



Evaluating and Categorizing the Reliability of Distribution Coefficient
Values in the Sorption Database (3)

Michael OCHS, Tadahiro SUYAMA, Susanne KUNZE, Yukio TACHI
and Mikazu YUI

Geological Isolation Research Unit
Geological Isolation Research and Development Directorate

February 2010

Japan Atomic Energy Agency

日本原子力研究開発機構

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

(Received December 9, 2009)

Sorption of radionuclides in bentonites and rocks is one of the key processes in the safe geological disposal of radioactive waste. Japan Atomic Energy Agency (JAEA) has developed sorption database (JAEA-SDB) which includes extensive compilation of sorption K_d data by batch experiments, extracted from published literatures. JA EA published the first SDB as an important basis for the H12 performance assessment (PA), and has been continuing to improve and update the SDB in view of potential future data needs, focusing on assuring the desired quality level and practical applications to K_d -setting for the geological environment. The JA EA-SDB includes more than 24,000 K_d data which are related with various conditions and methods, and different reliabilities. Accordingly, the quality assuring (QA) and classifying guideline/criteria has been developed in order to evaluate the reliability of each K_d value. The reliability of K_d values of key radionuclides for bentonite and mudstone system has been already evaluated. To use these QA information, the new web-based JA EA-SDB was published in March, 2009.

In this report, the QA/classification of selected entries for key radionuclides (Th, Np, Am, Se and Cs) in the JA EA-SDB was done following the approach/guideline defined in our previous report focusing granite rocks which are related to reference systems in H12 PA and possible applications in the context of URL activities, and Fe-oxide/hydroxide, Al-oxide/hydroxide existing widely in geological environment. As a result, the reliability of 1,373 K_d values was evaluated and classified. This classification scheme is expected to make it possible to obtain quick overview of the available data from the SDB, and to have suitable access to the respective data for K_d -setting in PA.

Keywords: Sorption Database, Distribution Coefficient, K_d , Reliability, Quality Assurance, Geological Disposal

* BMG ENGINEERING LTD, Switzerland

*Collaborating Engineer

収着データベースに登録された収着分配係数の信頼度評価 (3)

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

Michael OCHS*, 陶山 忠宏*, Susanne KUNZE*, 舘 幸男, 油井 三和

(2009 年 12 月 9 日受理)

放射性廃棄物の地層処分安全評価において、人工バリアであるベントナイトや天然バリアである岩石中での核種の収着現象は、核種の移行遅延を支配する重要な現象である。日本原子力研究開発機構 (JAEA) では、バッチ法収着試験によって得られた収着分配係数を、公開文献から抽出・整理した収着データベース (JAEA-SDB) の整備を進めてきた。最初の収着データベースを、地層処分研究開発第 2 次取りまとめの性能評価の重要な基盤情報として整備して以降、将来の性能評価におけるニーズへの対応を念頭に、データベースに含まれる K_d データの信頼度評価、実際の地質環境に対する K_d 設定におけるデータベース適用に着目して、データベースの改良・更新を継続的に実施してきている。JAEA-SDB に登録されている K_d データは 24,000 データを超え、様々な実験条件や手法によって得られた信頼度の異なるデータが含まれる。このため、個々の K_d データの信頼性を評価することを目的に、信頼度評価とそのレベル分けに関するガイドライン/基準が開発された。これまでに、このガイドラインに基づき、ベントナイト系および泥岩系の主要核種の K_d データを対象に信頼度評価を実施した。2009 年 3 月には、これらの信頼度評価に関する情報、信頼度情報に基づくデータ抽出機能等を拡充した Web アプリケーションによるデータベースとして公開した。

本報告書では、JAEA-SDB に含まれる重要核種(Th, Np, Am, Se, Cs)の K_d データのうち、第 2 次取りまとめの性能評価におけるレファレンスケース、深地層研究施設との関連から花崗岩系に着目するとともに、地質環境に広く存在する鉄やアルミニウムの酸化物/水酸化物系を対象として、これまでに報告してきた手法に従って信頼度評価を実施した。その結果として、1,373 の K_d データに対して、新たな信頼度情報が付与された。この信頼度評価手法は、収着データベースから利用可能な関連データ群を速やかに抽出し、 K_d データ設定の際に参照すべきデータを適切に選定する上で、有効な手法となると考えられる。

核燃料サイクル工学研究所 (駐在) : 〒319-1194 茨城県那珂郡東海村村松 4-33

* BMG ENGINEERING LTD, スイス連邦共和国

※技術開発協力員

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1. Introduction

Sorption of radionuclides in buffer materials (bentonites) and rocks is one of the key processes in the safe geological disposal of radioactive waste. Japan Atomic Energy Agency (JAEA) has developed sorption database (JAEA-SDB) which includes extensive compilation of sorption K_d data by batch experiments, extracted from published literatures. JAEA published the first SDB as an important basis for the H12 performance assessment (PA) (Shibutani et al., 1999). JAEA has been and is continuing to improve and update the SDB in view of potential future data needs.

As part of this on-going development program, JAEA has focused on;

- keeping the databases up-to-date (Suyama and Sasamoto, 2004; Saito et al., 2007),
- assuring the desired quality level (Ochs et al., 2007; Saito et al., 2008),
- testing the usefulness of the SDB to K_d -setting for possible PA-related applications (Ochs et al., 2008).

The JAEA-SDB includes more than 24,000 K_d data which are related with various conditions and methods, and different reliabilities. Accordingly, the quality assuring (QA) and classifying guideline/criteria has been developed in order to evaluate the reliability of each K_d value (Ochs et al., 2007; Saito et al., 2005). The reliability of K_d values of key radionuclides for bentonite system (Ochs et al., 2007) and mudstone system (Saito et al., 2008) has been already evaluated. To use these QA information and to extract reliable data based on QA/classification, the new web-based JAEA-SDB has developed and published in March, 2009 (Tachi et al., 2009).

In this report, the QA/classification of selected entries for key radionuclides (Th, Np, Am, Se, Cs) in the JAEA-SDB was done following the approach/guideline defined in our previous report (Ochs et al., 2007; Saito et al., 2008) focusing granite rocks which are related to reference systems in H12 PA and possible applications in the context of URL activities, and Fe-oxide/hydroxide, Al-oxide/hydroxide existing widely in geological environment.

In the chapter 2, the QA criteria and classification scheme defined in our previous report (Ochs et al., 2007) are described. And in the chapter 3, classifications of selected entries for granite, Fe-oxide/hydroxide, Al-oxide/hydroxide in the JAEA-SDB are described by each item. In the appendix, the details of the evaluation and classifications for the selected entries of the SDB are listed.

2. Reliability of JAEA-SDB: Classification Guideline

2.1 Introduction, description of main criteria

The reliability of K_d values in the JAEA-SDB can be assessed using the following three main criteria. The three main criteria are listed in the expected sequence of application during a classification of entries in the JAEA-SDB. Criteria I-a and I-b are related to documentation and data entry, whereas the technical and scientific quality of an entry is addressed by criteria II and III.

Criteria I — Completeness of documentation and type of K_d information:

- a) It needs to be verified that the documentation of each entry is detailed enough to allow further examination according to the main criteria II-III. At this point, only the completeness of the documentation is examined; the appropriateness of the reported data and approaches is evaluated under criteria II below.
- b) This point takes also into account that the reliability of data input to the JAEA-SDB will be substantially high if K_d values are directly available in table format in comparison to literature that reports e.g. %-adsorbed values in a graph. The latter way of reporting requires the operator to i) manually read values off a graph and ii) to calculate K_d from the %-adsorbed and Solid/water ratio (s/w) values given, which significantly increases the likelihood of an operator error during data input.

Criteria II — Quality of reported data

This is the most important issue from a technical and scientific point of view. This criteria encompasses an evaluation of the appropriateness of the experimental system to produce reliable K_d data. The methods used (or lacking) for determining experimental uncertainty are also examined for each literature source. Further, it is considered whether the data represent single-point measurements or are part of e.g. an isotherm, which would provide additional support for their reliability.

Criteria III — Consistency of data:

While the previous two main criteria address the reliability of each K_d entry in the JAEA-SDB, criteria No. III requires an examination of the level of support that other K_d values in similar systems can lend to the entry under consideration. Any disagreement with data from related systems will have to be evaluated as well. It could be argued that this kind of data examination may be left to the user of the JAEA-SDB. However, the classification of data entries in the JAEA-SDB in terms of reliability adds an aspect of quality that is above that for a pure compilation, and users may expect that the listed K_d values passed some kind of check for internal consistency.

Internal consistency means that data from different sources should not be in obvious disagreement. An example would be the dependency on pH of K_d values for a certain radionuclide, which should be approximately similar in all studies. Similarly, if many studies indicate e.g. stronger sorption of U(IV) than of Th(IV), for any study that indicates the opposite an appropriate explanation should be given. If no good reason can be found, such deviations make a study less reliable. These types of considerations will only be possible for sufficiently well researched elements.

2.2 Description of checkpoints within each main criteria

2.2.1 General

Each entry in the JAEA-SDB (each K_d value identified in the JAEA-SDB by a unique ID) should be evaluated and classified individually. Because many studies report K_d values under different experimental conditions, it is not sufficient to evaluate all data based on a given reference globally. Depending on conditions, different entries related to a given study may receive a different rating.

2.2.2 Criteria I: Completeness of documentation and type of K_d information

The checkpoints under I-a are used for a screening prior to a further classification. Failure to satisfy these checkpoints will not be used (unreliable).

I-a.1 Are all mandatory fields completed? Here it is only verified that all fields have been completed by the operator; an entry "not reported" is counted, therefore. The following entries are considered mandatory:

- element
- solid phase
- solution composition
- atmosphere
- pH (or other information that allows to derive pH, e.g. portlandite equilibrium)
- pe/redox condition (only in case of redox-sensitive systems)
- method of pe control (only in case of redox sensitive systems and imposed reducing conditions)
- initial radionuclide (RN) concentration (except for RN that are not solubility controlled)
- method for phase separation
- type of experiment, if different from batch

- In case of missing entries, the corresponding K_d is excluded from further evaluation and classified as unreliable (until remedied by operator). If all fields are completed, proceed to I-a.2.

I-a.2 Is all mandatory information provided? Here it is evaluated whether critical information is provided or lacking completely. The quality of the information provided is evaluated under criteria II. In addition to the information listed under I-a.1, further mandatory information includes:

- units

- In case of missing mandatory information, the corresponding K_d is excluded from further evaluation and classified as unreliable. If all fields are completed, proceed to I-b.

I-b Does the type of K_d information provided require manipulation by the operator?

- The following levels are distinguished:

- class 1: table with K_d values given
- class 2: table with % sorbed given
table with residual concentration given
- class 3: linear graph K_d
- class 4: linear graph % sorbed
linear graph residual concentration
- class 5: logarithmic graph K_d
- class 6: logarithmic graph % sorbed
logarithmic graph residual concentration

2.2.3 Criteria II: Technical and scientific quality of reported data

It is generally assumed that the entries presently contained in the JAEA-SDB correspond to a minimum quality standard; i.e. are assumed to be basically reliable. The different checkpoints regarding experimental quality are designed to distinguish different levels of reliability. However, if in case of critical checkpoints even the requirements leading to the lowest rating are not met, the respective entry should be classified as unreliable (indicated for each checkpoint).

II-a Solid phase (substrate)

It is evaluated whether the solid phase has been sufficiently characterized. This is equally important for properly designing experiments, as well as for using the measured K_d values. In general, three types of key information are

required:

- Information about major mineral composition.
- Information about accessory minerals or impurities.
- Information about surface characteristics: Minimum is a measure of sorption capacity per mass of sorbent, such as CEC or a different measure of site density per mass.

However, the amount of information required to sufficiently characterize a given solid phase also depends on the complexity of the substrate:

1. It needs to be known whether a substrate consists of a single pure mineral phase, or whether it contains impurities or additional minerals. In general, some measure of site density per mass (e.g. CEC) needs to be known to properly design experiments, in particular with respect to achieving reasonable surface loading.
2. In case of simple substrates (pure minerals), no further information is necessary.
3. In case of complex substrates (i.e., where significant impurities are present, or where a substrate is composed of several minerals), and in particular in case of natural samples, detailed information on composition has to be provided in addition.
4. In cases where sample treatment (such as crushing or sieving) had been performed, the respective information on particle size also needs to be provided (see II-f). Where any chemical treatments (e.g. acid washing to remove calcite; but also change of redox conditions in case of redox-sensitive substrates, see II-c) had been applied, the applied method and resulting mineralogy should be given as well.
5. In case of many commercially available substrates (e.g., MX-80 or Kunigel-V1 bentonite; standard clay minerals from the Clay Minerals Society, such as SWy-1; Min-U-Sil SiO₂, etc.) detailed solid phase information is widely known and can be retrieved from a large number of publications. Therefore, characterization of such solids is not required for each entry in the JAEA-SDB; i.e., level A or B can be reached even if such information is not reported. Note that this holds only when such solids have been used as received. Where washing procedures etc. have been applied, the procedures and resulting changes still need to be documented.

→ Three levels of reliability:

- A) Major and minor mineralogy as well as surface characteristics are known.
For example: The substrate is a single, well-defined mineral; or comprehensively characterized complex mineral assemblage. Either no sample treatment has been carried out, or it is described in detail and the result are documented.
- B) Major mineralogy as well as surface characteristics are known.
For example: The substrate is a single mineral that may contain impurities (such as a non-purified clay mineral) or a complex mineral assemblage where additional impurities could be present. Sample treatment may have led to minor changes in mineralogy.
- C/D) Information on both major mineralogy or surface characteristics is lacking.
For example: There is no information on CEC (or another measure of sorption capacity); or the substrate is a natural clay sample where it is not clear whether it is smectite, kaolinite, or illite; or a non-characterized soil or crushed rock. Sample treatment may have led to major changes in mineralogy that are not documented.

II-b Adjustment and control of pH

One of the most important solution parameters controlling radionuclide(RN) sorption is pH. It needs to be known to interpret K_d values, but also for proper experimentation: The pH needs to be known to evaluate the solubility limits of radionuclides and some major ions, as well as the stability of certain mineral phases (in particular carbonates). Further, pH has to be approximately constant during a sorption experiment in order to reach equilibrium of sorption reactions. There are two basically different approaches in sorption experiments with regard to pH control:

1. The pH is not controlled, but allowed to reach an equilibrium value according to the experimental conditions and is then measured at the end of the experiment. In this case, it is important that the pH has been verified after experimentation, in order to know its equilibrium value.
2. The pH is controlled during the experiment by acid-base addition and/or buffers. Where it is desired to determine K_d values as a function of pH, this cannot be avoided. In this case, it needs to be

shown (or known from the literature) that the added acids, bases, or buffers do not interfere with RN reactions at the surface (which obviously influence sorption) or with RN reactions in solution (which influence sorption through changing the RN speciation). Therefore, use of a non-inert pH buffer at unspecified concentration levels leads to a classification as unreliable.

- Four levels of reliability:
- A) To achieve rating A it is sufficient, but required, that the pH is verified at the end of the experiment. This is based on the assumption that equilibrium or at least a stable state of near-equilibrium conditions has been achieved (see also II-a, II-d, and II-j). In such systems, a determination of the experimental end pH will represent an adequate measure of the actual equilibrium pH. Second, rating A is given where the successful use of inert buffers has been demonstrated (e.g. by measuring K_d in the presence and absence of buffers at some pH, or by showing through speciation calculations that the buffer does not influence RN behavior). In some cases, level A may also apply if a non-inert buffer is part of the experimental setup (see the example of K_d determination as a function of carbonate concentration under point C).
 - B) The final pH is reported, but only a pH range (within 1 pH unit) is given instead of a discrete pH value (the same assumptions regarding equilibrium can be made as for level A above). Rating B also applies in cases where only the initial pH is provided, but the experimental system is well buffered (for example, because a inert buffer is used, or because of the presence of a natural buffer system, such as carbonate).
 - C) Only the initial pH is provided, no attempt is made to control final pH. All cases where non-inert pH-buffers are being added. Note that this refers to the addition of an additional complexing ligand, such as acetate, for the control of pH. On the other hand, if a sorption experiment is carried out where K_d is measured as a function of carbonate concentration and this is simultaneously used to control pH, level A applies (given that the effect of carbonate on K_d is documented).
 - D) Only a range (within 1 pH unit) of initial pH is provided, no information on final pH is given.

- If a lower quality than required for level D is evident, the respective entry is excluded from further evaluation as unreliable. If a non-inert buffer (e.g. acetate or carbonate) is used at unspecified concentration levels, the respective entry is excluded from further evaluation as unreliable.

II-c Redox conditions

Here it needs to be differentiated between systems that are not redox-sensitive and systems that are. Within the redox-sensitive systems, it needs to be further taken into account whether only the sorbing RN is redox-sensitive or whether other components of the system (such as solid phase or groundwater components) are redox-sensitive as well.

In this sense, checkpoint II-c deals with the redox control of the sorbing RN, not with redox control of an overall redox-sensitive system. If the experimental system comprises a range of redox-sensitive dissolved (e.g. organics) and solid (e.g. Fe- and Mn-phases) components, imposing redox conditions different from the original level may influence many redox-equilibria simultaneously. In such a case it can be very difficult to ascertain equilibrium or to know which solid phases are present. Such effects on solution and solid phase chemistry are addressed by checkpoints II-a and II-d. It also needs to be pointed out in this context that "imposed redox condition" does not necessarily refer only to imposing reducing conditions by adding a reducing agent, it also includes imposing oxidizing conditions by e.g. transferring a reduced natural sediment to the laboratory and exposing it to O₂ (as a matter of fact, the latter may be the more common problem).

Given the focus of this checkpoint on redox control of sorbing radionuclides explained above, two different requirements on data quality can be distinguished. Levels of reliability reflect the degree to which these two requirements are met:

1. Reliability regarding control and confirmation of the redox status of the sorbing RN.
2. Reliability regarding the absence of unwanted side effects, such as changes in RN speciation induced by the addition of a reducing agent.

→ Two levels of reliability:

A/B) Level A/B applies to entries in the JAEA-SDB where it is demonstrated that both of the above requirements are met: This

includes the following cases:

- Systems which are not redox-sensitive in terms of sorption and where no reducing agents needed to be added (i.e., where the sorbing RN can take on only one oxidation state in aqueous solutions).
- Redox-sensitive systems that have been pre-equilibrated with and are being kept at ambient conditions.
- Experiments where reducing conditions are imposed on redox-sensitive RN (in otherwise stable systems) and where similar results are obtained using several reducing agents.

