0.050	4.224 ± 0.285
PuSO ₄ ⁺	-1341.825 ± 2.852 *	Pu ³⁺ + SO ₄ ²⁻ ⇌ PuSO ₄ ⁺	3.300 ± 0.150	-18.837 ± 0.856
Pu(SO ₄) ₂ ⁻	-2088.112 ± 2.942 *	Pu ³⁺ + 2 SO ₄ ²⁻ ⇌ Pu(SO ₄) ₂ ⁻	3.700 ± 0.150	-21.120 ± 0.856
PuN ₃ ²⁺	-240.316 ± 3.399 *	Pu ³⁺ + N ₃ ⁻ ⇌ PuN ₃ ²⁺	1.670 ± 0.100	-9.532 ± 0.571
PuNO ₂ ²⁺	-623.171 ± 3.087 *	Pu ³⁺ + NO ₂ ⁻ ⇌ PuNO ₂ ²⁺	2.100 ± 0.200	-11.987 ± 1.142
PuNO ₃ ²⁺	-697.370 ± 2.950 *	Pu ³⁺ + NO ₃ ⁻ ⇌ PuNO ₃ ²⁺	1.330 ± 0.200	-7.592 ± 1.142
PuPO ₄ (am,hydr)	-1745.975 ± 4.630 *	Pu ³⁺ + PO ₄ ³⁻ ⇌ PuPO ₄ (am,hydr)	24.790 ± 0.600	-141.500 ± 3.425
PuH ₂ PO ₄ ²⁺	-1733.260 ± 4.222 *	Pu ³⁺ + H ₂ PO ₄ ⁻ ⇌ PuH ₂ PO ₄ ²⁺	3.000 ± 0.500	-17.124 ± 2.854
PuCO ₃ ⁺	-1152.548 ± 3.548 *	Pu ³⁺ + CO ₃ ²⁻ ⇌ PuCO ₃ ⁺	8.000 ± 0.400	-45.664 ± 2.283
Pu(CO ₃) ₂ ⁻	-1708.418 ± 4.423 *	Pu ³⁺ + 2 CO ₃ ²⁻ ⇌ Pu(CO ₃) ₂ ⁻	12.900 ± 0.600	-73.634 ± 3.425
Pu(CO ₃) ₃ ³⁻	-2248.305 ± 6.417 *	Pu ³⁺ + 3 CO ₃ ²⁻ ⇌ Pu(CO ₃) ₃ ³⁻	15.000 ± 1.000	-85.621 ± 5.708
PuHCO ₃ ²⁺	-1183.524 ± 3.197 *	Pu ³⁺ + HCO ₃ ⁻ ⇌ PuHCO ₃ ²⁺	3.100 ± 0.300	-17.695 ± 1.712
Pu ₂ (CO ₃) ₃ (am)	-2836.992 ± 8.348 *	2 Pu ³⁺ + 3 CO ₃ ²⁻ ⇌ Pu ₂ (CO ₃) ₃ (am)	16.700 ± 1.100	-95.324 ± 6.279
PuCO ₃ OH(am)	-1379.406 ± 6.322 *	Pu ³⁺ + CO ₃ ²⁻ + OH ⁻ ⇌ PuCO ₃ OH(am)	20.200 ± 1.000	-115.302 ± 5.708
PuCO ₃ OH•0.5H ₂ O(cr)	-1510.534 ± 3.941 *	Pu ³⁺ + CO ₃ ²⁻ + 0.5 H ₂ O(l) + OH ⁻ ⇌ PuCO ₃ OH•0.5H ₂ O(cr)	22.400 ± 0.500	-127.860 ± 2.854
PuSiO(OH) ₃ ²⁺	-1877.129 ± 3.101 *	Pu ³⁺ + Si(OH) ₄ (aq) ⇌ PuSiO(OH) ₃ ²⁺ + H ⁺	-1.680 ± 0.180	9.590 ± 1.027
PuSCN ²⁺	-493.704 ± 5.114 *	Pu ³⁺ + SCN ⁻ ⇌ PuSCN ²⁺	1.300 ± 0.300	-7.420 ± 1.712

* Determined by the authors

Table 8 Solubility product and hydrolysis constants for samarium(III) and actinium(III) comparing with those for americium(III) and plutonium(III) selected by the OECD/NEA

element	method ^{*1}	medium	T (K)	log K	ref.
$M^{3+} + 3 H_2O(l) \Leftrightarrow M(OH)_3(s) + 3 H^+$					
Sm	sol	0.1 M Sm(NO ₃) ₃	298.15	-18.48 (I = 0) ^{*2}	23
	sol	0.1 M Sm(ClO ₄) ₃	298.15	-18.92 (I = 0) ^{*2}	23
	sol	0.045 M Sm(ClO ₄) ₃	298.15	-19.99 (I = 0) ^{*2}	24
	sol	< 0.1 M Sm(NO ₃) ₃	293.15	-17.68 (I = 0) ^{*2}	25
	sol	(2 – 6) × 10 ⁻⁴ M SmCl ₃	293.15	-17.29 (I = 0) ^{*2}	26
	sol	0.002 – 4.0 M NaCl	298.15	-16.13 (I = 0) ^{*2}	27
	sol	1 M NaClO ₄	n.s.	-17.5 (I = 1)	18
	sol	0.1 M NaClO ₄	r.t.	-16.4 (I = 0)	19
Ac	sol	0.001 M NH ₄ NO ₃	r.t.	fresh: -23.35 ± 0.23 ^{*3} old: -21.11 ± 0.14 ^{*3}	21
Am	(I = 0 by the OECD/NEA)		298.15	am: -16.9 ± 0.8 cr: -15.6 ± 0.6	5
Pu	(I = 0 by the OECD/NEA)		298.15	cr: -15.8 ± 1.5	5

$M^{3+} + H_2O(l) \Leftrightarrow MOH^{2+} + H^+$					
Sm	pot	0.001 M sulfate	298.15	-8.90	28
	pot	0.3 M NaClO ₄	298.15	-8.36	29
	sol	1.0 M NaClO ₄	r.t.	-7.50	18
	ext	0.1 M LiClO ₄	298.15	-4.40	30
	sol	0.1 M NaClO ₄	r.t.	-7.2 (I = 0)	19
Am	(I = 0 by the OECD/NEA)		298.15	-7.2 ± 0.5	5
Pu	(I = 0 by the OECD/NEA)		298.15	-6.9 ± 0.3	5

$M^{3+} + 2 H_2O(l) \Leftrightarrow M(OH)_2^+ + 2 H^+$					
Sm	sol	1.0 M NaClO ₄	r.t.	-15.0	18
	sol	0.1 M NaClO ₄	r.t.	≤ -15.0 (I = 0)	20
Am	(I = 0 by the OECD/NEA)		298.15	-15.1 ± 0.7	5

$M^{3+} + 3 H_2O(l) \Leftrightarrow M(OH)_3(aq) + 3 H^+$					
Sm	sol	1.0 M NaClO ₄	r.t.	-22.7	18
	sol	0.1 M NaClO ₄	r.t.	-24.9 (I = 0)	19
Am	(I = 0 by the OECD/NEA)		298.15	-26.2 ± 0.5	5

$M^{3+} + 4 H_2O(l) \Leftrightarrow M(OH)_4^- + 4 H^+$					
Sm	sol	1.0 M NaClO ₄	r.t.	-36.7	31

^{*1} sol: solubility, pot: potentiometry, ext: solvent extraction

^{*2} Determination of log K^o was performed by Diakonov *et al.*³²⁾

^{*3} Recalculated by the authors

Table 9 Thermodynamic data for samarium(III) selected by the authors for the JAEA-TDB