C/D) Level C/D applies to entries in the JAEA-SDB where meeting the above requirements may not have been demonstrated, but can be assumed with high certainty. This includes the following cases:

- Reducing conditions imposed on redox-sensitive RN (in otherwise stable systems) using one reducing agent that can be estimated (e.g. from experience or from the literature) to be effective and to be sufficiently inert with respect to influencing RN behavior.
- In cases where complexing reducing agents have been used, level C/D still can be achieved if the influence of the reducing agent on RN speciation has been estimated.
- All cases where redox conditions may be less well defined than for level A/B, but where it can be assumed that no significant artifacts regarding RN behavior are introduced and where the oxidation state of RN has been measured independently (in some cases, this may include low-O₂ conditions with a subsequent confirmation of RN oxidation state). Evaluating the reliability of such measurements is likely to require an expert decision by the operator.

→ If a lower quality than required for level C/D is evident, the respective entry is excluded from further evaluation as unreliable. For example, cases where it has been attempted to achieve reducing conditions only by minimizing the level of O₂ (e.g., by performing experiments in a N₂ atmosphere) generally should be labeled "unreliable" (except where the oxidation state of a RN somehow has been confirmed, see description of level C/D). Also, if a strongly complexing reducing agent (such as many organic acids) is used at unspecified concentration levels, the respective entry is excluded from further evaluation as unreliable.

II-d Final solution composition

Note that solution composition includes dissolved carbonate concentration, which may be controlled through, or expressed as $p\text{CO}_2$. Added pH-buffers or reducing agents are also included, and are addressed in checkpoints II-b and II-c.

→ Two levels of reliability:

A/B) The final solution composition is known (either from direct measurements or from the initial experimental setup and speciation calculations) and corresponds to equilibrium or is otherwise well constrained. All major components are included in the analysis. Relevant minor components (e.g. traces of carbonate or of other complexing ligands) may only be estimated. Some minor components may be unknown. In case of natural water samples, solutions are (or can be) shown to be charge balanced (within 5 %). The information on final solution composition can be obtained from i) analyses of the actual sorption samples or from ii) using pre-equilibrated solutions that had been analyzed prior to the actual sorption experiments.

C/D) The critical major solution components are known, or can be estimated approximately. There may be unknown minor components and/or less critical major components. In case of natural water samples, solutions are approximately charge balanced (within 10 %).

→ If a lower quality than required for level C/D is evident, the respective entry is excluded from further evaluation as unreliable.

II-e Temperature

Here, it is evaluated whether temperature is specified and kept constant.

→ Two levels of reliability:

A/B) Temperature is approximately specified (e.g. room temperature) and constant, or varied in a controlled fashion.

C/D) Temperature is not specified at all (i.e., it is not clear whether the experiments had been performed at room temperature or not).

II-f Liquid/Solid ratio (L/S) and grain size

It is evaluated whether enough solid had been added to avoid a significant influence by the vessel walls (see II-m), and to ensure sample reproducibility and representativeness in case of complex substrates, especially in case of

large grain sizes: It is estimated that in cases where less than ca. 100 mg of solid (this value depends on grain size) has been added to each experimental vessel, sample reproducibility and representativeness becomes difficult to achieve in case of complex or crushed samples.

→ Two levels of reliability:

A/B) Enough solid had been added to each vessel to assume that

- a) [surface area sorbent] » [surface area vessel], i.e. that at least 5 m² of sorbent surface had been added to each vessel, and to assume that
- b) samples are reproducible and representative.

What is enough substrate clearly depends on specific surface area and homogeneity. Fulfilling the above two requirements is typically not a problem in case of relatively homogeneous sorbents with a high specific surface area (such as clay minerals or bentonite), where "enough" may mean at least ca. 100 mg. On the other hand, "enough" may mean at least one to several grams in case of rocks (depending on specific surface area, grain size and complexity of the sample).

C/D) Any other than the above.

II-g Sorption value

It is evaluated whether an appropriate experimental design had been employed to avoid sorption values near 0% or 100%, which can lead to higher experimental uncertainty. This problem can be addressed by choosing an appropriate L/S ratio (see II-f) or/and an appropriate initial concentration of RN ([RN]) (see II-h). However, the choice of [RN] is more restricted by solubility and analytical detection limits.

A) The sorption value is in the range of 5% - 95% sorbed.

B) The sorption value is inside the range of 2% - 98% sorbed.

C/D) Any other than the above.

II-h Initial RN concentration ([RN])

This parameter is used to evaluate the likelihood of a possible supersaturation of RN-phases:

→ Three levels of reliability:

A) RN is not solubility limited, or initial [RN] was clearly (at least a

factor of 5) below the solubility limit. Note that factor 5 does not take into account uncertainties in RN solubility; i.e., if the solubility of a given RN cannot be estimated with more certainty than e.g. 10^{-6} to 10^{-8} M, then initial [RN] has to be $\leq 2 \times 10^{-9}$ M for rating A to apply.

- B) Initial [RN] was clearly below the solubility limit, but maybe less than a factor of 5 (see above).
- C/D) [RN] was very small, and in all likelihood below their maximum solubility, but the solubility limit cannot be established clearly due to missing information (solution composition) or lacking thermodynamic data.
- Note that the solubility limit can be defined on either thermodynamic calculations or on experimental data obtained under the relevant conditions.
- If initial RN concentration had been clearly above the respective solubility limit, the respective entry is excluded from further evaluation as unreliable.

II-i Phase separation

Here, the appropriateness of phase separation is evaluated: Note that in cases where colloids or other artifacts are important, different phase separation methods will not lead to the same results. Identical or very similar results with different efficient methods are probably the best direct proof of absence of important colloid effects; hence such studies are rated A. Rating B would be given for methods that can be presumed to remove colloids, but where no direct proof as in A is given.

- Three levels of reliability:
- A) Identical (very similar) results are obtained with different methods of phase separation, where at least one method needs to be efficient in terms of colloids removal (ultrafiltration or high-speed centrifugation). Accordingly, the best comparison would be between two efficient methods, such as ultrafiltration and high-speed centrifugation. Note that such a comparison of phase separation methods is not required for each individual K_d value: For example: If the absence of artifacts has been demonstrated for some representative samples of a study by comparing an efficient and a standard method of phase separation, the rating A may be given to all datapoints of this study,

even if they correspond to the standard method only.

- B) Only one, but efficient method (high-speed centrifugation, ultrafiltration) is used, and there is no evidence for artifacts such as colloid effects or significant sorption to the filter.
- C/D) Only one general method (normal centrifugation, membrane filtration with nominal pore sizes of 0.01~0.45 μm) is used, and there is no evidence for artifacts such as colloid effects or significant sorption to the filter.
- If no phase separation is used, or in case of obvious evidence for artifacts (colloid effect, adsorption on filter) the respective entry is excluded from further evaluation as unreliable.

II-j Reaction time

- Two levels of reliability:
- A/B) Identical (similar) results are obtained with different reaction times, or some other demonstration of near-equilibrium is provided (e.g. separate kinetic experiments).
- C/D) Only one, but reasonably long reaction time is used. What is “reasonably long” is highly dependent on the experimental system: In general, the time needed to reach equilibrium will increase with the complexity of the sorbing substrate and the strength of sorption. Sorption of Sr onto a pure clay mineral through ion exchange can be assumed to be complete within a day; sorption of a trivalent actinide onto a complex substrate may need several days to weeks for completion. In the absence of kinetic information, operator expert decisions will be required to assess this point. If possible, reaction times reported for similar systems included in the JAEA-SDB could be used to evaluate what is reasonably long. Further, even for the most simple systems a reaction time of 1 day is considered as minimum requirement.
- If the requirement for level C/D is not met (i.e., if the reaction time cannot be assumed to be reasonably long), the respective entry is excluded from further evaluation as unreliable.

II-k Agitation method

- Two levels of reliability:

- A/B) Appropriate agitation is required in all cases, except where enough kinetic information is provided to show that equilibrium has been reached. Shaking is the preferred method, as use of stir bars can lead to abrasion of samples. In case of simple and well crystallized substrates (such as Al-oxide) or of substrates with very small grain size that are easily suspended, stir bars can also be accepted.
- C/D) Any other than the above.

II-1 RN loading

Ideal are values as a function of RN loading (i.e., K_d values that form part of an isotherm), otherwise low loading is preferred. RN loading (e.g. in moles RN/kg substrate) refers to the amount of RN adsorbed in relation to the amount of different surface sites available. It is known from classical isotherms (e.g. Langmuir) that a linear sorption can only be assumed if sufficient unoccupied sites are present. In case of simple substrates (including some bentonites), the linear portion of an isotherm extends to fairly high RN loading. There are other cases where K_d depends significantly on RN loading over many orders of RN concentration.

- Three levels of reliability:
- A) At least one isotherm has been determined (for a constant solution composition and L/S), and at least some experiments have been carried out using trace level RN concentration (i.e., at least some data are included within a linear sorption region).
- B) No isotherm is available, but at least a limited variation of initial [RN] or L/S has been carried out, and some experiments have been carried out using trace level RN concentration (i.e., some data are included within a linear sorption region).
- C/D) No variation as in A or B has been carried out.

II-m Reaction vessels

High-density polyethylene (HDPE) or Teflon are preferred over normal PE, which is preferred over glass, which may lead to sorption of radionuclides by the vessel walls. Especially at high or very low pH, glass dissolution and release of dissolved or colloidal silica may also occur. On the other hand, glass is more gas-tight (especially than PE); if that is of experimental relevance. Corrections for sorption on vessel walls should not be necessary if blank tests

show that it can be neglected.

Correction for sorption on vessel walls may be needed to estimate K_d values correctly in some cases, but only in cases where a) sorption on the vessel is much stronger than on the solid sorbent, or b) if the vessel offers a significant surface area in comparison to the sorbent (see II-f). If that is not the case, the sorption on the added solid will be much greater than on the vessel in a system where both solid and vessel are present. It is further an erroneous assumption that sorption on the vessel will be same in i) the absence of the solid (no competition for RN by solid) as ii) in the presence of the solid (strong competition for RN by solid). The sorption on the walls is typically much smaller in ii) than in i). Therefore, the overall mistake is often bigger if sorption on the vessel wall is accounted for than if it is neglected.

If effects of vessel walls are corrected for, it has to be done by extracting any RN sorbed to vessel walls after experimentation (e.g. by acid washing) and establishing a complete mass balance.

→ Three levels of reliability:

- A) An appropriate vessel has been used (taking into account sorption as well as tightness with respect to CO_2 or O_2 , where required), and corrections for sorption on vessel wall have been performed or no sorption on vessel wall has been observed by blank tests. If effects of vessel walls are corrected for, it has to be done by extracting any RN sorbed to vessel walls after experimentation (e.g. by acid washing) and establishing a complete mass balance. If the sorption on vessel wall has been determined as significantly lower (at least two orders of magnitude in terms of K_d) than the actual K_d value and thus corrections for sorption on vessel wall have not been performed, such a case would also correspond to level A
- B) An appropriate vessel has been used, and corrections for sorption on vessel walls have not been performed.
- C/D) The vessel used may have been not appropriate (this is often the case with glass, see above), or corrections for sorption on vessel wall have been performed based on a blank test only (i.e., without verifying that sorption on vessel walls is relevant in the presence of a solid added, thus possibly leading to overcorrection).

II-n Uncertainty estimates

In general, uncertainties based on repeated experiments (i.e., actual observations of K_d) are preferred over uncertainties based on error propagation, as the latter is an estimate based on a type of extrapolation. Thus, the difference between levels of reliability is mainly based on the amount of actual information gained by repetitions: For level A, the entire experiment is repeated; for level B, only sampling and analysis are repeated; for C, no repetitions are carried out.

Values that are based on repetitive experiments are preferred over single experimental data points. Note, however, that this checkpoint refers to single-point K_d values and may be overruled by data being part of e.g. pH-edge, isotherm, kinetic experiment, etc., which may provide independent evidence of good reproducibility or systematic errors (see checkpoint II-o).

→ Four levels of reliability:

- A) Uncertainties in K_d are derived based on entire, replicated sorption experiments (i.e., at least duplicate experiments).
- B) Uncertainties in K_d are derived based on single sorption experiments that are sampled and analyzed repeatedly. This may be supplemented by error propagation.
- C) Uncertainties in K_d are based on error propagation of estimated analytical and/or procedural uncertainties.
- D) No error estimate is given, no repeated sampling is done.

II-o Parameter variation

Studies with a systematic variation of key parameters are much more valuable and reliable than single K_d measurements. In this context, key parameters are those that influence sorption (for example, chemical parameters such as RN concentration, pH, $p\text{CO}_2$, but also temperature, L/S, or grain size in case of crushed substrates), but not parameters that only help to determine the experimental framework (such as vessel type or reaction time). In particular, variation of key parameters allows improved detection of experimental problems and systematic errors. Especially the latter are not detected by repeating experiments under identical conditions. In the application of this checkpoint, care has to be taken to take into account the characteristics of the particular system studied. For example, more parameter variation may be required to show clear trends in a complicated

system in comparison to a simpler one. On the other hand, the pH and carbonate concentration in experiments with calcite are quite constrained by the solid itself, and only limited variations are possible.

→ Four levels of reliability:

- A) Both RN surface loading (isotherm) as well as a chemical parameter, such as pH or $p\text{CO}_2$ (edge), or e.g. [Na] in case of ion exchange, are varied systematically.
- B) Either RN concentration (isotherm) and/or chemical parameters, such as pH or $p\text{CO}_2$ (edge), or e.g. [Na] in case of ion exchange (i.e., at least two parameters in total), are varied. These variations are less systematic than in A, but still allow to observe trends.
- C) As B, but only one parameter in total is varied.
- D) No parameter variation is done.

2.2.4 Criteria III: Consistency of data

Here it will be evaluated whether data from a particular study can be supported by other studies. Comparisons should only be made with studies that are at least as (or more) reliable than the study under investigation, based on criteria I and II. In many cases, only approximate consistencies or inconsistencies may be apparent, because of different conditions used in the different studies.

- Therefore, the evaluation of criteria III will only be reported in the form of a comment. Any such comments will be included both in a classification report as well as in the corresponding rating summary sheets.
- If the K_d values under investigation are clearly inconsistent with the majority of related reliable studies, and if the reason for this observation cannot be explained, they may also be labeled unreliable based on criteria III. As this requires an expert decision by the operator, the underlying reasoning needs to be clearly documented.

2.3 Overall classification

The above criteria are applied to an overall classification system as follows:

- The three criteria I-III are evaluated separately, the respective results are reported separately as well.
- Criteria I: The checkpoints under I-a are used in a yes/no screening fashion, entries not fulfilling I-a are labeled as unreliable and are not evaluated further.
- Criteria I-b is then used to assign classes 1-6 for documentation.

- Criteria II: a) The datasets that pass Criteria I are again classified according to a 6-level system, where classes 1-6 represent the highest and lowest levels of reliability. To ensure a minimum quality level, certain checkpoints are regarded as critical (marked with * in Table 2.3.1). If the quality of the data does not correspond to the respective minimum requirements, the entries are not to be used and are classified as unreliable.
- b) To facilitate transparent averaging of all checkpoints, the following numerical system is suggested: A=3, B=2, C=1, D=0 (A/B=3 and C/D=0 in some cases).
- c) Initially, checkpoints II-b, II-c, II-d, and II-h are evaluated (indicated in bold letters below). If an entry is rated unreliable for any of these checkpoints, it is excluded from further evaluation.
- d) Weighting of individual checkpoints at this level is done according to the factors given in Table 2.3.1 below.
- e) The total sum of points obtained for Criteria II is then used to indicate the level of reliability. With the present system, the maximum number of points would be 183, leading to an overall classification as follows (Table 2.3.2):

Table 2.3.1 Weighting of individual checkpoints under Criteria II.

checkpoint	description	weighting factor
II-a	solid phase (substrate)	$A \cdot C/D \times 2$
*II-b	pH	$A \cdot D \times 8$
*II-c	redox conditions	$A/B \cdot C/D \times 8$
*II-d	final solution composition	$A/B \cdot C/D \times 8$
II-e	temperature	$A/B \cdot C/D \times 1$
II-f	L/S, grain size	$A/B \cdot C/D \times 2$
II-g	sorption value	$A \cdot C/D \times 2$
*II-h	initial RN concentration	$A \cdot C/D \times 8$
*II-i	phase separation	$A \cdot C/D \times 8$
*II-j	reaction time	$A/B \cdot C/D \times 2$
II-k	agitation	$A/B \cdot C/D \times 1$
II-l	RN loading	$A \cdot C/D \times 2$
II-m	reaction vessel	$A \cdot C/D \times 1$
II-n	uncertainty estimates	$A \cdot D \times 2$
II-o	parameter variation	$A \cdot D \times 8$

* indicates critical checkpoints with minimum requirements;

bold letters indicate the checkpoints to be evaluated initially

Table 2.3.2 Overall classes of reliability for Criteria II

points	rating
183-151	class 1
150-121	class 2
120-91	class 3
90-61	class 4
60-31	class 5
30-0	class 6

- Criteria III: Criteria III is used to qualitatively assess consistency with other studies. In case of clear inconsistencies, an entry may be labeled as unreliable.
- Overall, the following classification system is used, with Criteria II as the main basis for assessing the reliability of entries in the JAEA-SDB.

Table 2.3.3 The classification system

Criteria	classification
I-a	accept/reject
I-b	6 classes of K_d information
II	6 classes of data quality and reliability
III	qualitative level of consistency with other studies

3. Classification of selected entries for granite, Fe-, Al-oxide/hydroxide in the JAEA-SDB

This section presents the classification results for selected entries in the JAEA-SDB covering the datasets for the sorption of Th, Np, Am, Se and Cs on granite and Fe-, Al-oxide/hydroxide.

- An overview of the results as well as the corresponding numerical rating is given in the Appendix.
- For transparency and ease of presentation, all results of Criteria I and II are presented in tabular form, using the format of the following table throughout. The results pertaining to Criteria III are discussed subsequently and are illustrated in the form of plots of K_d vs. a relevant master variable (typically pH), where applicable.
- According to the established classification guideline, criteria I and checkpoints II-b, II-c, II-d, II-h were evaluated first. Classification and final numerical rating were only completed when an entry was evaluated as reliable based on these checkpoints. Otherwise, entries were labeled "unreliable" and were excluded from further evaluation. For most reliable entries, criteria III was evaluated as well.

3.1 Criteria I and II

Data table Element/#: REF: original reference JAEA-SDB version # – DATA: element/solid sorbent, datapoint # GUIDELINE: Revision # (date)		
Checkpoint ¹ "SDB"/"REF"	Evaluation	Rating
I-a.1	Are all mandatory fields completed?	Yes/No
I-a.2	Is all mandatory information provided?	Yes/No
I-b	Type of K _d information	class 1-6
II-a	Solid phase (substrate)	A-C/D
II-b	Adjustment and control of pH	A-D
II-c	Redox conditions.	A/B-C/D
II-d	Final solution composition	A/B-C/D
II-e	Temperature	A/B-C/D
II-f	Solid/water ratio (L/S) and grain size	A/B-C/D
II-g	Sorption value	A-C/D
II-h	Initial RN concentration [RN]	A-C/D
II-i	Phase separation	A-C/D
II-j	Reaction time	A/B-C/D
II-k	Agitation method	A/B-C/D
II-l	RN loading	A-C/D
II-m	Reaction vessels	A-C/D
II-n	Uncertainty estimates	A-D
II-o	Parameter variation	A-D

- ¹ Application of the checkpoint to the information given in the JAEA-SDB is indicated with "SDB".
"REF" indicates the additional application to the original reference indicated in each table.