Species	$\Delta_f G_m^\circ$ (kJ·mol ⁻¹)	Reaction	$\log_{10} K^\circ$	$\Delta_f G_m^\circ$ (kJ·mol ⁻¹)
Sm(cr)	0.000			
Sm ³⁺	-666.600 ± 1.000 *			
SmOH ²⁺	-862.642 ± 3.024 **	Sm ³⁺ + H ₂ O(l) ⇌ SmOH ²⁺ + H ⁺	-7.200 ± 0.500	41.098 ± 2.854
Sm(OH) ₂ ⁺	-1054.689 ± 4.120 **	Sm ³⁺ + 2 H ₂ O(l) ⇌ Sm(OH) ₂ ⁺ + 2 H ⁺	-15.100 ± 0.700	86.191 ± 3.996
Sm(OH) ₃ (aq)	-1281.554 ± 4.676 **	Sm ³⁺ + 3 H ₂ O(l) ⇌ Sm(OH) ₃ (aq) + 3 H ⁺	-26.200 ± 0.500	149.551 ± 2.854
Sm(OH) ₃ (am)	-1228.469 ± 3.027 **	Sm ³⁺ + 3 H ₂ O(l) ⇌ Sm(OH) ₃ (am) + 3 H ⁺	-16.900 ± 0.800	96.466 ± 4.566
Sm(OH) ₃ (cr)	-1288.975 ± 3.570 **	Sm ³⁺ + 3 H ₂ O(l) ⇌ Sm(OH) ₃ (cr) + 3 H ⁺	-15.600 ± 0.600	89.045 ± 3.425
SmF ²⁺	-967.530 ± 2.587 **	Sm ³⁺ + F ⁻ ⇌ SmF ²⁺	3.400 ± 0.400	-19.407 ± 2.283
SmF ₂ ⁺	-1262.753 ± 2.054 **	Sm ³⁺ + 2 F ⁻ ⇌ SmF ₂ ⁺	5.800 ± 0.200	-33.107 ± 1.142
SmCl ²⁺	-799.187 ± 1.021 **	Sm ³⁺ + Cl ⁻ ⇌ SmCl ²⁺	0.240 ± 0.030	-1.370 ± 0.171
SmCl ₂ ⁺	-924.810 ± 1.066 **	Sm ³⁺ + 2 Cl ⁻ ⇌ SmCl ₂ ⁺	-0.740 ± 0.050	4.224 ± 0.285
SmSO ₄ ⁺	-1429.441 ± 1.381 **	Sm ³⁺ + SO ₄ ²⁻ ⇌ SmSO ₄ ⁺	3.300 ± 0.150	-18.837 ± 0.856
Sm(SO ₄) ₂ ⁻	-2175.728 ± 1.559 **	Sm ³⁺ + 2 SO ₄ ²⁻ ⇌ Sm(SO ₄) ₂ ⁻	3.700 ± 0.150	-21.120 ± 0.856
SmN ₃ ²⁺	-327.932 ± 2.308 **	Sm ³⁺ + N ₃ ⁻ ⇌ SmN ₃ ²⁺	1.670 ± 0.100	-9.532 ± 0.571
SmNO ₂ ²⁺	-710.787 ± 1.817 **	Sm ³⁺ + NO ₂ ⁻ ⇌ SmNO ₂ ²⁺	2.100 ± 0.200	-11.987 ± 1.142
SmNO ₃ ²⁺	-784.986 ± 1.574 **	Sm ³⁺ + NO ₃ ⁻ ⇌ SmNO ₃ ²⁺	1.330 ± 0.200	-7.592 ± 1.142
SmPO ₄ (am,hydr)	-1833.591 ± 3.900 **	Sm ³⁺ + PO ₄ ³⁻ ⇌ SmPO ₄ (am,hydr)	24.790 ± 0.600	-141.500 ± 3.425
SmH ₂ PO ₄ ²⁺	-1820.876 ± 3.406 **	Sm ³⁺ + H ₂ PO ₄ ⁻ ⇌ SmH ₂ PO ₄ ²⁺	3.000 ± 0.500	-17.124 ± 2.854
SmCO ₃ ⁺	-1240.164 ± 2.523 **	Sm ³⁺ + CO ₃ ²⁻ ⇌ SmCO ₃ ⁺	8.000 ± 0.400	-45.664 ± 2.283
Sm(CO ₃) ₂ ⁻	-1796.034 ± 3.652 **	Sm ³⁺ + 2 CO ₃ ²⁻ ⇌ Sm(CO ₃) ₂ ⁻	12.900 ± 0.600	-73.634 ± 3.425
Sm(CO ₃) ₃ ³⁻	-2335.921 ± 5.912 **	Sm ³⁺ + 3 CO ₃ ²⁻ ⇌ Sm(CO ₃) ₃ ³⁻	15.000 ± 1.000	-85.621 ± 5.708
SmHCO ₃ ²⁺	-1271.140 ± 1.999 **	Sm ³⁺ + HCO ₃ ⁻ ⇌ SmHCO ₃ ²⁺	3.100 ± 0.300	-17.695 ± 1.712
Sm ₂ (CO ₃) ₃ (am)	-3012.224 ± 6.693 **	2 Sm ³⁺ + 3 CO ₃ ²⁻ ⇌ Sm ₂ (CO ₃) ₃ (am)	16.700 ± 1.100	-95.324 ± 6.279
SmCO ₃ OH(am)	-1467.022 ± 5.809 **	Sm ³⁺ + CO ₃ ²⁻ + OH ⁻ ⇌ SmCO ₃ OH(am)	20.200 ± 1.000	-115.302 ± 5.708
SmCO ₃ OH•0.5H ₂ O(cr)	-1598.150 ± 3.050 **	Sm ³⁺ + CO ₃ ²⁻ + 0.5 H ₂ O(l) + OH ⁻ ⇌ SmCO ₃ OH•0.5H ₂ O(cr)	22.400 ± 0.500	-127.860 ± 2.854
SmSiO(OH) ₃ ²⁺	-1964.745 ± 1.842 **	Sm ³⁺ + Si(OH) ₄ (aq) ⇌ SmSiO(OH) ₃ ²⁺ + H ⁺	-1.680 ± 0.180	9.590 ± 1.027
SmSCN ²⁺	-581.320 ± 4.465 **	Sm ³⁺ + SCN ⁻ ⇌ SmSCN ²⁺	1.300 ± 0.300	-7.420 ± 1.712
NaSm(CO ₃) ₂ •5H ₂ O(cr)	-3289.922 ± 3.131 **	Sm ³⁺ + 2 CO ₃ ²⁻ + 5 H ₂ O(l) + Na ⁺ ⇌ NaSm(CO ₃) ₂ •5H ₂ O(cr)	21.000 ± 0.500	-119.869 ± 2.854

* Taken from the literature ¹⁶⁾ with addition of uncertainties by the authors

** Determined by the authors

Table 10 Stability constants of the chloride and bromide complexes of some lanthanoids and actinoids with reaction of $M^{3+} + x L^- \rightleftharpoons ML_x^{3-x}$ (x : 1 and 2) at $3.0 \text{ mol}\cdot\text{dm}^{-3}$ LiCl or LiBr solutions ²²⁾

anion	metal	β_1	β_2
Cl ⁻	Sm	0.41 ± 0.04	0.25 ± 0.03
	Eu	0.52 ± 0.02	0.22 ± 0.02
	Gd	0.56 ± 0.02	0.21 ± 0.02
	Tb	0.45 ± 0.02	0.26 ± 0.02
	Ac	0.44 ± 0.02	0.31 ± 0.02
	Am	0.55 ± 0.03	0.22 ± 0.02
	Cm	0.56 ± 0.03	0.20 ± 0.02
	Bk	0.59 ± 0.02	0.25 ± 0.02
	Cf	0.61 ± 0.04	0.25 ± 0.03
Br ⁻	Sm	0.33 ± 0.04	0.24 ± 0.03
	Eu	0.38 ± 0.02	0.23 ± 0.01
	Gd	0.37 ± 0.02	0.26 ± 0.02
	Tb	0.41 ± 0.03	0.22 ± 0.01
	Ac	0.42 ± 0.02	0.29 ± 0.01
	Am	0.30 ± 0.03	0.28 ± 0.02
	Cm	0.39 ± 0.02	0.22 ± 0.02
	Bk	0.15 ± 0.04	0.29 ± 0.03
	Cf	0.30 ± 0.04	0.30 ± 0.03