3.1.1 Americium

Data table Am/1: REF: Allard and Beall (1979)* JAEA-SDB version 4 - DATA: Am/Granitic rocks; granite, #42188 GUIDELINE: Revision 4b (May 19, 2005) *REMARK: K_d value is based on prediction and therefore excluded from classification.		
Checkpoint	Evaluation	Rating
I-a.1 SDB	All mandatory fields are completed.	Yes
I-a.2 SDB	The datapoint is not evaluated, since it is predicted and not measured.	No, unreliable

Data table Am/2: REF: Allard et al. (1978)* JAEA-SDB version 4 - DATA: Am/Granitic rocks; granite, #42222, 42223 GUIDELINE: Revision 4b (May 19, 2005) *REMARK: Checkpoints I-b, II-b, II-c and II-i should be updated/revised.		
Checkpoint	Evaluation	Rating
I-a.1 SDB	All mandatory fields are completed.	Yes
I-a.2 SDB	All mandatory information is provided.	Yes
I-b SDB REF	K_d values are provided in a table in [m ³ /kg] There are five K_d values reported. The K_d values indicated in the SDB do not correspond to the reported values in the reference	class 1 (update SDB)
II-a SDB	As solid phase granite is indicated. Major mineralogy and surface characteristics are not reported.	C/D
II-b SDB REF	Initial and final pH values are indicated. Apparently for examinations concerning complex formation and solubility a pH of 7 to 9 was applied. Seemingly no pH values are reported for the sorption experiments, but it is assumed that experiments had been performed at a pH of 7 to 9.	(update SDB) C (tentative)
II-c SDB REF	Redox state of Am is indicated as +III. Experiments had been performed under aerobic and under reducing conditions with Fe(II/III) present in solution. Eh values are indicated to be -0.15 to -0.21 V for experiment #42222. Am is not redox sensitive. Eh values are reported to be -0.15 to -0.27 V in a pH range of 7 ~9.	A/B
II-d SDB REF	It is indicated that experiments had been performed in synthetic groundwater aq293. Final solution composition is reported. There are datapoints of sorption experiments with another synthetic groundwater aq1105 available. For datapoint #42222 the concentration of reducing agent Fe(II/III) in solution is not reported.	unreliable

Data table Am/3: REF: Allard et al. (1979b) JAEA-SDB version 4 - DATA: Am/Granitic rocks; granite, #42259-42264 GUIDELINE: Revision 4b (May 19, 2005)		
Checkpoint	Evaluation	Rating
I-a.1 SDB	All mandatory fields are completed.	Yes
I-a.2 SDB	All mandatory information is provided.	Yes
I-b SDB	A table with log K_d values is provided.	class 1
II-a SDB	As solid phase granite is indicated. Mineralogy and surface characteristics are not reported.	C/D

II-b	SDB	Initial pH values are reported.	C
II-c	SDB	Oxidation state of Am is not reported. Since experiments had been performed under aerobic conditions, it is assumed that americium was in the oxidation state (+III). Americium is not redox sensitive. Eh values are not reported.	A/B
II-d	SDB	Detailed composition of two synthetic groundwaters is indicated.	A/B
II-e	SDB	A reaction temperature of 25°C and 65°C is indicated.	A/B
II-f	SDB REF	A L/S ratio of 10~50 mL/g is indicated. An apparent surface to mass ratio of <10 m ² /kg is reported. Assumed that this is the specific surface of granite, with 1~3 g of solid phase per reaction vial the total surface is 0.01~0.03 m ² /vial.	C/D
II-g	SDB	Sorption values are calculated from K _d and L/S are all >99%.	C/D
II-h	SDB REF	An initial Am concentration of $<1.0 \times 10^{-8}$ M is indicated. Based on speciation calculations (for 25°C) with Phreeqci 2.14.3 using the data in the NAGRA-PSI thermodynamic database (Hummel et al., 2002) the indicated Am concentration is at a pH 8.2 clearly below the solubility limit in both solutions, aq293 and aq1105.	A
II-i	SDB REF	It is indicated that samples had been centrifuged for 50 min. at 7,000 rpm and filtration over 0.2 µm membrane filter. It is reported that the filtration did not change the sorption values.	A
II-j	SDB REF	A contact time of 7 and 180 days is indicated. The K _d values of equal experiments but different reaction times differ by a factor of about three. Since there is only the initial pH value provided and the reaction time of 7 days is considered to be reasonable long, the data with a reaction time of 180 days are assessed as unreliable. •#42261, 42262 •#42259, 42260, 42263, 42264 The natural groundwaters contain 0.5 and 20 mg/L of iron. Reported K _d values of Th and Am show a significant increase at a contact time of 180 days, whereas K _d values of Cs do not differ much from the values measured after 7 days. On the basis of this information, sorption of Am and Th onto iron oxides is very likely during a contact time of 180 days.	unreliable C/D
II-k	REF	The samples were shaken.	A/B
II-l	SDB	No variation in [Am] or the L/S is indicated.	C/D
II-m	REF	The experiments were carried out in glass bottles. Corrections for sorption on the vessel walls have not been bone.	C/D
II-n	REF	No error information is available.	D
II-o	REF	Sorption was measured at two different temperatures.	C

Data table Am/4: REF: Allard et al. (1980)*

JAEA-SDB version 4 - DATA: Am/Granitic rocks; granite, #42525-42528

GUIDELINE: Revision 4b (May 19, 2005)

*REMARK: Due to incorrect K_d values in the SDB, classification was mainly performed on the basis of information of the reference. Checkpoints I-a.2, II-a, II-b, II-f and II-i should be updated/revised.

Checkpoint	Evaluation	Rating
I-a.1 SDB	All mandatory fields are completed.	Yes

I-a.2	SDB	All mandatory information is provided. Incorrect K_d values were transmitted from the reference to the SDB.	No, (update SDB)
I-b	REF	A graph with logarithmic K_d values is provided.	class 5
II-a	SDB REF	As solid phases the climax stock and the westerly granite are indicated. It is indicated that CEC or BET values are not reported. Surface characteristics (CEC and BET) of the mineral components are reported.	(update SDB) A
II-b	SDB REF	Indicated pH values do not correspond to the information in the reference. Initial and final pH values are reported.	(revise SDB) A
II-c	SDB REF	It is indicated that no information about the oxidation state is reported. Am in the oxidation state (III) is reported. Am is not redox sensitive. It is assumed that experiments had been performed under ambient conditions, no oxidizing or reducing agents had been added to the reaction mixture.	(update SDB) A/B
II-d	SDB	Experiments had been performed in synthetic groundwater. Final solution composition is indicated.	A/B
II-e	SDB	It is indicated that experiments had been performed at 22 °C.	A/B
II-f	SDB REF	It is indicated that the amount of solution and solid phase is not reported. Rating is done based on the indicated L/S ratio of 0.08~0.1 L/g. Specific surface at a particle size of 0.044 to 0.063 mm of climax stock granite and westerly granite is about 8 to 8.5 m ² /g.	(update SDB) A/B
II-g	SDB	The sorption values will be classified after the update of SDB.	—
II-h	SDB REF	An initial Am concentration of 2.0×10^{-9} M is indicated. Based on speciation calculations (for 25°C) with Phreeqi 2.14.3 using the thermodynamic data in NAGRA-PSI (Hummel et al., 2002) the initial Am concentration is clearly below the solubility limit.	A
II-i	SDB REF	It is indicated, that no separation procedure is reported. Samples had been centrifuged for 1h at 4,000g.	(update SDB) C/D
II-j	SDB	A contact time of 5 days is indicated.	C/D
II-k	REF	No agitation method is indicated.	C/D
II-l	SDB	No variation in [Am] or the L/S is indicated.	C/D
II-m	REF	There is no information about the reaction vessel. Blank measurements had been performed, but no correction for the adsorption to the vessel walls was made, since this was deemed unnecessary.	C/D
II-n	REF	There is no error information reported.	D
II-o	REF	No parameter variation is indicated.	D

Data table Am/5: REF: Barney and Anderson (1979)* JAEA-SDB version 4 - DATA: Am/Granitic rocks; granite, #44233-44237 GUIDELINE: Revision 4b (May 19, 2005) *REMARK: Update of SDB required for checkpoint II-b.		
Checkpoint	Evaluation	Rating
I-a.1 SDB	All mandatory fields are completed.	Yes
I-a.2 SDB	All mandatory information provided? Information about the pH (initial and final), the groundwater composition and the mineral composition is missing. See checkpoints II-a, II-b and II-d for annotations.	No
I-b SDB	A table with K_d values is given.	class 1
II-a SDB REF	As solid phase granite#1 and granite#2 is indicated. Mineralogy is not reported. Specific surface area for granite#1 is given. The 'granite' used for experiments was fresh crushed quartz monzonite porphyry from the Nevada test site and a weathered one. Only qualitative mineralogy is reported in a previous report.	C/D
II-b SDB REF	It is indicated that no pH is reported. It is reported that pH was 8.4 on average and about constant over 91 days.	B (update SDB)
II-c SDB REF	Redox conditions are not indicated. Initial Eh values are listed. Am is not redox sensitive. Experiments had been performed under aerobic conditions.	A/B
II-d SDB	As water type groundwater is indicated. The solution composition is not indicated. From dissolution curves for elemental components of granite in synthetic groundwater at different times it is concluded that no equilibrium was reached even after a contact time of 92 days.	unreliable

Data table Am/6: REF: Barney and Brown (1979)* JAEA-SDB version 4 - DATA: Am/Granitic rocks; granite, #44319-44321 GUIDELINE: Revision 4b (May 19, 2005) *REMARK: Update required for checkpoint I-a.2.		
Checkpoint	Evaluation	Rating
I-a.1 SDB	All mandatory fields are completed.	Yes
I-a.2 SDB	All mandatory information is provided. Information about the pH, synthetic groundwater composition and redox conditions are provided.	No (update SDB)
I-b SDB	The K_d values are listed in a table in [mL/g].	class 1
II-a SDB REF	As solid phase granite#1, #2 and #3 are indicated. Mineralogy is not indicated. For granite#1 BET and CEC, and for granite#2 CEC is indicated. The 'granite' used for experiments was crushed quartz monzonite porphyry from Nevada test site. There are two granite samples A and B reported with qualitative information about mineralogy. K_d values are given for a fresh and two types of weathered granite samples. However it is not clear from the data, if these samples correspond to granite A or B.	C/D (tentative)
II-d SDB	The solution components of used synthetic groundwater are indicated in the SDB under the category of solid phase. From dissolution curves for elemental components of granite in	unreliable

	synthetic groundwater at different times it is concluded that no equilibrium was reached even after a contact time of 150 days. Therefore the datapoints are considered as unreliable.	
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Data table Am/7: REF: Baston et al.(1998) JAEA-SDB version 4 –DATA: Am / Granitic rocks, Granodiorite, #65946-65951 GUIDELINE: Revision 4b (May 19, 2005)		
Checkpoint	Evaluation	Rating
I-a.1 SDB	All mandatory fields are completed.	Yes
I-a.2 SDB	All mandatory information is provided.	Yes
I-b SDB	Tables with K_d are given.	class 1
II-a SDB REF	The solid phase is indicated as granodiorite. Mineral composition of granodiorite is reported in Berry et al.(2007).	A
II-b SDB REF	Final pH values are reported. No use of any pH-buffer is reported. The pH value is monitored every 7 days, the pH adjusted back to the appropriate value.	A
II-c SDB REF	Experiments are performed under N_2 . The oxidation state of Am is reported as III. Final Eh values are provided, as well as the reducing agent used ($Na_2S_2O_4$) at an initial concentration of 2.5×10^{-3} M. O ₂ levels are reportedly <1 ppm. All solutions are de-oxygenated by bubbling an argon(96%) /hydrogen(4%) mixture through them before posting into the glovebox. Also, Am is not a redox sensitive element.	A/B
II-d SDB REF	A de-ionized water after equilibration with graodiorite is reported as input solution; main solution compositions are indicated in the additional file “solution composition”. Samples are filtered using a 10000MWCO filter prior to analysis.	A/B
II-e SDB	A temperature of 60°C is reported.	A/B
II-f SDB	It is indicated that L/S ratio of 5 mL/g had been used, but that the specific solid mass and solution volume are not reported. Assuming that the solution volume is ≥ 20 mL would mean a corresponding solid mass of at least 1 g. This is accepted as reasonable.	A/B
II-g SDB	Based on the information provided in the JAEA-SDB, all K_d values can be calculated: • #65946, #65947 : 95%<%-sorbed values<98% • #65948-65951 : %-sorbed values >99%.	B C/D
II-h SDB	1.2×10^{-10} M is indicated as initial Am concentration. Based on the data in Rai et al.(1999b), as well as on speciation calculations using the thermodynamic data in Guillaumont et al.(2003), it is estimated that the initial Am concentration is below the respective solubility limit, but possibly by less than a factor of 5.	B
II-i SDB REF	Filtration through 10000 MWCO and 45 μ m membranes, as well as centrifugation at 1100 g for 2.5 h is reported. Three methods of phase separation are used: 1) centrifugation at 1100 g for 2.5 h, 2) centrifugation at 1100 g for 2.5 h followed by filtration through 0.45 μ m membranes, and 3) centrifugation at 1100 g for 2.5 h followed by filtration through 0.45 μ m membranes	A

		and then by filtration through 10000 MWCO filters. It appears that the resulting K_d values are slightly dependent on the method of phase separation: surprisingly, the highest K_d is generally obtained with centrifugation alone, whereas filtration with 10000 MWCO membranes leads to the lowest values. However, the respective variation is of about the same magnitude as observed for different L/S. Therefore, it may be considered to be within the overall experimental uncertainties.	
II-j	SDB	A reaction time of 122 days (four months) is reported. This reaction time is reasonably long.	C/D
II-k	REF	The experiments are gently agitated on a shaker table.	A/B
II-l	SDB	No variation of L/S ratio or of the initial Am concentration is reported.	C/D
II-m	REF	The experiments are carried out in polypropylene centrifuge tubes. And corrections for sorption on vessel walls have been performed.	A
II-n	SDB REF	It is indicated that each experiment is done in duplicate. Error estimates are given for each replicate, based on analytical uncertainties.	A
II-o	SDB	No relevant parameter variation is indicated.	D

Data table Am/8: REF: Berry et al. (2007)*

JAEA-SDB version 4 – DATA: Am/Granitic rocks; granodiorite, #46906-46911

GUIDELINE: Revision 4b (May 19, 2005)

*REMARK: Update of SDB required for checkpoint I-a.2.

Checkpoint		Evaluation	Rating
I-a.1	SDB	All mandatory fields are completed.	Yes
I-a.2	SDB REF	Oxidation state of Am is not indicated. It is reported that the major aqueous species measured was $\text{Am}(\text{OH})_2^+$ with oxidation state +III.	Yes (tentative) (update SDB)
I-b	SDB	A table with K_d values is given.	class 1
II-a	SDB REF	As solid phase granodiorite is indicated. Mineral composition is reported, CEC or BET are not indicated. Surface characteristics are not reported.	C/D
II-b	SDB	Final pH values are indicated.	A
II-c	SDB REF	It is indicated that reducing conditions had been applied with final Eh values of -510 mV and -520 mV. Am is not redox sensitive. It is indicated that sodium dithionite ($\text{Na}_2\text{S}_2\text{O}_4$) as reducing agent was added to the reaction mixtures. The effect of sodium dithionite on Am is difficult to estimate since no experiments with an other reducing agent had been done. For this reason rating C/D is applied.	C/D
II-d	SDB REF	The solution composition of distilled water after equilibration with granodiorite at 60°C is indicated. It is assumed that the same $\text{Na}_2\text{S}_2\text{O}_4$ concentration as in the batch experiments of Uranium was applied (2.5×10^{-3} M).	A/B
II-e	SDB	A temperature of 60°C is indicated.	A/B
II-f	SDB	A L/S of 5 mL/g is indicated. Although any information about the specific surface area is lacking, 1 g of solid per reaction vial is assumed to be enough.	A/B

II-g	SDB	The sorption values are calculated from K_d and L/S ratios: • # 46906 and 46907 (97%) • # 46908-46911 (100%)	B C/D
II-h	SDB	An initial Am concentration of 1.2×10^{-10} M is reported. Based on speciation calculations (for 60°C) with Phreeqi 2.12.5 using the thermodynamic data in the NAGRA-PSI thermodynamic database (Hummel et al., 2002) the initial Am concentration is clearly below (factor >5) the solubility limit at the reported pH of 9.6 (due to the $\text{AmSiO}(\text{OH})_3^{2+}$ and $\text{Am}(\text{CO}_3)_2^{2-}$ species).	A
II-i	SDB REF	Centrifugation only and centrifugation combined with two different filtration procedures were applied (0.45 μm and 10,000 MWCO). The more effective the separation procedure, the higher were the K_d values. These results indicate colloid formation or sorption to the filter membranes and data of 0.45 μm filtration are considered as unreliable: • # 46908/46911 (due to consistency with other data considered as reliable, expert decision) • # 46906/46907/46909/46910	B unreliable
II-j	SDB	A contact time of 120 days is indicated.	C/D
II-k	REF	Tubes were gently agitated continuously in a shaker.	A/B
II-l	SDB	No isotherm is available. No variation in L/S or [Am] is indicated.	C/D
II-m	REF	One blank tube without solid phase was monitored regularly to test for a steady-state concentration of radionuclide. Where a significant sorption to the vessel walls was observed in the blank test, the corresponding vessel walls of tubes containing geologic material were investigated. This was in order to confirm that sorption was genuinely onto the solid phase and not onto the vessel walls.	A
II-n	SDB REF	Error estimates are indicated. Error estimates are based on the statistics of counting.	C
II-o	SDB	No parameter variation had been performed.	D

Data table Am/9: REF: Daniels (1981)*		
JAEA-SDB version 4 - DATA: Am/Granitic rocks; granite, #49978-50001		
GUIDELINE: Revision 4b (May 19, 2005)		
*REMARK: Only 24 out of 48 listed datapoints in the reference are indicated in the SDB.		
Update of SDB required for checkpoints I-a.2, II-a and II-c.		
Checkpoint	Evaluation	Rating
I-a.1 SDB	All mandatory fields are completed.	Yes
I-a.2 SDB	Is all mandatory information provided? It is indicated that there is no information about the solid/solution ratio provided.	No (update SDB)
REF	Experimental details are given elsewhere in a cited reference.	
I-b SDB	A table with K_d values is given.	class 1
II-a SDB	As solid phase granite#1 and #2 are indicated. Mineral compositions are not reported. Surface characteristics are not reported. Fraction sizes of the granite samples are indicated.	B (tentative)
REF	Mineralogy in volume percent is given in Erdal et al. (1979c). Surface areas of different fraction sizes are listed, however, not for	

		the fraction sizes indicated in the SDB.	
II-b	SDB	Initial and final pH values are listed.	A
II-c	SDB	Oxidation state of Am is not reported. It is indicated that experiments had been performed under aerobic and under controlled atmosphere conditions. Eh values are not reported. Am is not redox sensitive.	A/B (update SDB)
	REF	Controlled atmosphere condition was nitrogen-atmosphere containing <0.2 ppm oxygen and <20 ppm carbon dioxide.	
II-d	SDB	As water type groundwater#1 is indicated. Final solution compositions are not given. It is reported that for experiments the same conditions were used as in three other cited references described. In the cited references several batches of groundwaters are listed. From the provided information of references it is not possible to clearly assign a groundwater to the given datapoints, therefore all datapoints are classified as unreliable.	unreliable

Data table Am/10: REF: Erdal et al. (1979c)* JAEA-SDB version 4 - DATA: Am/Granitic rocks: granite, #50897-50904 GUIDELINE: Revision 4b (May 19, 2005) *REMARK: Additional datapoints listed in the reference should be entered to the SDB (only 8 out of 47 in SDB). Update of SDB required for checkpoints.			
Checkpoint		Evaluation	Rating
I-a.1	SDB	All mandatory fields are completed.	Yes
I-a.2	SDB	All mandatory information is provided.	Yes
I-b	SDB	A table with K_d values is given.	class 1
II-a	SDB	As solid phase granite#1 and #2 are indicated. Major mineral composition and surface characteristics (CEC/surface area) are reported.	B (revise SDB)
	REF	The mineral composition is given in volume percent and not as in the SDB indicated in percent by weight.	
II-b	SDB	pH values are indicated as follows: •#50904 only initial pH value indicated •#50899, 50902 only final pH values indicated •#50897, 50898, 50900, 50901, 50903 initial and final pH given	C A A
II-c	SDB	Am(III) is indicated and experiments had been performed under atmospheric conditions. Am is not redox sensitive.	A/B
II-d	SDB	Pre-equilibrated synthetic groundwater and its composition is indicated for the datapoints listed in the SDB.	(revise SDB) A/B
	REF	It is reported (p.48) that for experiments at ambient temperature the groundwater batch #3 was used and for the experiments at 70°C the groundwater batch #2. Compositions given in the SDB do not correspond to these data.	
II-e	SDB	A reaction temperature of 22°C and 70°C is indicated.	A/B
II-f	SDB	It is indicated that for reactions 1 g of solid was added to 20 mL of solution. With the given surface area of 4.0 and 3.3 m ² /g, measured with the ethylene glycol method for granite#1 and #2 respectively, rating C/D is applied.	C/D
II-g	SDB	The sorption values are calculated from K_d and L/S ratio are all >98%.	C/D

II-h	SDB REF	An initial Am concentration of $<1.0 \times 10^{-6}$ M is reported. Based on speciation calculations (for both, 22 and 70°C) with Phreeqci 2.14.3 using the thermodynamic data in the NAGRA-PSI thermodynamic database (Hummel et al., 2002) the initial Am concentration is clearly below (factor>5) the solubility limited at the reported pH of 8.4 due to the $\text{AmSiO}(\text{OH})_3^{2+}$ and $\text{Am}(\text{CO}_3)_2^{2-}$ species.	A
II-i	SDB	Centrifugation for 1 hour at 16,000 rpm is indicated.	B
II-j	SDB REF	A contact time of 7 and 56 days is indicated. There is a clear trend of higher K_d values with extended reaction times, what indicates that alteration of the solid phase during the experiments are reasonable. The authors explained the trend of sorption values with a change in mineralogy as well (page 24), therefore datapoints are considered as unreliable.	unreliable

Data table Am/11: REF: Ikeda and Amaya (1998)* JAEA-SDB version 4 – DATA: Am/Granitic rocks; granodiorite, #53535-53542 GUIDELINE: Revision 4b (May 19, 2005) *REMARK: Checkpoints I-b and II-a should be updated in SDB.			
Checkpoint		Evaluation	Rating
I-a.1	SDB	All mandatory fields are completed.	Yes
I-a.2	SDB	All mandatory information is provided.	Yes
I-b	SDB	A table with logarithmic K_d values is given, but for datapoints # 53535-53538 limiting K_d values are provided. Datapoints # 53539-53542 however are listed in SDB with error estimates.	class 1 (revise SDB)
II-a	SDB REF	As solid phase granodiorite is indicated. Mineral composition and surface characteristics are not reported. Information about major mineral composition and chemical composition are given. A BET of 0.7 m ² /g is reported.	B (update SDB)
II-b	SDB	Initial and final pH values are indicated.	A
II-c	SDB REF	It is indicated that reducing conditions had been applied with final Eh values of –210 mV and –320 mV. Am is not redox sensitive and an oxidation state (+III) is reported. Sodium dithionite ($\text{Na}_2\text{S}_2\text{O}_4$) as reducing agent was added to the reaction mixtures. The effect of sodium dithionite on Am is difficult to estimate since no experiments with an other reducing agent had been done. For this reason rating C/D is applied.	C/D
II-d	SDB REF	As water type seawater and distilled water are indicated. The solutions are 2×10^{-4} M and 1.2×10^{-3} M in sodiumdithionite, to keep reducing conditions. Final solution compositions are not given, but it is supposed that no essential changes take place in the case of seawater. Major mineralogy and chemical composition of the granodiorite are available. Final solution composition with distilled water and the reported L/S can be estimated approximately.	A/B C/D
II-e	SDB	A temperature of 26°C is indicated.	A/B
II-f	SDB	It is indicated that for reactions 1 g of solid was added to either 39, 49 or 50 mL of solution. With a BET value of 0.7 m ² /g, rating C/D is applied.	C/D
II-g	SDB	The sorption values (calculated from K_d and L/S ratios) are all >98%.	C/D

II-h	SDB	Initial Am concentrations of 1.5×10^{-10} and 1.6×10^{-10} M are reported. Based on the data in Rai et al. (1999b) it is assumed that initial [Am] was clearly below the respective solubility limit for the reported data around pH 6. For the data around pH 8 Am is likely below the solubility limit. • # 53535-53538 • # 53539-53542	A C/D
II-i	SDB	Two different filtration procedures were applied and similar results are reported: filtration with 0.45 µm membranes and with 10,000 MWCO-filters.	A
II-j	SDB	A reaction time of 26 and 33 days is indicated. No further (kinetic) information is provided.	C/D
II-k	REF	Samples were manually shaken every one to two weeks.	C/D
II-l	REF	No isotherm is available. Limited variation of L/S is indicated for experiments with seawater. No variation in L/S or [Am] had been indicated for experiments with distilled water. • # 53535-53538 • # 53539-53542	C/D B
II-m	REF	The experiments were carried out in teflon vessels. There is no information about blank measurements or sorption on vessel walls given.	B (tentative)
II-n	SDB REF	It is indicated that replicates are not reported. Error information is available for datapoints # 53539-53542. Two repetitions are reported (probably concerning datapoints # 53539-53542 only). No repetitions are reported for datapoints # 53535-53538.	A (tentative) D
II-o	SDB	No parameter variation had been done for experiments with distilled water. L/S had been varied for experiments performed with seawater.	D C

Data table Am/12: REF: Kitamura et al. (1999a) JAEA-SDB version 4 – DATA: Am/Granitic rocks; granite, #62982-63016 GUIDELINE: Revision 4b (May 19, 2005)		
Checkpoint	Evaluation	Rating
I-a.1	SDB All mandatory fields are completed.	Yes
I-a.2	SDB All mandatory information is provided.	Yes
I-b	SDB The K_d values are extracted from a graph with distribution coefficients as a function of pH.	class 3
II-a	SDB As solid phase granite is indicated. Mineral composition is not indicated. Mesh size and specific surface area are reported. REF The granite sample had been a biotite granite from Inada, Ibaraki, Japan, purchased from Nichika Co. Granite samples had been crushed and washed with 0.5 M HCl. Sample treatment may have led to minor changes.	B
II-b	SDB Final exact pH values are indicated. Inert NaClO ₄ electrolyte solution had been used and the pH was adjusted by addition of either HClO ₄ or NaOH.	A
II-c	SDB Am with the oxidation state (+III) is reported. It is indicated that experiments had been performed under inert Ar atmosphere. Am is not redox sensitive.	A/B

	REF	Experiments had been performed in an argon filled glove box to avoid contamination and complexation by carbonate.	
II-d	SDB	0.01 M and 0.1 M NaClO ₄ electrolyte solutions are indicated. It is assumed that no changes of the solution composition had taken place during the equilibration procedure due to antecedent sample treatment (see checkpoint II-a).	A/B
II-e	SDB	A temperature of 24°C is indicated.	A/B
II-f	SDB	It is indicated that 0.1 g of granite powder was added to 4.0 mL of electrolyte solution. Based on the given BET value of 0.11 m ² /g, the surface area of added granite is about 0.011 m ² .	C/D
II-g	SDB	The sorption values are calculated from K _d and L/S ratios: <ul style="list-style-type: none"> • # 62982 to # 62986 and # 62997 to 63007 (26%~94% sorption) • # 62987 and # 63008 (97% and 98% sorption) • # 62988 to # 62996 and # 63009 to # 63016 (>98% sorption) 	A B C/D
II-h	SDB	An initial Am concentration of 1.8×10^{-10} M is reported. Based on the data in Rai et al. (1999b) and calculations with Phreeqci 2.12.5 using the thermodynamic data in the NAGRA PSI thermodynamic database (Hummel et al., 2002), the initial [Am] was clearly below the respective solubility limit (by a factor >5) for the reported data.	A
II-i	SDB	It is indicated that the samples had first been centrifuged at 3000 rpm and then filtered with 0.45 µm membranes.	B
II-j	SDB	A reaction time of 7 days is indicated. No further (kinetic) information is provided.	C/D
II-k	REF	Samples were shaken during the contact time.	A/B
II-l	SDB	No isotherm is available. No variation in L/S or [Am] had been indicated	C/D
II-m	REF	The experiments were carried out in polypropylene tubes. There is no information about blank measurements or sorption on vessel walls given.	B (tentative)
II-n	SDB	It is indicated that replicates are not reported and no error information is available.	D
II-o	SDB	Variation of pH over a range of 2 to 12 at two different electrolyte concentrations had been performed.	B

Data table Am/13: REF: Nakayama et al. (1986)*		
JAEA-SDB version 4 – DATA: Am/Granitic rocks; granite, #56795-56806		
GUIDELINE: Revision 4b (May 19, 2005)		
* REMARK: Update of SDB required for checkpoints I-a.2 and II-c.		
Checkpoint	Evaluation	Rating
I-a.1 SDB	All mandatory fields are completed.	Yes
I-a.2 SDB	It is indicated that redox state of Am and reaction temperature are not reported.	Yes (tentative) (update SDB)
REF	Batch sorption experiments had been performed at room temperature with Am(III).	
I-b SDB	A table with K _d values is given.	class 1
II-a SDB	As solid phase Inada and Rokko granite are indicated. Mineral compositions are not reported. Mesh sizes of the granite samples are indicated. BET is given for datapoints # 56795-56799.	C/D
REF	Major and minor mineralogy are not reported.	

II-b	SDB REF	Final limiting pH values are indicated. Approximate pH values are reported (e.g. pH ~7).	B
II-c	SDB REF	It is indicated that experiments had been performed under aerobic conditions. Eh values are not reported. Am is not redox sensitive. The oxidation state of Am is not indicated. It is reported that Am(III) was used for the experiments.	A/B (update SDB)
II-d	SDB REF	As water type preequilibrated water and distilled water are indicated. Final solution compositions are not given. Final solution compositions are not reported. Since information about mineral composition including impurities is lacking as well, it is impossible to estimate the final solution composition.	unreliable

Data table Am/14: REF: Pinnioja et al. (1984)* JAEA-SDB version 4 - DATA: Am/Granitic rocks; granite, #57264, #57265 GUIDELINE: Revision 4b (May 19, 2005) *REMARK: Checkpoints II-e, II-f, II-m and II-n should be updated.			
Checkpoint		Evaluation	Rating
I-a.1	SDB	All mandatory fields are completed.	Yes
I-a.2	SDB	All mandatory information is provided.	Yes
I-b	REF	K _d is given in tabular form	class 1
II-a	SDB	As solid phases tonalite and rapaviki granite are indicated. Major mineralogy and BET are known. The soil was pretreated with synthetic groundwater 3~4 times so that minor impurities had been washed out.	A
II-b	SDB	Only initial pH-values are reported for the artificial groundwater.	C
II-c	SDB	It is indicated that experiments had been performed under oxidizing conditions (air). Am(III) is not redox sensitive.	A/B
II-d	SDB REF	Allard water is indicated as synthetic groundwater and its composition is tabulated. Details about experimental procedure for the batch experiments are described elsewhere: Before labeling, the soil was equilibrated with the groundwater by sequential shaking with three to four portions of 100 mL of water.	A/B
II-e	SDB REF	It is indicated that temperature is not reported. It is reported that experiments had been performed at 20°C.	(update SDB) A/B
II-f	SDB REF	A solid to liquid ratio of 10 mL/g is indicated. The respective amounts are not reported. It is reported that 10 g of wet soil were added to 100 mL of groundwater. With a BET of 0.27 m ² /g (tonalite) and 0.54 (granite) a surface area of 2.7 respectively 5.4 m ² /g per reaction vial are obtained: •#57264 (tonalite) •#57265 (granite)	(update SDB) C/D A/B
II-g	SDB	Sorption is in all cases calculated to be >99% sorbed.	C/D
II-h	SDB REF	Initial [Am] of 1.1×10^{-9} M is indicated. Based on speciation calculations (for 20°C) with Phreeqi 2.14.3 using the thermodynamic data in NAGRA-PSI (Hummel et al., 2002) the initial Am concentration is clearly below the solubility limited.	A

II-i	REF	It is reported that samples were centrifuged at 13,000 g and filtered over 0.45 µm membranes.	B
II-j	SDB	An equilibration time of 7 days is indicated. Before labeling the soil was equilibrated with the groundwater.	C/D
II-k	REF	Samples had been shaken during experiments.	A/B
II-l	SDB	No variation in [Am] or the L/S is indicated.	C/D
II-m	REF	Polycarbonate centrifuge tubes were used for equilibration as well as phase separation. Corrections for adsorption to the tube walls had been made, but proceeding is not described in detail.	(update SDB) C/D
II-n	SDB REF	It is indicated that no error estimates are reported. It is reported that errors are based on 2 to 4 parallel K _d determinations.	(update SDB) A
II-o	REF	No parameter variation is indicated.	D

Data table Am/15: REF: Suksi et al. (1987)* JAEA-SDB version 4 - DATA: Am/Granitic rocks; granite, #59374, #59375 GUIDELINE: Revision 4b (May 19, 2005) *REMARK: Update of SDB required for			
Checkpoint		Evaluation	Rating
I-a.1	SDB	All mandatory fields are completed.	Yes
I-a.2	SDB	Oxidation state of Am is not indicated. It is reported that the major aqueous species measured was Am(OH) ₂ ⁺ with oxidation state +III.	Yes (tentative) (update SDB)
I-b	SDB	A table with K _d values is given.	class 1
II-a	SDB REF	As solid phase granite are indicated. Mineral composition is reported, CEC or BET are not indicated. Surface characteristics are not reported.	C/D
II-b	SDB	Final pH values are indicated.	A
II-c	SDB REF	It is indicated that reducing conditions had been applied with final Eh values of -390 mV. Am is not redox sensitive and an oxidation state (+III) is reported. Sodium dithionite (Na ₂ S ₂ O ₄) as reducing agent was added to the reaction mixtures. The effect of sodium dithionite on Am is difficult to estimate since no experiments with an other reducing agent had been done. For this reason rating C/D is applied.	C/D
II-d	SDB REF	The solution composition of granite equilibrated distilled water (equilibration at 60°C) is indicated. It is assumed that the same Na ₂ S ₂ O ₄ concentration as in the batch experiments of Uranium was applied (2.5×10^{-3} M).	A/B
II-e	SDB	A temperature of 60°C is indicated.	A/B
II-f	SDB	A L/S of 5 mL/g is indicated. Although any information about the specific surface area is lacking. 1g of solid per reaction vial is assumed to be enough.	A/B
II-g	SDB	The sorption values (calculated from K _d and L/S ratio) are all >99.8%.	C/D
II-h	SDB REF	An initial Am concentration of 1.0×10^{-10} M is indicated. Based on speciation calculations (for 60°C) with Phreeqc 2.14.3 using the thermodynamic data in the NAGRA-PSI thermodynamic database (Hummel et al., 2002) the initial Am concentration is clearly below	A

		(factor>5) the solubility limited at the reported pH of 9.2 (due to the $\text{AmSiO}(\text{OH})_3^{2+}$ and $\text{Am}(\text{CO}_3)_2^-$ species.	
II-i	SDB	Centrifugation only and centrifugation combined with two different filtration procedures were applied (0.45 μm and 10,000 MWCO). The more effective the separation procedure, the higher were the K_d values. These results indicate colloid formation or sorption to the filter membranes.	unreliable

Data table Am/16: REF: Allard and Beall (1979)*			
JAEA-SDB version 4 – DATA: Am/Other minerals; Al-oxide/-hydroxide, #42201, #42205			
GUIDELINE: Revision 4b (May 19, 2005)			
* REMARK: Checkpoints II-h and II-j should be revised in SDB.			
Checkpoint	Evaluation	Rating	
I-a.1 SDB	All mandatory fields are completed.	Yes	
I-a.2 SDB	All mandatory information is provided.	Yes	
I-b SDB	A table with ranges of logarithmic K_d values is given.	class 5	
II-a SDB REF	As solid phases corundum and gibbsite are reported. CEC or BET values are not reported. Surface characteristics of the pure minerals are not reported. Samples had been obtained from Ward's Natural Science Establishment and were not further treated. Approximate surface characteristics of the pure solids can be obtained from the literature.	B	
II-b SDB	Final pH values were measured and a pH range is reported.	B	
II-c SDB	It is indicated that no redox conditions are reported. Am(III) is not redox sensitive.	A/B	
II-d SDB	It is indicated that the solution consisted of solid-equilibrated artificial groundwater. The final solution composition is reported.	A/B	
II-e SDB	It is indicated that experiments had been performed at room temperature.	A/B	
II-f SDB	Rating is done based on the indicated L/S ratio (0.067~0.1 L/g).	C/D	
II-g SDB	The sorption values (calculated from K_d and L/S ratios) result in 94% and 97%: • # 42201 • # 42205	A B	
II-h SDB REF	An initial Am concentration of 1.0×10^{-5} to 1.0×10^{-4} M is indicated. An initial Am concentrations of about 10^{-9} M is reported. Based on speciation calculations (for 25°C) with Phreeqci 2.12.5 using the thermodynamic data in JNC-TDB_011213c2 and NAGRA-PSI thermodynamic database (Hummel et al., 2002) the initial Am concentration is clearly below the solubility limit.	A (revise SDB)	
II-i SDB	It is indicated that samples had been centrifuged for 60 min. at 4,000g max.	C/D	
II-j SDB REF	A contact time of 7 days is indicated. A reaction time of 5 days after addition of the radionuclide is indicated. Before spiking the solutions, the synthetic groundwater was pre-equilibrated with the pre-washed solid during 5 days.	C/D (revise SDB)	
II-k REF	No agitation method is indicated.	C/D	
II-l SDB	No variation in [Am] or the L/S is indicated.	C/D	