Table 11 Thermodynamic data for actinium(III) selected for the JAEA-TDB *

Species	$\Delta_f G_m^\circ$ (kJ·mol ⁻¹)	Reaction	log ₁₀ K°	$\Delta_f G_m^\circ$ (kJ·mol ⁻¹)
Ac(cr)	0.000			
Ac ³⁺	-640.152 ± 25.104			
AcOH ²⁺	-836.194 ± 25.420	Ac ³⁺ + H ₂ O(l) ⇌ AcOH ²⁺ + H ⁺	-7.200 ± 0.700	41.098 ± 3.996
Ac(OH) ₂ ⁺	-1028.241 ± 25.624	Ac ³⁺ + 2 H ₂ O(l) ⇌ Ac(OH) ₂ ⁺ + 2 H ⁺	-15.100 ± 0.900	86.191 ± 5.137
Ac(OH) ₃ (aq)	-1202.021 ± 25.420	Ac ³⁺ + 3 H ₂ O(l) ⇌ Ac(OH) ₃ (aq) + 3 H ⁺	-26.200 ± 0.700	149.551 ± 3.996
Ac(OH) ₃ (am)	-1277.938 ± 27.125	Ac ³⁺ + 3 H ₂ O(l) ⇌ Ac(OH) ₃ (am) + 3 H ⁺	-16.900 ± 4.800 **	119.298 ± 10.274
AcF ²⁺	-941.082 ± 25.346	Ac ³⁺ + F ⁻ ⇌ AcF ²⁺	3.400 ± 0.600	-19.407 ± 3.425
AcF ₂ ⁺	-1236.305 ± 25.246	Ac ³⁺ + 2 F ⁻ ⇌ AcF ₂ ⁺	5.800 ± 0.400	-33.107 ± 2.283
AcCl ²⁺	-772.739 ± 25.139	Ac ³⁺ + Cl ⁻ ⇌ AcCl ²⁺	0.240 ± 0.230	-1.370 ± 1.313
AcCl ₂ ⁺	-898.362 ± 25.146	Ac ³⁺ + 2 Cl ⁻ ⇌ AcCl ₂ ⁺	-0.740 ± 0.250	4.224 ± 1.427
AcSO ₄ ⁺	-1402.993 ± 25.187	Ac ³⁺ + SO ₄ ²⁻ ⇌ AcSO ₄ ⁺	3.300 ± 0.350	-18.837 ± 1.998
Ac(SO ₄) ₂ ⁻	-2149.280 ± 25.197	Ac ³⁺ + 2 SO ₄ ²⁻ ⇌ Ac(SO ₄) ₂ ⁻	3.700 ± 0.350	-21.120 ± 1.998
AcN ₃ ²⁺	-301.484 ± 25.242	Ac ³⁺ + N ₃ ⁻ ⇌ AcN ₃ ²⁺	1.670 ± 0.300	-9.532 ± 1.712
AcNO ₂ ²⁺	-684.339 ± 25.227	Ac ³⁺ + NO ₂ ⁻ ⇌ AcNO ₂ ²⁺	2.100 ± 0.400	-11.987 ± 2.283
AcNO ₃ ²⁺	-758.538 ± 25.211	Ac ³⁺ + NO ₃ ⁻ ⇌ AcNO ₃ ²⁺	1.330 ± 0.400	-7.592 ± 2.283
AcPO ₄ (am,hydr)	-1807.143 ± 26.760	Ac ³⁺ + PO ₄ ³⁻ ⇌ AcPO ₄ (am,hydr)	24.790 ± 4.600 **	-118.670 ± 9.133
AcH ₂ PO ₄ ²⁺	-1794.428 ± 25.468	Ac ³⁺ + H ₂ PO ₄ ⁻ ⇌ AcH ₂ PO ₄ ²⁺	3.000 ± 0.700	-17.124 ± 3.996
AcCO ₃ ⁺	-1213.716 ± 25.340	Ac ³⁺ + CO ₃ ²⁻ ⇌ AcCO ₃ ⁺	8.000 ± 0.600	-45.664 ± 3.425
Ac(CO ₃) ₂ ⁻	-1769.586 ± 25.528	Ac ³⁺ + 2 CO ₃ ²⁻ ⇌ Ac(CO ₃) ₂ ⁻	12.900 ± 0.800	-73.634 ± 4.566
Ac(CO ₃) ₃ ³⁻	-2309.473 ± 26.048	Ac ³⁺ + 3 CO ₃ ²⁻ ⇌ Ac(CO ₃) ₃ ³⁻	15.000 ± 1.200	-85.621 ± 6.850
AcHCO ₃ ²⁺	-1244.692 ± 25.267	Ac ³⁺ + HCO ₃ ⁻ ⇌ AcHCO ₃ ²⁺	3.100 ± 0.500	-17.695 ± 2.854
Ac ₂ (CO ₃) ₃ (am)	-2982.160 ± 51.632	2 Ac ³⁺ + 3 CO ₃ ²⁻ ⇌ Ac ₂ (CO ₃) ₃ (am)	16.700 ± 5.100 **	-72.492 ± 11.987
AcCO ₃ OH(am)	-1463.407 ± 27.581	Ac ³⁺ + CO ₃ ²⁻ + OH ⁻ ⇌ AcCO ₃ OH(am)	20.200 ± 5.000 **	-92.470 ± 11.416
AcSiO(OH) ₃ ²⁺	-1938.297 ± 25.224	Ac ³⁺ + Si(OH) ₄ (aq) ⇌ AcSiO(OH) ₃ ²⁺ + H ⁺	-1.680 ± 0.380	9.590 ± 2.169
AcSCN ²⁺	-554.872 ± 25.580	Ac ³⁺ + SCN ⁻ ⇌ AcSCN ²⁺	1.300 ± 0.500	-7.420 ± 2.854