II-m	REF	There is no information about the reaction vessel. Based on blank measurements adsorption to the vessel walls had been corrected.	C/D
II-n	REF	No error information is available.	D
II-o	SDB	It is indicated that no error information is available.	D

Data table Am/17: REF: Allard and Beall (1979)*			
JAEA-SDB version 4 – DATA: Am/Other minerals; Fe-oxide/-hydroxide, #42207, #42210			
GUIDELINE: Revision 4b (May 19, 2005)			
* REMARK: Data of checkpoints II-h and II-j should be revised/corrected in SDB.			
Checkpoint		Evaluation	Rating
I-a.1	SDB	All mandatory fields are completed.	Yes
I-a.2	SDB	All mandatory information is provided.	Yes
I-b	SDB	It is indicated that logarithmic K_d values are given, but only ranges of K_d values are provided, therefore rating class 5 is applied.	class 5
II-a	SDB	As solid phases hematite and magnetite are reported. CEC or BET values are not reported.	A
	REF	Surface characteristics of the pure minerals are known. Samples had been obtained from Ward's Natural Science Establishment and were not treated further.	
II-b	SDB	Final pH values were measured and a pH range is reported.	B
II-c	SDB	It is indicated that no redox conditions are reported. Am(III) is not redox sensitive.	A/B
	REF	It is assumed that experiments had been performed under ambient conditions.	
II-d	SDB	The groundwater composition (Allard water) is indicated.	A/B
	REF	It is indicated that the solution consisted of solid-equilibrated artificial groundwater. The resulting solution composition is reported.	
II-e	REF	It is indicated that experiments had been performed at room temperature.	A/B
II-f	REF	Rating is done based on the indicated L/S ratio (0.067~0.1 L/g).	A/B
II-g	SDB	The sorption values (calculated from K_d and L/S ratios) result in 97% and 98%.	B
II-h	SDB	An initial Am concentration of 1.0×10^{-5} to 1.0×10^{-4} M is indicated.	A (revise SDB)
	REF	An initial Am concentrations of about 10^{-9} M is reported. Based on speciation calculations (for 25°C) with Phreeqci 2.12.5 using the thermodynamic data in JNC-TDB_011213c2 and NAGRA-PSI the initial Am concentration is clearly below the solubility limit.	
II-i	SDB	It is indicated, that samples had been centrifuged for 60 min. at 4,000g max.	C/D
II-j	SDB	A contact time of 7 days is indicated.	C/D (revise SDB)
	REF	A reaction time of 5 days is indicated after addition of the radionuclide. Before spiking the solutions, the synthetic groundwater was pre-equilibrated with the pre-washed solid during 5 days.	
II-k	REF	No agitation method is indicated.	C/D
II-l	SDB	No variation in [Am] or the L/S is indicated.	C/D
II-m	REF	There is no information about the reaction vessel. Blank measure-	C/D

		ments had been performed to correct adsorption to the vessel walls.	
II-n	SDB	It is indicated that no error information is available.	D
II-o	REF	No parameter variation is indicated.	D

Data table Am/18: REF: Degueldre et al. (1994)* JAEA-SDB version 4 – DATA: Am/Other minerals; Fe-oxide/-hydroxide, #50234, #50235 GUIDELINE: Revision 4b (May 19, 2005) * REMARK: In the reference a pre-study (to determine the effect of colloid concentration) and main studies (batch sorption experiment and dialysis test) are reported. It is unclear to which study the SDB entries correspond to. Update SDB for additional datapoints (only 2 out of 6 datapoints available).			
Checkpoint		Evaluation	Rating
I-a.1	SDB	All mandatory fields are completed.	Yes
I-a.2	SDB	All mandatory information is provided.	Yes
I-b	SDB	A graph with log K_d at different L/S and a graph with log K_d at different carbonate concentrations is provided. It is not clear which data the given K_d 's in the SDB do correspond to.	class 5 (update SDB)
	REF	Dialysis test experiments and batch sorption measurements are described.	
II-a	SDB	Hematite is reported as mineral phase. CEC or surface area is not reported. However surface characteristics of hematite are known.	B
II-b	SDB	Final pH values are given.	A
	REF	0.01 M Tris-buffer was added at the experimental setup to adjust pH to 8.	
II-c	SDB	No redox conditions are indicated. It is assumed that experiments had been performed under ambient conditions. Am is not redox sensitive.	A/B (tentative)
II-d	SDB	It is indicated that the solution consisted of 0.01 M carbonate and 0.001 M Tris-buffer.	A/B
	REF	It is indicated that solutions consisted of 0.01 M carbonate and 0.01 M Tris-buffer for dialysis experiments. For batch reaction experiments the Tris-buffer was 0.001 M in concentration. Due to the simplicity of the given solutions, the final solution composition can be estimated.	
II-e	SDB	Temperature is not specified.	C/D
II-f	SDB	A solution/solid ratio of 3125 and 1,000,000 mL/g is indicated. It is not indicated how much solid was used per reaction vial.	C/D
	REF	It is not clear how much solid per reaction vial was used.	
II-g	SDB	Rating is done based on %-sorbed values calculated from the information given in the SDB: • #50234 (26% sorbed) • #50235 (>99.9% sorbed)	A C/D
II-h	SDB	The initial Am concentration is indicated to be 8.5×10^{-10} M. Based on Phreeqc-2.12.5 calculations (database: JNC-TDB_011213c2 and NAGRA-PSI) for the indicated solution, the initial [Am] is below the calculated solubility limit of 3.9×10^{-6} M.	A/B (update SDB)
	REF	For batch sorption experiments an initial Am concentration of 3.6×10^{-9} M is given.	

II-i	SDB REF	Filtration over 30 nm pored filters is indicated. A polycarbonate membrane with a pore size of 30 nm was used as membrane in the dialysis tests. Batch reaction mixtures were filtered with polycarbonate filters of 30 nm pore size.	C/D
II-j	SDB	It is indicated that a contact time of 5 days had been used.	C/D
II-k	REF	For mixing the samples were allowed to equilibrate on a shaking mashine during the whole reaction time of at least 5 days.	A/B
II-l	SDB	No isotherm is available, but dialysis tests had been setup with different L/S.	B
II-m	REF	Polyethylene test tubes are indicated for the dialysis tests. It is asumed that batch reaction experiments were setup equally. Corrections for sorption on vessel walls had been performed by substraction of blank tests.	C/D
II-n	SDB REF	It is indicated that no error estimation is reported. All tests, including the blanks were run in duplicate and uncertainty bars are given in the graphs.	A (update SDB)
II-o	SDB	Experiments had been performed with different L/S and carbonate concentrations.	B

Data table Am/19: REF: Higgo et al. (1983)*			
JAEA-SDB version 4 – DATA: Am/Other minerals; Fe-oxide/-hydroxide, #53056-53060			
GUIDELINE: Revision 4b (May 19, 2005)			
* REMARK: Checkpoints II-a, II-b, II-e, II-f and II-n should be revised/updated in SDB			
Checkpoint	Evaluation		Rating
I-a.1	REF	All mandatory fields are completed.	Yes
I-a.2	REF	All mandatory information is provided.	Yes
I-b		K _d is given in tabular form.	class 1
II-a	SDB REF	As solid phases amorphous Mn and Fe are indicated. Specific surface area and CEC values are given. Amorphous Mn hydroxides and Fe oxihydroxides are reported. Major and minor mineralogy of these compounds is known. Sample treatment may have led to minor changes (see II-j).	C/D (revise SDB)
II-b	SDB REF	It is indicated that exact final pH values are reported. A final pH between 7.7 and 8.2 is reported.	B (revise SDB)
II-c	SDB REF	It is indicated that no redox conditions are reported. Am(III) is not redox sensitive. It is reported that the samples were never allowed to dry out, and that Eh was not controlled. Due to the Fe- or Mn-(hydr)oxide containing solids, it can be assumed that at least slightly oxidizing conditions were prevalent throughout.	A/B
II-d	SDB REF	Seawater is indicated. The critical major components are approximately known. Minor components may be unknown. Charge balance cannot be calculated, but seawater can be expected to be well poised.	C/D
II-e	SDB REF	It is indicated that temperature is not reported. It is reported that temperature was kept at 4°C at all times.	(update SDB) A/B
II-f	SDB REF	It is indicated that this information is not provided. It is reported that 50~100 mg of solid were added to 30 mL of seawater. This equals a L/S ratio of 0.3~0.6 m ³ /kg.	(update SDB) C/D

II-g	SDB	Sorption is in all cases calculated to be >99% sorbed.	C/D
II-h	SDB	Initial [Am] ranging from 2.0×10^{-10} M to 1.8×10^{-9} M is indicated. Based on the data in Rai et al. (1999b) it is estimated that initial [Am] was below the respective solubility limit, but maybe by a factor <5.	B
	REF	Higgo et al. (1983) report that a small Am-fraction (in a more concentrated solution, no details given) may not be in true solution, based on filtration with $0.025 \sim 0.22$ μ m membranes. Based on the above and information in the REF, it is estimated that this result may be related to colloids in the seawater; rating B is retained.	
II-i	SDB	Centrifugation (7,000 rpm/180 min) is indicated.	C/D
II-j	SDB	K_d values measured after various equilibration times (7, 28 and 56 days) show no tendency to approach equilibrium. However a reaction time of 28 or 56 days is considered to be reasonably long to reach near equilibrium. It is assumed that more complex reactions may have had occurred due to instability of the solid phase.	C/D
II-k	REF	Agitation by an automatic shaker is reported.	A/B
II-l	SDB	No substantial variation in [Am] or the L/S is indicated.	C/D
II-m	REF	Polycarbonate centrifuge tubes were used for equilibration as well as phase separation. No correction for wall effects was done.	B
II-n	SDB	Error estimates are indicated, but it is not indicated whether samples had been replicated.	(update SDB) C
	REF	It is reported that errors are based on analytical counting statistics only.	
II-o	SDB	No significant parameter variation is indicated.	D

Data table Am/20: REF: Righetto et al. (1988)*

JAEA-SDB version 4 – DATA: Am/Other minerals; Al-oxide/-hydroxide, #58542-58544

GUIDELINE: Revision 4b (May 19, 2005)

* REMARK: Only three datapoints are listed in the SDB, due to the original selection of data in the context of sorption onto bentonite. Additional information about sorption of Am on aluminum oxide e.g. in presence of carbonate in solution is provided in the reference. Update of SDB required for checkpoints II-c, II-f, II-l, and II-o.

Checkpoint	Evaluation	Rating
I-a.1	SDB All mandatory fields are completed.	Yes
I-a.2	SDB All mandatory information is provided.	Yes
I-b	SDB A linear graph with % sorbed is given.	class 4
II-a	SDB As solid phase aluminum oxide is reported. CEC and BET values are indicated. REF The solid phase (Aluminium oxide C) was purchased from Degussa.	A
II-b	SDB Final discrete pH-values are indicated and a NaClO ₄ electrolyte solution was used for the experiments.	A
II-c	SDB It is indicated that Am in the oxidation state III was used. No information about the redox/atmospheric conditions are provided. REF Experiments had been performed under oxic conditions. However, Am(III) is not redox sensitive.	A/B (update SDB)
II-d	SDB It is indicated that the solution was 0.1 M in NaClO ₄ (post equilibration).	A/B
II-e	REF Temperature is not specified, but it is assumed that experiments	C/D

		were done under ambient conditions.	
II-f	SDB REF	The indicated L/S ratio of 1000 L/g is incorrect. Rating is done based on the indicated L/S ratio (100 L/g). With a BET of 130 m ² /g and assumed that 0.01 g per reaction vial were used, a surface of 1.3 m ² /vial is obtained.	C/D (revise SDB)
II-g	SDB	The sorption values are calculated from K _d and L/S ratios and range from 12% to 96%. • # 58542/58543 (55% / 12%) • # 58544 (96%)	A B
II-h	SDB	An initial Am concentration of 5×10^{-10} M is reported. Based on the data in Rai et al. (1999b) it is assumed that initial [Am] was below the respective solubility limit by a factor of about 1,000.	A
II-i	SDB	It is indicated that samples had been centrifuged for 60 min. at 55,000 rpm (ultracentrifugation).	B
II-j	SDB REF	The radionuclide was allowed to react for 7 days. The radionuclide was added after one month of pre-equilibration time. It is reported that reaction time was determined by preliminary kinetic runs.	A/B
II-k	REF	The samples were mechanically shaken.	A/B
II-l	SDB REF	No variation in [Am] or the L/S is indicated. Experiments with a different L/S are reported.	B (update SDB)
II-m	REF	Reactions had been done in polyallomer ultracentrifuge tubes "quick seal" of Beckman. Parallel experiments without centrifugation were performed to quantify the nuclide adsorption on the tube walls. Apparently no corrections had been done.	B
II-n	SDB	No error information is available.	D
II-o	SDB REF	pH had been varied. Additional experiments are reported (datapoints not in SDB) where sorption on aluminum oxide at different electrolyte and carbonate concentrations had been studied.	C (maybe update SDB)

3.1.2 Cesium

Data table Cs/1: REF: Allard et al. (1979b)		
JAEA-SDB version 4 - DATA: Cs/Granitic rocks; granite, #42301-42312		
GUIDELINE: Revision 4b (May 19, 2005)		
Checkpoint	Evaluation	Rating
I-a.1 SDB	All mandatory fields are completed.	Yes
I-a.2 SDB	All mandatory information is provided.	Yes
I-b SDB	A table with log K_d values is provided.	class 1
II-a SDB	As solid phase granite is indicated. Mineralogy and surface characteristics are not reported.	C/D
II-b SDB	Initial pH values are indicated.	C
II-c SDB	Experiments had been performed under aerobic conditions. Cs is not a redox sensitive element.	A/B
II-d SDB	Detailed compositions of two synthetic groundwaters Aq293 and Aq1105 are indicated.	A/B
II-e SDB	A temperature of 25 and 65°C is indicated.	A/B
II-f SDB REF	A L/S ratio of 10~50 mL/g is indicated. An apparent surface to mass ratio of 3 m ² /kg is reported for Cs on granite. Assumed that this is the specific surface of granite, the total surface is at most 0.01 m ² /vial with 1~3 g of solid phase per reaction vial.	C/D
II-g SDB	Rating is done based on %-sorbed values calculated from the information given in the SDB. Calculating with the least L/S of 100, the following sorption values are obtained: •#42303(96%) and #42301(97%) •#42301, 42302, 42305-42312(67~93%)	B A
II-h SDB	Initial [Cs] is reported to be 1.0×10^{-8} to 1.0×10^{-5} M. Cs is not solubility limited.	A
II-i SDB	It is indicated that samples had been centrifuged for 50 minutes at 7,000 rpm and filtered over 0.2 µm membrane filter. It is reported that filtration did not change the sorption values.	A
II-j SDB	A contact time of 7 and 180 days is indicated. The K_d values for Cs are for both reaction times in the same range, not as for Th and Am.	A/B
II-k REF	The samples were shaken.	A/B
II-l SDB	There are two initial Cs indicated. No variation in L/S is reported.	B
II-m REF	The experiments were carried out in glass bottles. Corrections for sorption on the vessel walls have not been done.	C/D
II-n REF	No error estimates are indicated for the K_d values. Number of replicates is not reported.	D
II-o REF	Experiments had been done with two different [Cs] and at two different reaction temperatures.	B

Data table Cs/2: REF: Andersson et al. (1983b)*			
JAEA-SDB version 4 - DATA: Cs/Granitic rocks; granite, gneiss, #43989-44010			
GUIDELINE: Revision 4b (May 19, 2005)			
*REMARK: Designation of the different solid phases is incorrect and not consistent (checkpoint II-a). It is recommended to keep original designations. Checkpoints II-a, II-f and II-i of SDB should be update/revised.			
Checkpoint		Evaluation	Rating
I-a.1	SDB	All mandatory fields are completed.	Yes
I-a.2	SDB	All mandatory information is provided.	Yes unreliable
	REF	It is indicated that for datapoints #43991-43993, 43995, 43997, 43999, 44001, 44004 and 44005 no L/S, no pH and no contact time is reported. It is not clear from the information provided, if experiments with different ionic medium (K _a values in table 7, p.20) were made with the same experimental conditions as described for batch experiments. These datapoints are classified as unreliable.	
I-b	SDB	Table with K _a values is given.	class 1
II-a	SDB	As solid phase gneiss, and granite#2 to #6 are indicated. Major mineralogy of granite#2 to #4 is given. Surface characteristics and CEC are not indicated. No information at all is given for granite#6. Granite #4 correspond to datapoint #44010 and granite#6 to datapoint #44008.	C/D (revise SDB)
	REF	As solid phases Stripa granite, Finisjön granite, Studsvik gneiss and Blekinge gneiss are reported.	
II-b	SDB	For datapoints #44007 to 44010 a final pH within a range of 1 pH unit is given. For all other datapoints a final pH within a range of 2 to 4 pH units are given, therefore these datapoints are considered as unreliable and not further classified.	D unreliable
II-c	SDB	It is indicated that experiments had been performed under aerobic conditions. Cs is not redox sensitive.	A/B
II-d	SDB	Initial solution composition (synthetic groundwater) is indicated.	C/D
	REF	The final solution composition is not reported, but can be estimated based on major mineral components and initial solution composition.	
II-e	SDB	A temperature of 22°C is reported.	A/B
II-f	SDB	A L/S ratio of 10~20 mL/g is indicated.	C/D (revise SDB)
	REF	Experiments had been performed with 0.5 to 1 g of solid in 45 mL solution. This corresponds to a L/S of 45~90. Since there is no surface area reported, rating C/D is applied.	
II-g	SDB	The sorption values are calculated from K _a and L/S ratios: •#44007(88% sorption) •#44008 to 44010(>98% sorption)	A C/D
II-h	SDB REF	Initial [Cs] of 1.0×10 ⁻⁸ to 1.0×10 ⁻⁷ M is reported. Cs is not solubility limited.	A
II-i	SDB	It is indicated that centrifugation was used for phase separation. Samples had been centrifuged for 1 hour at 4,000g.	C/D (update SDB)

Data table Cs/3: REF: Barney and Anderson (1979)* JAEA-SDB version 4 - DATA: Cs/Granitic rocks: granite, #44250~44255 GUIDELINE: Revision 4b (May 19, 2005) *REMARK: Update required for checkpoint II-c.		
Checkpoint	Evaluation	Rating
I-a.1 SDB	All mandatory fields are completed.	Yes
I-a.2 SDB	All mandatory information is provided. Information about the pH (initial and final), the groundwater composition and the mineralogy is missing. See checkpoints II-a, II-b and II-d for annotations.	No
I-b SDB	Table with K _a values is given.	class 1
II-a SDB REF	As solid phase granite#1 and granite#2 is indicated. Mineralogy is not reported. Specific surface area for granite#1 is given. The 'granite' used for experiments was fresh crushed quartz monzonite porphyry from the Nevada test site and a weathered one. It is indicated that qualitative mineralogy is reported in a previous report.	C/D
II-b SDB REF	It is indicated that no pH is reported. It is reported that the pH was in average 8.4 and about constant over 91 days.	B (update SDB)
II-c SDB REF	Redox conditions are not indicated. Initial Eh values are listed. Cs is not redox sensitive. Experiments had been performed under aerobic conditions.	A/B
II-d SDB REF	As water type groundwater is indicated. The solution composition is not indicated. From dissolution curves for elemental components of granite in synthetic groundwater at different times it is concluded that no equilibrium was reached even after a contact time of 35 days. Sorption edge curves do affirm that equilibrium was not reached.	unreliable

Data table Cs/4: REF: Barney and Brown (1979)* JAEA-SDB version 4 - DATA: Cs/Granitic rocks: granite, #44328-44330 GUIDELINE: Revision 4b (May 19, 2005) *REMARK: Update of SDB required for checkpoint I-a.2, II-b and II-c.		
Checkpoint	Evaluation	Rating
I-a.1 SDB	All mandatory fields are completed.	Yes
I-a.2 SDB REF	All mandatory information is provided. It is indicated that there is no information about reaction temperature, pH, initial [Cs] and redox conditions. Necessary information for the mentioned points is reported.	No (update SDB)
II-a SDB REF	As solid phase granite#1, 2 and 3 are indicated. Mineralogy is not indicated. For granite#1 BET and CEC, for granite#2 CEC is indicated. The 'granite' used for experiments was fresh crushed quartz monzonite porphyry from the Nevada test site. There are two granite samples A and B reported with qualitative information about mineralogy. K _a values are given for a fresh and two types of weathered granite samples. However it is not clear from the data, if these samples correspond to granite A or B.	C/D (tentative)
II-b SDB	It is indicated that experimental pH is not reported.	B

	REF	It is reported that the pH was about constant over the contact time of 154 days and was averaged 8.4. Since the pH is an average value rating B is applied.	(update SDB)
II-c	SDB	It is indicated that redox conditions are not reported. Cs is not a redox sensitive element.	(update SDB) A/B
	REF	According the information provided by the authors it is assumed that experiments had been performed at aerobic conditions. It is reported that experiments had been made in sealed polyethylene bottles.	
II-d	SDB	Groundwater is indicated as water type. The final solution composition is not given.	unreliable
	REF	The composition of synthetic groundwater is reported. The dissolution curve for element components of granite in groundwater shows no equilibrium over a time period of 150 days. Also the sorption vs. time plot shows that equilibrium was not reached before 150 days. Since the datapoints indicated in the SDB correspond to a reaction time of 14 days, data are considered as unreliable.	

Data table Cs/5: REF: Benischek et al. (1992a)*		
IAEA-SDB version 4 - DATA: Cs/Granitic rocks; granodiorite, granite-gneiss, mylonite, #47310-47373		
GUIDELINE: Revision 4b (May 19, 2005)		
*REMARK: Necessary information e.g. pH values or solution composition are not entered in the IAEA-SDB. SDB should be revised for checkpoint II-a, II-b, II-d, II-I, II-j for further classification ¹ .		
Checkpoint	Evaluation	Rating
I-a.1 SDB	All mandatory fields are completed.	Yes
I-a.2 SDB	All mandatory information is provided.	No
REF	Necessary information e.g. about pH are not indicated in the IAEA-SDB, although reported in the reference.	(revise SDB)

Data table Cs/6: REF: Byegard et al.(1998)*		
IAEA-SDB version 4 –DATA: Cs/Granitic rocks; granite #62586-62603 and 62628-62630 and 62634-62636, diorite #62553-62573 and 62622-62627 and 62631-62633, mylonite #62616-62621		
GUIDELINE: Revision 4b (May 19, 2005)		
* REMARK: Data for mylonite # 62616-62621 are also included in this entry of the SDB, but should be categorized under clay or other minerals, not under granitic rocks		
Checkpoint	Evaluation	Rating
I-a.1 SDB	All mandatory fields are completed.	Yes
I-a.2 SDB	Not all mandatory information is provided. Missing is the information on phase separation.	No
REF	No phase separation technique was used. Spiked solutions were (incompletely) extracted from the solid phases, followed by some type of rinsing process and desorption. It is not described how the extraction was done. Based on the rating "No", the data cannot be used. According to II-i, all data would also be rated as unreliable.	

Data table Cs/7: REF: Daniels (1981)* JAEA-SDB version 4 - DATA: Cs/Granitic rocks; granite #50041-50062 GUIDELINE: Revision 4b (May 19, 2005) *REMARK: Update of SDB required for checkpoints II-a, II-b, II-d, II-f and II-g.		
Checkpoint	Evaluation	Rating
I-a.1 SDB	All mandatory fields are completed.	Yes
I-a.2 SDB	All mandatory information is provided. For datapoints #50041, 50046, 50050, 50052, 50055 and 50058 it is indicated that no information about pH is provided. See checkpoint II-b for details. For all other datapoints the information about L/S is not reported. It is mentioned that experimental conditions are reported elsewhere in cited reference.	No (update SDB)
REF		
I-b SDB	A table with K_d values is given.	class 1
II-a SDB	As solid phase granite#1 and #2 are indicated. Mineral compositions and surface characteristics are not reported. Fraction sizes of the granite samples are indicated.	B (update SDB)
REF	Mineralogy in volume percent of the climax stock granite samples is given in Erdal et al. (1979c). Surface areas of different fraction sizes are listed, however, not for the fraction sizes indicated in the SDB.	
II-b SDB	•It is indicated that for datapoints #50041, 50046, 50050, 50052, 50055 and 50058 no information about pH is reported. •Distinct initial pH values are indicated for datapoints #50042, 50043, 50048, 50049, 50051, 50054, 50056, 50057, 50061 and 50062. •Initial and final pH values are reported for datapoints #50044, 50045, 50047, 50053, 50059 and 50060.	(update SDB) D A
REF	An initial pH of about 8 is reported for the two synthetic groundwaters used for the experiments in the cited reference Erdal et al. (1980). Since this is not a distinct value, rating D is applied for datapoints #50041, 50046, 50050, 50052, 50055 and 50058.	C
II-c SDB	It is indicated that for datapoints #50041, 50046, 50050, 50052, 50055 and 50058 no information about redox conditions are reported. For all other datapoints either atmosphere or controlled atmosphere is indicated. Cs is not redox sensitive.	A/B
REF		
II-d SDB	As water type groundwater#1 and groundwater#2 are indicated. Final solution compositions are not given.	(update SDB) C/D
REF	It is reported that for experiments the same conditions were used as in three cited references. In Erdal et al. (1980) the initial composition of two synthetic groundwaters is described related to Cs batch experiments. Rating C/D is applied because the final solution compositions have to be estimated approximately.	
II-e SDB	•For datapoints #50041, 50046, 50050, 50052, 50055 and 50058 no reaction temperature is indicated. •For all others a reaction temperature is reported.	C/D A/B
II-f SDB	The used amount of solid and liquid for experiments is not reported.	C/D (update SDB)
REF	In the cited reference Erdal et al. (1979c) it is reported that for reactions 1 g of solid was added to 20 mL of solution. With the	

		given surface area of 4.0 and 3.3 m ² /kg, measured with the ethylene glycol method for granite#1 and #2 respectively, rating C/D is applied.	
II-g	SDB REF	Only for datapoints #50041, 50046, 50050, 50052, 50055 and 50058 a L/S is indicated. For all other datapoints it is indicated that the L/S is not reported. The sorption values calculated from indicated K _d and L/S ratios are >98%. With the given L/S of 20 mL/g in the cited Erdal et al. (1979c) the following sorption values are calculated: •#50048(54%), 50049(12%), 50051(95%), 50054(25%), 50056(8%), 50057(90%), 50059-50061(94%) •#50042-50045(96~98%), 50053(95%), 50062(95%) •#50047(>98%)	A B C/D
II-h	SDB REF	Initial Cs-concentration of 1.02×10^{-10} to 1.87×10^{-3} M is indicated. Cs is not solubility limited. For datapoints #50044, 50045, 50047, 50053, 50059 and 50090 no [Cs] _{init} is reported.	A unreliable
II-i	SDB REF	Only for datapoints #50042, 50043, 50048, 50049, 50051, 50054, 50056, 50057, 50061 and 50062 the separation method is indicated. These samples had been filtered over 0.45 µm membrane. For the datapoints without any separation technique indicated in the SDB it is assumed that samples had been centrifuged for one hour at 16,000 rpm, and afterwards filtered over 0.45 µm membrane, as described in the cited reference Erdal et al. (1979c).	C/D (update SDB) B
II-j	SDB REF	Reaction times of 21, 42 and 84 days are indicated. It is reported that there is an increase in sorption with time (p.19) and that the changes that take place in granite with time are more effective in changing the sorption of cesium than are the low oxygen and carbon oxide concentrations present in the controlled atmosphere experiment. Therefore the data are considered as unreliable.	unreliable

Data table Cs/8: REF: Erdal et al.(1979a)* JAEA-SDB version 4 –DATA: Cs/Granitic rocks; granite, #50772-50786 GUIDELINE: Revision 4b (May 19, 2005) * REMARK: The extraction of datapoints is not systematical and comprehensive, and not all datapoints given in the reference are listed in the SDB. It is noted in the REF that experiments of the same batches measured several months later give different results (by a factor of three). Revision of the SDB required for checkpoints II-b, II-c, II-d, II-i, II-j, II-n		
Checkpoint	Evaluation	Rating
I-a.1 SDB	All mandatory fields are completed.	Yes
I-a.2 SDB	All mandatory information is provided	Yes
I-b SDB	The K _d values are listed in tables.	class 1
II-a SDB REF	Granite samples of different fraction sizes and with a specific surface area of 0.1 to 0.95 m ² /g is indicated. Major composition of the granite is indicated. The granite samples had been a Climax Stock granite from the Nevada test site. It had been crushed to fraction sizes of 106~150,	B update SDB

		250~355, and 500~850 μm .	
II-b	SDB REF	It is indicated that initial and final pH values are reported. However, initial pH values for the Cs batch experiments are reported in the reference to be 7.69 for the experiments at ambient temperature (p.24). The data of batch sorption experiments at 70°C show clearly (p. 32 and 41) that steady state was not reached after a contact time of more than 60 days. Changes in the solid phase cannot be excluded as the noted in the REF (p.24). The datapoints measured at 70°C are therefore considered as unreliable. • # 50776, 50777, 50780, 50781, 50784, and 50785	A revise SDB unreliable
II-c	SDB	It is indicated that experiments had been performed under aerobic conditions. Cs is not a redox sensitive element. For the Eh values zero instead of n.r. is indicated in the SDB.	A/B (revise SDB)
II-d	SDB	Different synthetic groundwaters are indicated. The initial composition of the solutions is given. The final solution composition is not reported but can be estimated based on the information about the main mineral composition. There may be minor solution components that cannot be estimated. Remark: it seems to be unclear how the different groundwaters were assigned to the different datapoints in the SDB, since it is not clearly tabulated in the reference.	C/D (tentative) (verify SDB)
II-e	SDB	A reaction temperature of 22°C is indicated.	A/B
II-f	SDB REF	A L/S of 20 mL/g is indicated. Based on the given surface area of 0.1 to 0.95 m ² /g, the mass of 1 g granite used in the experiment has a surface area of maximum 0.95 m ² .	C/D
II-g	SDB	The sorption values were calculated based on the information given in the SDB. • # 50773, 50775, 50779, 50783 (86~93%) • # 50772, 50774, 50778, 50782, 50786 (95~97%)	A B
II-h	SDB	Initial [Cs] is indicated (1.4×10^{-9} mol/L). Cs is not solubility limited.	A
II-i	SDB REF	It is indicated that no separation method is reported. Samples had been centrifuged for one hour at 16,000 rpm, and then filtered through a 0.45 μm membrane.	B (revise SDB)
II-j	SDB	Contact times of 56 and 66 days are indicated. The measurements of the two batches (both experiments measured at ambient temperature) several months later differ by a factor of about three.	A/B (update SDB)
II-k	REF	The reaction vessels were shaken.	A/B
II-l	REF	No variation of either Cs concentration or in L/S had been performed.	C/D
II-m	REF	The experiments had been performed in polyethylene tubes and corrections for sorption on vessel walls had not been made.	B
II-n	SDB REF	It is indicated that no information is reported. No replicate measurements had been made. Standard deviations are given.	C (update SDB)
II-o	REF	No parameter variation was performed.	D

Data table Cs/9: REF: Erdal(1980)* JAEA-SDB version 4 –DATA: Cs/Granitic rocks, granite # 51198, 51199 GUIDELINE: Revision 4b (May 19, 2005) * REMARK: Update or revision of SDB required for checkpoints II-i and II-n.		
Checkpoint	Evaluation	Rating
I-a.1 SDB	All mandatory fields are completed.	Yes
I-a.2 SDB	All mandatory information is provided.	Yes
I-b REF	A table with K_d values is given.	class 1
II-a SDB	Granite is reported as mineral phase without detailed mineralogical composition. Surface area or CEC are not provided. Fraction sizes are given.	C/D (tentative)
REF	At least partly, this information is given (see II-f).	update SDB
II-b SDB	Initial and final pH values are reported.	A
II-c SDB	It is indicated that experiments had been performed under anoxic conditions. Cs is not redox sensitive.	A/B
II-d SDB	As water type groundwater is indicated. Final solution compositions are not given.	update SDB C/D (tentative)
REF	It is indicated that the same groundwater was used for experiments as described in cited references. However there are different groundwater compositions (synthetic groundwater and groundwaters after equilibration) given in the cited literature. It is assumed that the synthetic groundwater was used.	
II-e SDB	A temperature of 32°C is indicated.	A/B
II-f SDB	A L/S of 20 mL/g is indicated.	A/B C/D
REF	Based on the table with given specific surface areas at different fraction sizes of Climax granite core 7, the mass of 1 g granite used for an experiment had a surface area of about 3 to 11 m ² . • # 51198 (<75 µm, assuming 1 g > 5 m ²) • # 51199 (75~500 µm, assuming 1 g < 5 m ²)	
II-g SDB	The sorption values were calculated based on the information given in the SDB. • # 51198 (97%) • # 51199 (99%)	B C/D
II-h SDB	Initial [Cs] is reported. Cs is not solubility limited.	A
II-i SDB	It is indicated that no separation method is reported.	C/D (revise SDB)
REF	Supernatant had been several times centrifuged at 12,000 rpm.	
II-j SDB	A reaction time of 20.63 days is indicated.	C/D
REF	The kinetics of sorption are not reported.	
II-k REF	Samples had been shaken.	A/B
II-l SDB	No isotherm, no variation of the Cs concentration and no variation of L/S is indicated.	C/D
II-m REF	Polypropylene tubes were used for experiments and no corrections for sorption on the vessel walls had been performed.	B
II-n SDB	It is indicated that three replicates and error estimates are reported.	C (revise SDB)
REF	The error estimates given are the standard deviations for a single measurement of the K_d values. Replicate measurements or experiments are not reported.	
II-o REF	No parameter variation is done.	D

Data table Cs/10: REF: Eriksen and Locklund(1987)* JAEA-SDB version 4 –DATA: Cs/Granitic rocks; granite, #51424-51444 GUIDELINE: Revision 4b (May 19, 2005) * REMARK: Update required for checkpoints I-a.2, I-b, II-a, II-b, II-c, II-d, II-i, II-j. It is not clear which data exactly are taken from the REF (read off from which graphs, for which contact times, etc.). This needs to be clarified (see II-j).		
Checkpoint	Evaluation	Rating
I-a.1 SDB	All mandatory fields are completed.	Yes
I-a.2 SDB	Not all mandatory information is provided. It is indicated that pH values, contact time, phase separation methods, atmosphere conditions, and reaction temperature are not reported.	revise SDB Yes (tentative)
REF	The missing information is available.	
I-b SDB	It is indicated that K_d values are calculated	class 3 (tentative) to be verified
REF	K_d values are from linear graphics. Except for the point # 51439, all datapoints are given as a function of $1/d$ with d as the arithmetic mean of the particle size fraction. The quality of graphs is questionable. It is assumed that data has been read off correctly by the operator.	
II-a SDB	Fourteen granite samples are reported as solid phases (different fraction sizes). Mineral composition and surface characteristics are not indicated.	C/D (update SDB)
REF	The granite samples should be specified more precisely. Granitic drill cores from the Stripa mine were used for the experiments. The cation exchange capacities of the mean fraction sizes (d) of the samples are given in a plot CEC versus $1/d$.	
II-b SDB	It is indicated that no pH values are reported.	D (revise SDB)
REF	The initial pH of the artificial groundwater is given. It is 8 to 8.2.	
II-c SDB	It is indicated that redox conditions or Eh values are not reported. Cs is not redox sensitive.	A/B (revise SDB)
REF	The Eh of artificial groundwater is 260 mV, and the groundwater was used under aerobic conditions.	
II-d SDB	It is indicated that synthetic groundwater was used for experiments. Initial or final composition of the groundwater however is not given.	update SDB C/D
REF	The composition of the artificial groundwater is tabulated. Rating C/D is applied because the final solution compositions have to be estimated approximately.	
II-e SDB	Temperature is not reported.	C/D
REF	No additional information is available.	
II-f SDB	A liquid/solid ratio of 30 mL/g is reported.	C/D
REF	It is reported that standard-scale experiments used 3 mL of solution and 0.1 g of solid. BET values of the samples are not reported. Since BET values of granite are usually below 5 m ² /g rating C/D is applied.	
II-g REF	The sorption value (calculated from K_d and L/S ratios) ranges between 17% and 90%.	A
II-h SDB	Initial [Cs] is reported as 1.1×10^{-9} mol/L. Since Cs is not solubility limited, the datapoints are classified as A.	A
II-i SDB	Centrifugation without any further details is indicated.	update SDB
REF	It is reported that filtration (not specified) was applied for	

		separation.	C/D
II-j	SDB	It is indicated that no reaction time is reported (except datapoint # 51439).	C/D (tentative) revise SDB
	REF	Contact times of 48 hours and 7 days are reported. From graphs it seems that equilibrium was reached after about 100 min. It needs to be verified that the data entered in the SDB are read off for the correct conditions.	
II-k	REF	There is no information about the agitation method.	C/D
II-l	REF	No variation in L/S or initial Cs concentration is indicated.	C/D
II-m	REF	The experiments were carried out in polypropylene tubes. Corrections for sorption on the vessel wall had been performed, but no details are provided.	C/D
II-n	SDB	It is indicated that no error estimates are reported.	D
	REF	Experimental error bars are given in the graphics, but there is no information about their derivation, therefore rating D is applied.	
II-o	REF	No parameter variation was done.	D