* All the obtained values except for $\Delta_f G_m^\circ$ of Ac³⁺ (-640.152 ± 25.104 kJ·mol⁻¹) should be treated as a tentative value

** Larger uncertainties than those for americium(III), curium(III) and samarium(III)

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
物質の量	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 基本単位	
	名称	記号
面積	平方メートル	m ²
体積	立法メートル	m ³
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
質量濃度 ^(a) , 濃度	モル毎立方メートル	mol/m ³
質量濃度	キログラム毎立法メートル	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	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	ジーメンズ	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)	°C	K	K
光束流	ルーメン	lm	cd sr ^(c)	cd
放射線種の放射能 ^(f)	ベクレル ^(d)	Bq	lm/m ²	m ⁻² cd 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及び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
粘り度	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	接頭語	記号	乗数	接頭語	記号
10 ²⁴	ヨタ	Y	10 ¹	デカ	d
10 ²¹	ゼタ	Z	10 ²	ヘンチ	c
10 ¹⁸	エクサ	E	10 ³	ミリア	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=60s
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/10800) rad
秒	"	1"=(1/60)'=(π/648000) rad
ヘクタール	ha	1 ha=1 hm ² =10 ⁴ m ²
リットル	L, l	1 L=11.1 dm ³ =10 ³ cm 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=0.1 MPa=100 kPa=10 ⁵ Pa
水銀柱ミリメートル	mmHg	1 mmHg=133.322 Pa
オングストローム	Å	1 Å=0.1 nm=100 pm=10 ⁻¹⁰ m
海里	M	1 M=1852 m
バイン	b	1 b=100 fm 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。
ベベル	B	
デジベル	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 =0.1 Pa 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=1 cd cm ⁻² =10 ⁴ cd m ⁻²
フォト	ph	1 ph=1 cd sr cm ⁻² 10 ⁴ lx
ガリ	Gal	1 Gal=1 cm s ⁻² =10 ⁻² ms ⁻²
マクスウェル	Mx	1 Mx=1 G cm ² =10 ⁸ Wb
ガウス	G	1 G=1 Mx cm ⁻² =10 ⁻⁴ T
エルステッド ^(c)	Oe	1 Oe ≐ (10 ³ /4π) A m ⁻¹

(c) 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=1 cGy=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	f	1 f=エルミ=1 fm=10 ⁻¹⁵ m
メートル系カラット		1メートル系カラット=200 mg=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	cal	1 cal=4.1868 J (「15°C」カロリ), 4.1868 J (「IT」カロリ), 4.184 J (「熱化学」カロリ)
マイクロン	μ	1 μ=1 μm=10 ⁻⁶ m