Data table Cs/11: Eriksen and Locklund (1989)* JAEA-SDB version 4 –DATA: Cs/Granitic rocks; granite, #51452 GUIDELINE: Revision 4b (May 19, 2005) * REMARK: Only one datapoint of several available ones with crushed granite is entered into the SDB. There is an experiment reported with ¹³⁷ Cs-solution on Stripa granite coupons where equilibrium was not reached even after 120 days of contact time. These data are unreliable and should not be entered to the SDB. Update of SDB required for checkpoints I-a.2, II-a, and II-c.		
Checkpoint	Evaluation	Rating
I-a.1 SDB	All mandatory fields are completed.	Yes
I-a.2 SDB	All mandatory information is provided. An incorrect K _d value is given.	No (correct SDB)
I-b SDB	A table with K _d values is provided	class 1
II-a SDB	Crushed Stripa Granite is indicated as solid phase. BET is given, but information about mineralogy is not reported.	B (revise SDB)
	REF The BET indicated in SDB is not the same given in the reference.	
II-b SDB	An initial pH value of 8 to 8.2 is indicated.	D
	REF No further information is available.	
II-c SDB	It is indicated that atmospheric conditions of the experiment are not reported. An initial Eh value is indicated to be 260 mV. Cs is not a redox sensitive element.	A/B (update SDB)
	REF It is reported that groundwater was aerated.	
II-d SDB	The composition of synthetic groundwater is indicated.	C/D
	REF No further information is available. It is assumed that final solution composition can be approximately estimated.	
II-e SDB	A temperature of 20°C is indicated.	A/B
II-f SDB	A liquid/solid ratio of 30 is indicated. It is indicated that 3 mL of solution with 0.1 g of solid phase were used for the experiments.	C/D
	REF Based on a BET of 0.25 m ² /g for crushed Stripa granite, rating C/D is given.	
II-g REF	The sorption value (calculated from K _d and L/S ratio) is 52%.	A

II-h	SDB	The initial [Cs] is 1.0×10^{-9} mol/L. Since Cs is not solubility limited, the datapoint is classified as A.	A
II-i	SDB	Filtration over a 0.5 μ m membrane is indicated.	C/D
II-j	SDB REF	A contact time of 120 days is indicated. There is only one datapoint of the sorption on Stripa granite of the same particle size available. Measurements on intact Stripa granite did not reach equilibrium after 120 days. It cannot be excluded that this could be due to changes in the solid phase, therefore changes in crushed granite samples cannot be excluded as well.	unreliable (tentative)
II-k	REF	Gentle agitation of the tubes is reported.	A/B
II-l	SDB	No variation of initial [Cs] or L/S is indicated.	C/D
II-m	REF	Polypropylene tubes had been used for experiments and the results are corrected for the amount of radionuclide sorbed onto the tube walls. It is not reported how the sorption onto the tube walls had been measured, therefore rating C/D is applied.	C/D
II-n	SDB	An error estimate is indicated	C
II-o	REF	No parameter variation had been performed.	D

Data table Cs/12: REF: Fujikawa and Fukui (1997a)*

JAEA-SDB version 4 – DATA: Cs/Granitic rocks; granite, #51751-51762

GUIDELINE: Revision 4b (May 19, 2005)

* REMARK: Update of SDB for checkpoint I-a.2.

Checkpoint	Evaluation	Rating
I-a.1	SDB All mandatory fields are completed.	Yes
I-a.2	SDB Information about major mineral composition and CEC or BET is lacking.	unreliable
	REF A reference is cited (Fujikawa and Fukui, 1991), where mineral composition and surface characteristics are provided.	(update SDB)

Data table Cs/13: REF: Huitti et al.(1998)*

JAEA-SDB version 4 –DATA: Cs/Granitic rocks; granite, mica gneiss, tonalite # 53346-53523

GUIDELINE: Revision 4b (May 19, 2005)

* REMARK: For final classification a revision of SDB for checkpoints II-b, II-d, and II-i is necessary.

Checkpoint	Evaluation	Rating
I-a.1	SDB All mandatory fields are completed.	Yes
I-a.2	SDB All mandatory information is provided	Yes
I-b	SDB Table with K_d values is given	class 1
II-a	SDB Granite, mica gneiss and tonalite are reported as mineral phases. Mineralogy and BET characteristics for the phases are indicated. CEC and composition of opaque fraction is not indicated. It is not clear whether crushing had any effect on final composition.	B
II-b	SDB Only initial pH values are indicated in SDB, and for several datapoints only a range of initial pH. REF Final pH values (incl. uncertainties) after equilibration are reported for the different reported waters.	revise SDB A
II-c	SDB It is indicated that experiments had been performed at ambient conditions. Cs is not a redox sensitive element.	A/B
II-d	SDB Fresh groundwater and saline groundwater are indicated, but no	revise SDB

REF		solution compositions are given. All solutions used for experimentation were synthetic groundwaters. The fresh reference water was the Allard water and modified Allard water. The saline reference water was the synthetic saline groundwater from Olkiluoto, and a brine reference water and a dilution of it. Chemical composition of the waters after equilibration is reported.	A/B
II-e	SDB	Reactions had been performed at room temperature.	A/B
II-f	SDB	A L/S ratio of 10 mL/g is indicated. For the experiments 3.5 g of the solid phase were used per reaction vial. Based on a BET of 1.55 m ² /g for mica gneiss a total surface area of > 5.0 m ² is reached and rating A/B is given. In case of granite and tonalite with a BET of 0.4 respective 0.28 m ² /g, rating C/D is given: • # 53405-53464 (mica gneiss) • # 53346-53404 (granite) and 53465-53523 (tonalite)	A/B C/D
II-g	SDB	The sorption values are calculated from K _d and L/S ratios: • # 53346-53378, 53380-53383, 53385/86, 53389-53397, 53399-53403, 53405/06, 53408-53412, 53414, 53416-53422, 53452/53, 53455-53459, 53461-53463, 53466-53475, 53483/88/90, 53492-53503, 53506-53517, 53519-53522 (9~95% sorption) • # 53424-53426, 53429/30, 53433/34, 53436-53442, 53478, 53480-53482, 53484-53487, 53489/91, 53504/05, (95~98% sorption) • # 53379/84/87/88/98, 53404/07/13/15/23/27/28/31/32/35, 53443-53451, 53454/53460/64/65/76/77/79, 53518/23 (98~100% sorption)	A B C/D
II-h	SDB	Initial [Cs] is reported. Cs is not solubility limited.	A
II-i	SDB	Centrifugation is indicated. Separation was performed in a centrifuge at 6500 g for 30 minutes.	D (update SDB)
II-j	SDB REF	A reaction time of 21 days is indicated. It is reported that a steady state was achieved in 7 to 10 days.	A/B
II-k	REF	Samples were mixed continuously for 15 minutes each hour during the equilibration.	A/B
II-l	SDB	Isotherms for the three solid phases and the different synthetic waters are available. A variation in L/S had not been performed.	A
II-m	REF	Polypropylene centrifuge tubes were used for experiments. Blank tests and corrections for sorption on vessel walls had not been done.	B
II-n	SDB REF	Uncertainties are not reported, and it is indicated that information about replicates is not given. It is reported that four parallel samples were set up. Three of them were spiked with radioactive Cs, the fourth was used for chemical analysis of the water. Each of the parallel measurements is entered to the SDB so that error estimates could be calculated.	update SDB A (tentative)
II-o	SDB	Isotherms for each solid phase and water system are available. A systematic variation in pH had not been performed, but different salinities are indicated.	B

Data table Cs/14: REF: Kitamura et al. (1997) JAEA-SDB version 4 – DATA: Cs/Granitic rocks; granite, #53971-53977 GUIDELINE: Revision 4b (May 19, 2005)		
Checkpoint	Evaluation	Rating
I-a.1 SDB	All mandatory fields are completed.	Yes
I-a.2 SDB	All mandatory information is provided.	Yes
I-b SDB REF	The K_d values are extracted from graphs with a logarithmic scale. Not all datapoints from the literature are listed in the SDB.	class 5 (update SDB)
II-a SDB REF	Granite with a specific surface area of 0.11 m ² /g is indicated. The granite sample had been a biotite granite from Inada, Ibaraki, Japan. It had been crushed to a mesh size of 32 to 60.	B
II-b SDB	Final pH values are reported within 1 to 2 pH units. Inert NaClO ₄ electrolyte solution had been used and the pH was adjusted by addition of either HClO ₄ or NaOH. <ul style="list-style-type: none"> Final pH values of datapoints # 53971 to 53973 are reported to be in a range of 1 pH unit. For datapoints # 53974 to 53977 a final pH within 2 units is given. Therefore it was decided to give rating C. 	B C
II-c SDB REF	There is no information about redox conditions. It is indicated that experiments had been performed in an argon filled glove box to avoid contamination of carbonate. Cs is not a redox sensitive element.	A/B (update SDB)
II-d SDB REF	The initial composition of the solution is given (0.01 M and 0.1 M NaClO ₄). The initial composition of the electrolyte is given. The final solution composition is not reported and cannot be estimated due to lacking information about the mineral composition. Based on an indicated L/S of 40 mL/g, components of the rock are assumed not to be important with regard to the final solution composition in case of 0.1 M NaClO ₄ -solution. In case of the 0.01 M NaClO ₄ however, there may be minor solution components that cannot be estimated. <ul style="list-style-type: none"> Datapoints # 53971, # 53973 to 53975 Datapoints # 53972, 53976, 53977 	 A/B C/D
II-e SDB	A reaction temperature of 24°C is indicated.	A/B
II-f SDB REF	A L/S of 40 mL/g is indicated. Based on the given BET of 0.11 m ² /g, the mass of 0.1 g granite used in the experiment has a surface area of about 0.011 m ² .	C/D
II-g SDB	The sorption value (calculated from K_d and L/S ratios) ranges between 10% and 64%.	A
II-h SDB	Initial [Cs] is reported (2.5×10^{-6} mol/L). Cs is not solubility limited.	A
II-i SDB REF	Centrifugation is reported as separation method. Centrifugation at 5,000 rpm for 10 minutes is reported as separation method.	C/D
II-j SDB	A contact time of 7 days is indicated.	C/D
II-k REF	The reaction vessels were shaken.	A/B
II-l REF	No isotherms, no variation of the Cs concentration is indicated.	C/D
II-m REF	Polypropylene tubes were used as reaction vessels. Since not	B

		reported, it is assumed that no corrections for sorption to the vessel walls had been performed.	
II-n	REF	No replicates and no error estimates are reported.	D
II-o	REF	pH value is varied.	C

Data table Cs/15: REF: Maclean et al.(1978)* JAEA-SDB version 4 –DATA: Cs/Granitic rocks; granite #56174-56182 GUIDELINE: Revision 4b (May 19, 2005) * REMARK: An update of SDB is required for checkpoints II-b, II-i, and II-n.			
Checkpoint		Evaluation	Rating
I-a.1	SDB	All mandatory fields are completed.	Yes
I-a.2	SDB	All mandatory information is provided	Yes
I-b	SDB	Table with K_d values is given	class 1
II-a	SDB	Climax Stock granite, Westerly Granite, and Climax Shear Zone granite of different mesh sizes were used for batch experiments. Mineralogy is not indicated. BET characteristics are given for some of the datapoints. Due to the crushing, minor changes in the mineralogy may have had occurred.	C/D
	REF	No further information is available	
II-b	SDB	The indicated pH of synthetic groundwater does not correspond to the given pH in the reference.	revise SDB C
	REF	Initial pH value of the synthetic groundwater of granite is reported to be 7.8 ± 0.3 .	
II-c	SDB	It is indicated that experiments had been performed under aerobic conditions. Cs is not a redox sensitive element.	A/B
II-d	SDB	Synthetic groundwater is indicated and the chemical composition of the water is given.	C/D
	REF	Samples were pre-washed repeatedly. The final solution composition is not given, but can be estimated approximately. Due to the pre-washing, concentrations of major cations should not have been changed significantly.	
II-e	SDB	Reactions had been performed at 25°C.	A/B
II-f	SDB	A L/S ratio of 15 mL/g is indicated. For the experiments 1 g of the solid phase were used per reaction vial. Based on a BET of 4.37 m ² /g reported for Climax Shear Zone 1 (sieved with a mesh of 100~325 µm), rating C/D is given. For the granite samples with a BET>5 m ² /g rating A/B is given. For all datapoints without any information about the surface characteristics rating C/D is applied in analogy to the data for Climax Shear Zone 1 sample. • #56176/79 • #56174/75/77/78, 56180-56182	A/B C/D
II-g	SDB	The sorption values are calculated from K_d and L/S ratios: • #56181 (93% sorption) • #56174, 56182 (96~97% sorption) • #56175-56180 (98~99% sorption)	A B C/D
II-h	SDB	Initial [Cs] is reported. Cs is not solubility limited.	A
II-i	SDB	Filtration through a 0.1 µm membrane is indicated.	update SDB
	REF	Samples were first centrifuged at 3000 rpm for 20 to 60 minutes	

		and the supernatant solution was then filtered through a 0.1 μm nucleopore filter. While the phase separation method involved two steps, none of them is very effective for colloid removal.	C/D
II-j	SDB	A reaction time of 7 days is indicated.	C/D
II-k	REF	Samples were shaken continuously in a shaker-table (130 oscillations/min.).	A/B
II-l	SDB	No isotherm was determined and no variation in L/S had been performed.	C/D
II-m	REF	Polycarbonate centrifuge tubes with polypropylene screw caps were used for experiments. Blank tests had been made and sorption onto vessel walls had been considered by using the equation by Serne et al. (1977) for R_d calculations, possibly leading to overcorrection.	C/D
II-n	SDB	It is indicated that three replicates had been made, but no error estimates are reported.	update SDB
	REF	It is reported that three parallel samples were set up. Error estimates for the R_d values are given.	A
II-o	SDB	No parameter variation is indicated.	D

Data table Cs/16: REF: Sato et al. (1997) JAEA-SDB version 4 – DATA: Cs/Granitic rocks; granodiorite, #58950-58958 GUIDELINE: Revision 4b (May 19, 2005)			
Checkpoint	Evaluation		Rating
I-a.1	SDB	All mandatory fields are completed.	Yes
I-a.2	SDB	All mandatory information is provided.	Yes
I-b	REF	A table with K_d values is provided	class 1
II-a	SDB	Three granodiorite samples are reported as solid phases (intact granodiorite, altered granodiorite and fracture fillings). CEC values (2.0, 1.9 and 17.3 meq/100 g) are provided.	A (tentative) (update SDB)
	REF	Kurihashi granodiorite of the Kamaishi In Situ Test Site had been used for the experiments. It is assumed that mineralogy and detailed composition of the granodiorite samples are known. BET values are reported in the reference.	
II-b	SDB	Final pH values are reported (after a contact time of 30 days, which can be assumed to be enough for reaching equilibrium).	A
II-c	SDB	It is indicated that experiments had been performed under aerobic conditions. Eh values are not reported. Cs is not a redox sensitive element.	A/B
II-d	SDB	The final solution composition of the equilibrated groundwater is provided.	A/B
	REF	In situ groundwater sampled from the Kamaishi In Situ Test Site was used for the sorption experiments.	
II-e	SDB	Temperature is reported to be 23°C.	A/B
II-f	SDB	A liquid/solid ratio of 100 mL/g is reported.	C/D
	REF	It is reported that standard-scale experiments used 100 mL of solution and 1.0 g of solid. With BET values of 0.7 m ² /g (intact granodiorite) and 1.9 m ² /g (altered granodiorite, fracture fillings) rating C/D is applied.	
II-g	REF	The sorption value (calculated from K_d and L/S ratios) ranges	A

		between 15% and 53%.	
II-h	SDB	Initial [Cs] is reported as 8.6×10^{-5} mol/L. Since Cs is not solubility limited, the datapoints are classified as A.	A
II-i	SDB	Standard filtration over a 0.45 μ m filter is reported as separation method.	C/D
II-j	SDB	A contact time of 30 days is indicated. This reaction time is reasonably long.	C/D
II-k	REF	There is no information about the agitation method.	C/D
II-l	REF	No variation in L/S or initial Cs concentration is indicated.	C/D
II-m	REF	The experiments were carried out in teflon bottles. Corrections for sorption on the vessel wall had been performed by measurement of tracer concentration in the blank solution. This may have led to overcorrection.	C/D
II-n	SDB REF	Error estimates are reported. Erroneously one replicate is indicated. Three replicates are reported and the error of K_d was calculated based on the analytical error.	C (revise SDB)
II-o	REF	No parameter variation was done.	D

Data table Cs/17: REF: Torstenfelt et al.(1981)* JAEA-SDB version 4 – DATA: Cs/Granitic rocks; granite, gneiss #61057-61135 GUIDELINE: Revision 4b (May 19, 2005) * REMARK: There are ten datapoints listed in table 7 of the reference, where a distinct pH is given for Cs on Stripa granite, but these datapoints are not listed in the SDB. After an update of SDB these datapoints will be classified.		
Checkpoint	Evaluation	Rating
I-a.1 SDB	All mandatory fields are completed.	Yes
I-a.2 SDB	All mandatory information is provided.	Yes
II-b SDB	For all datapoints only a range of pH of two pH units or larger is indicated as end pH. Therefore all datapoints # 61057-61135 are considered as unreliable. This is based on the complex nature of the sorbing substrate, which may include impurities whose contribution to solution chemistry may depend on pH. Similar pH ranges were accepted in case of simple substrates (hematite, magnetite).	unreliable

Data table Cs/18: REF: Yamagata et al. (1981)* JAEA-SDB version 4 – DATA: Cs/Granitic rocks; granite, #61752-61757 GUIDELINE: Revision 4b (May 19, 2005) * REMARK: Values of datapoint # 61755 is identical to # 61756. Either C_{init} or temperature value of datapoint # 61754 does not correspond to the indications of the reference. # 61755 and # 61754 are therefore not evaluated. Update of SDB required for checkpoints II-a, II-c, and II-d.		
Checkpoint	Evaluation	Rating
I-a.1 SDB	All mandatory fields are completed.	Yes
I-a.2 SDB	All mandatory information is provided.	Yes
I-b REF	A table with K_d values is provided	class 1
II-a SDB	Granite is indicated as solid phase containing 44% K-feldspar and 1% iron oxide. Surface characteristics are not reported.	B
REF	Crushed granite from Inada, Ibaraki Pref., Japan with three	update

		particle sizes is reported. Major and minor mineralogy are given. Rating B is applied, since BET or CEC can be estimated on the basis of known surface characteristics of the single minerals in the granite. Fe-oxide is not important for Cs-sorption.	SDB
II-b	SDB	Final pH values are indicated.	A
II-c	SDB	It is indicated that experiments had been performed under aerobic conditions. Eh values are indicated to be 0 mV. Cs is not a redox sensitive element.	A/B (revise SDB)
	REF	Initial and final Eh values are not reported.	
II-d	SDB	A “prepared Cs nitrate solution” without information about concentration is indicated. The final solution composition is not indicated.	C/D (update SDB)
	REF	Distilled water including CsNO ₃ from 1 to 1,000 ppm is indicated. Final solution composition can be estimated based on mineral composition.	
II-e	SDB	A temperature of 25°C is indicated.	A/B
II-f	SDB	A liquid/solid ratio of 10 is indicated. It is indicated that 200 mL of solution with 20 g of solid phase were used for the experiments.	A/B
II-g	REF	The sorption values (calculated from K _d and L/S ratios) range from 26% to 58%.	A
II-h	SDB	Initial [Cs] range from 7.52×10^{-5} to 7.52×10^{-4} mol/L. Since Cs is not solubility limited, the datapoints are classified as A.	A
II-i	SDB	Centrifugation at 4,000 rpm for 5 minutes is indicated.	C/D
II-j	SDB	A contact time of 16 days is indicated.	A/B
	REF	Diagrams of kinetic measurements indicate that steady state is reached around the indicated contact time.	
II-k	REF	Continuous stirring or shaking is reported.	A/B
II-l	SDB	A limited variation of initial [Cs] is indicated.	B
II-m	REF	Erlenmeyer glass vessels with stoppers were used for experiments. Information about corrections for sorption on vessel walls is not given.	C/D
II-n	SDB	No error estimates are indicated.	D
II-o	REF	Initial [Cs] had been varied.	C

Data table Cs/19: REF: Andersson et al. (1983b)

JAEA-SDB version 4 – DATA: Cs/Al-oxide/-hydroxide, #44020

GUIDELINE: Revision 4b (May 19, 2005)

Checkpoint	Evaluation	Rating
I-a.1	SDB All mandatory fields are completed.	Yes
I-a.2	SDB All mandatory information is provided	Yes
I-b	SDB A table with K _d values is given	class 1
II-a	SDB Corundum is reported as solid phase. CEC or surface characteristics are not given. Mineralogy and surface characteristics of corundum are known.	B
II-b	SDB A final pH range between 7 and 8 is reported (about 1 pH unit). REF The spiked solution was roughly adjusted to the desired level of pH with HCl or NaOH at the experimental setup.	B
II-c	SDB The experiment was performed under aerobic conditions. Cs is not a redox sensitive element.	A
II-d	SDB The initial composition of artificial groundwater is given.	A

	REF	The composition of the artificial groundwater is not significantly altered under the experimental conditions, except for pH.	
II-e	SDB	A temperature of 22±2°C is given.	A/B
II-f	SDB REF	A L/S ratio of 10 to 20 g/L is indicated A solid mass of 0.5 to 1 g was added to a liquid volume of 45 mL. Based on a BET of 2.95 m ² /g for Al ₂ O ₃ from other literature, rating C/D is given.	C/D
II-g	SDB	The %-sorbed (calculated with K _d and L/S ratio) is 0%	C/D
II-h	SDB	Initial [Cs] is reported. Cs is not solubility limited.	A
II-i	SDB REF	Centrifugation is indicated. Centrifugation at 4000 g (or 27,000 g for some clay systems) for 1 hour is indicated.	C/D
II-j	SDB REF	A reaction time of 1 to 7 days is indicated. One week as standard contact time is reported.	C/D
II-k	REF	Samples were shaken vigorously but short before centrifugation.	C/D
II-l	SDB	No variation of initial [Cs] or another parameter is reported.	C/D
II-m	REF	The reaction vessel was a polypropylene or glass vessel. It is not clear, if effect of vessel was corrected for.	C/D
II-n	SDB	Uncertainties are not reported, no information about replicates.	D
II-o	REF	No parameter variation had been performed. Only one datapoint with a K _d of 0 mL/g was measured.	D

Data table Cs/20: REF: Andersson et al. (1983b)*			
JAEA-SDB version 4 – DATA: Cs/Other minerals; Fe-oxide/-hydroxide, #44024, 44029-44031, 44034, 44035			
GUIDELINE: Revision 4b (May 19, 2005)			
* REMARK: Update required for checkpoint II-a			
Checkpoint	Evaluation	Rating	
I-a.1 SDB	All mandatory fields are completed.	Yes	
I-a.2 SDB	All mandatory information is provided	Yes	
I-b SDB	Table with K _d values is given	class 1	
II-a SDB REF	Hematite and magnetite are reported as mineral phases. Mineralogy or surface characteristics for these phases are not reported. CEC values for hematite and magnetite are given in a diagram. BET values can be found in the literature.	B (update SDB)	
II-b SDB REF	Final pH range is reported (about 2 pH units). The spiked solutions were roughly adjusted to the desired level of pH with HCl or NaOH at the experimental setup.	B	
II-c SDB	The experiments were performed under aerobic conditions. Cs is not a redox sensitive element.	A	
II-d SDB REF	The initial composition of artificial groundwater is given. The composition of the artificial groundwater is not significantly altered under the experimental conditions, except for pH.	A	
II-e SDB	A temperature of 22±2°C is given.	A/B	
II-f SDB REF	A L/S ratio of 10 to 20 g/L is indicated A solid mass of 0.5 to 1 g was added to a liquid volume of 45 mL. Based on a BET of 75 m ² /g for pure magnetite and a BET of ~10 m ² /g for pure hematite found in other literature, rating A/B is given.	A/B	

II-g	SDB	Based on the information given in the SDB, the %-sorbed values are between 11% and 40%.	A
II-h	SDB	Initial [Cs] is reported. Cs is not solubility limited.	A
II-i	SDB REF	Centrifugation is indicated. Centrifugation at 4000 g (or 27,000 g for some clay systems) for 1 hour is indicated.	C/D
II-j	SDB REF	A reaction time of 1 to 7 days is indicated. One week as standard contact time is reported.	C/D
II-k	REF	Samples were shaken vigorously but short before centrifugation.	C/D
II-l	SDB	No variation of initial [Cs] or an other parameter is reported.	C/D
II-m	REF	Experiments were performed in polypropylene or glass vessels. The sorption of the walls of the vials was measured and found to be negligible in the presence of crushed material with a large accessible surface.	A
II-n	SDB	Uncertainties are not reported, no information about replicates.	D
II-o	SDB	<ul style="list-style-type: none"> Distribution coefficients at different pH values are given for magnetite and hematite, datapoints # 44029 to 44031 and # 44034/44035 No pH variation for the sorption experiment with corrosion product Fe(OH)₃,. datapoint # 44024 	C D

Data table Cs/21: REF: Fujikawa and Fukui (1997a)*

JAEA-SDB version 4 – DATA: Cs/Other minerals; Fe-oxide/-hydroxide, #51799-51822

GUIDELINE: Revision 4b (May 19, 2005)

* REMARK: Data in SDB do not correspond to the given reference (Part I), they are from Part II, Radiochimica Acta 76, 163 (1997).

Checkpoint	Evaluation	Rating
I-a.1	SDB All mandatory fields are completed.	Yes
I-a.2	SDB All mandatory information is provided	Yes
I-b	SDB A table with K _d values is provided.	class 1
II-a	SDB Magnetite and hematite are reported as mineral phases. REF Mineralogy and characteristics of these compounds are determined. The solid phases were purchased from Nihon-Hikagaku Co.	A
II-b	SDB Final pH values are reported	A
II-c	SDB Redox conditions are not reported. However, Cs is not redox sensitive. REF It is indicated that experimental systems were oxic, with positive Eh values in all solutions.	A/B
II-d	SDB The initial concentration of simple input electrolyte solutions (NaCl, Na ₂ CO ₃ , NaHCO ₃ , Na ₂ SO ₄) is given. REF The final solution compositions are not reported, but can be estimated based on mineral (hematite, magnetite) and initial solution composition.	A/B
II-e	SDB A temperature of 15°C is indicated.	A/B
II-f	SDB L/S ratio of 40 mL/g is indicated REF Solid masses of 1.0 g were added to liquid volumes of ca 40 mL. Based on typical specific surface of FeOOH (the mass of 1 g α-FeOOH has a surface area between 18 to 40 m ²) rating A/B is given.	A/B

II-g	SDB	Rating is done based on %-sorbed values calculated from the information given in the SDB. The sorption values range from 76% to 98.2%: • # 51799 to 51801, # 51803 to 51810, # 51812 to 51822 (76.5% to 93.1%) • # 51802 (98.2%) • # 51811 (96.1)	A C/D B
II-h	SDB REF	Initial [Cs] is erroneously reported to be 5×10^{-3} M. According to the reference the initial [Cs] is 5×10^{-9} M. Cs is not solubility limited.	A (update SDB)
II-i	SDB REF	It is indicated that no specific separation is reported. It is mentioned that experiments had been performed in centrifuge tubes, therefore it is assumed that centrifugation was done prior to the measurement of the supernatant solutions.	C/D (tentative)
II-j	SDB	A reaction time of 210 days is indicated.	C/D
II-k	REF	It is indicated that the samples were kept at a dark place. There is no information about agitation of the samples.	C/D
II-l	SDB	Neither [Cs] nor L/S variation is indicated.	C/D
II-m	REF	Experiments were performed in polypropylene centrifuge tubes. Corrections for sorption on vessel walls had been performed by blank tests.	C/D
II-n	SDB	No error estimates are indicated for the K_d values.	D
II-o	SDB	No isotherm is recorded; pH is varied, but not systematically. Sorption was measured in four different electrolytes for three electrolyte concentrations.	C

Data table Cs/22: REF: Ohnuki (1994b)*			
JAEA-SDB version 4 – DATA: Cs/Other minerals; Fe-oxide/-hydroxide, #57010			
GUIDELINE: Revision 4b (May 19, 2005)			
* REMARK: Update SDB for checkpoint II-c			
Checkpoint		Evaluation	Rating
I-a.1	SDB	All mandatory fields are completed.	Yes
I-a.2	SDB	All mandatory information is provided.	Yes
I-b	SDB	Table with K_d values is given	class 1
II-a	SDB	FeOOH is reported as solid phase. The CEC or surface area is not reported.	B
	REF	The pure metal oxide/hydroxide was used for the experiment and mineralogy and surface characteristics can be found in the literature.	
II-b	SDB	The experiment was performed at a pH of 5.4 to 5.6 in Na-acetate buffer.	C
II-c	SDB REF	There is no information about the redox conditions. Based on the information in the paper, experiments were done under air; i.e., under oxidizing conditions. Moreover, Cs is not a redox-sensitive element.	A/B (update SDB)
II-d	SDB REF	Initial solution composition (0.01 M in sodium acetate) is indicated. The final solution composition is not reported, but can be estimated based on mineral (FeOOH) and initial solution composition.	C/D

II-e	SDB	A temperature of 20°C is reported	C/D
II-f	SDB REF	L/S ration of 100 mL/g is indicated. Based on typical specific surface of FeOOH (the mass of 1 g α -FeOOH has a surface area between 18 to 40 m ²) rating A/B is given.	A/B
II-g	SDB	The %-sorbed (calculated with K_d and L/S ratio) is 0% ($K_d = 0$ mL/g)	C/D
II-h	SDB	Initial [Cs] is reported. Cs is not solubility limited.	A
II-i	SDB REF	Centrifugation at 10,000 rpm for one hour has been used for phase separation. No further information is available.	B
II-j	SDB	No sorption was observed after a contact time of 10 days.	C/D
II-k	REF	There is no information, whether samples were agitated or not.	C/D
II-l	REF	Neither [Cs] not the L/S have been varied.	C/D
II-m	REF	Experiments were performed in polycarbonate-vessels. Cs sorption on vessel walls was less than 0.01% at 2.4×10^{-9} M Cs-conc. over 10 days.	A
II-n	SDB	Three replicates were performed.	A
II-o	REF	Cs does not adsorb to FeOOH ($K_d=0$ L/kg).	D

Data table Cs/23: REF: Ticknor et al. (1991)

JAEA-SDB version 4 – DATA: Cs/Fe-oxide/-hydroxide, #60786, 60788, 60789

GUIDELINE: Revision 4b (May 19, 2005)

Checkpoint	Evaluation	Rating
I-a.1 SDB	All mandatory fields are completed.	Yes
I-a.2 SDB REF	It is indicated that there is no information about [Cs], pH, etc. There is no information about the initial [Cs], pH, solid/solution ratio, contact time, number of replicates and error of K_d .	No unreliable

Data table Cs/24: REF: Torstenfelt et al. (1981)*

JAEA-SDB version 4 – DATA: Cs/Other minerals; hematite, magnetite,
#61163-61187, #61188-61196

GUIDELINE: Revision 4b (May 19, 2005)

* REMARK: Information about experimental procedures was taken from Torstenfelt et al. (1982), Chemical Geology 36, 123-137, due to missing original reference. Entries of JAEA-SDB were not compared for agreement with data of the original literature. It is assumed that experimental conditions in Torstenfelt et al. (1982) are the same as in the original reference. Update of SDB required for checkpoint II-a.

Checkpoint	Evaluation	Rating
I-a.1 SDB	All mandatory fields are completed.	Yes
I-a.2 SDB	All mandatory information is provided.	Yes
I-b SDB	Table with K_d values is given.	class 1
II-a SDB REF	Hematite and magnetite are reported as mineral phases. Mineralogy or surface characteristics for these phases are not reported. CEC values for hematite and magnetite are given in a diagram. BET values can be found in the literature.	B (update SDB)
II-b SDB	Final pH range is reported:	B

		<ul style="list-style-type: none"> • # 61167-61169/61171-61174/61188/61189/61192-61196 about 1 pH unit • all other datapoints about 2 pH units 	C
II-c	SDB	It is indicated that redox conditions are not reported. It is assumed that experiments were done at standard atmospheric conditions. Cs is not a redox sensitive element.	A
II-d	SDB	Artificial groundwater is indicated as water type. A detailed final solution composition is provided.	A
II-e	SDB	Reaction temperature is not specified. It is assumed that experiments had been performed at ambient temperature.	C/D
II-f	SDB REF	<p>A L/S ratio of 90 mL/g is indicated. For the experiments 0.5 g of the solid phase were used per reaction vial.</p> <p>Based on a BET of 75 m²/g for pure magnetite and a BET of ~10 m²/g for pure hematite found in other literature, rating A/B is given.</p>	A/B
II-g	SDB	<p>The sorption values are calculated from K_d and L/S ratios:</p> <ul style="list-style-type: none"> • # 61166-61170/61188-61192/61196 (5~8% sorption) • # 61163-61165/61172-61187/61193-61195 (2~4% sorption) • # 61171 (1% sorption) 	A B C/D
II-h	SDB	Initial [Cs] is reported. Cs is not solubility limited.	A
II-i	SDB REF	<p>Centrifugation is indicated.</p> <p>Centrifugation at 5,000 rpm for 1 hour is indicated.</p>	C/D (update SDB)
II-j	SDB	A reaction time of 1, 7, 30 and 90 days is indicated. Time has no/little effect on K _d values.	A/B
II-k	REF	Samples were gently shaken during the sorption experiments.	A/B
II-l	SDB	No variation of initial [Cs] or an other parameter is reported.	C/D
II-m	REF	Blank tests were performed to determine the sorption on the glass. However, no correction for this effect was done since this sorption was negligible in comparison to the sorption on the solid phase.	B
II-n	SDB	Uncertainties are not reported, information about replicates is not given.	D
II-o	SDB	Contact time and pH had been varied.	B

3.1.3 Neptunium

Data table Np/1: REF:Allarad et al.(1979b) JAEA-SDB version 4 – DATA:Np/Granitic rocks, #42381-42386 GUIDELINE: Revision 4b (May 19, 2005)		
Checkpoint	Evaluation	Rating
I-a.1 SDB	All mandatory information is completed.	Yes
I-a.2 SDB	All mandatory information is completed. The experiments are conducted under aerobic conditions. Therefore, the oxidation number of Np is V.	Yes
I-b SDB	A table with log K_d values is provided.	class 1
II-a SDB REF	Major minerals in the solid phase are reported. But mineralogical composition is not indicated in detail. And particle size (0.063~0.105mm) is reported. No further information is available.	C/D
II-b SDB	Initial pH value is given. The synthetic groundwaters used contained carbonate. It can be assumed that the bentonite contained some CaCO_3 as well. The initial pH of 8.2 corresponds to the equilibrium pH of atmospheric CO_2 in contact with CaCO_3 -saturated water. Since the experiments were carried out in normal atmosphere conditions (see II-c), it can be expected that the initial pH was relatively well buffered.	B
II-c SDB REF	All experiments were carried out under atmospheric (i.e. oxidizing) conditions. The oxidation number of Np under these conditions is V. The experimental systems were aerated.	A/B
II-d SDB	The composition of the synthetic input solutions are given, the experiments were reportedly carried out under aerated conditions.	C/D
II-e SDB	A temperature of 25 or of 65°C is specified for different datapoints.	A/B
II-f SDB REF	A L/S ratio of 10~50 mL/g is indicated. 1~3 g solid were added to 30~50 mL solution. Particle size of granite is indicated as 0.063~0.105mm.	A/B
II-g REF	Based on the information given in the SDB, and on a L/S ratio that may range from 10~50 mL/g (av. 30 mL/g), sorption values between 46~73% sorbed can be calculated.	A
II-h SDB REF	The initial Np concentration of $<10^{-8}$ M is indicated. The exact initial Np concentration is not reported. Following the solubility measurements given in Yamaguchi et al. (1991), the initial RN concentration can be considered to be by more than a factor of 5 below the solubility limit in the considered pH range.	B
II-i SDB	Centrifugation(7000 rpm/50min) and filtration(0.2 μm) are indicated as phase separation method. It is not clear whether filtration was done on centrifuged or on original samples, but it is reported that it did not influence the values. Two methods were used, but none of them is considered to be very efficient for removal of colloids.	C/D
II-j SDB	It is indicated that contact time was 7~180 days for different datapoints. Considering that there are also differences in temperature, as well as slight differences in solution composition, the K_d values	A/B

		measured for different reaction times do not differ significantly.	
II-k	REF	Samples were shaken for 8~12 hours.	A/B
II-l	SDB	All experiments were conducted at the same L/S and initial RN concentration.	C/D
II-m	REF	The experiments were carried out in glass vessels. No correction for sorption on vessel walls reported.	C/D
II-n	SDB	No information is reported.	D
II-o	SDB	Within the set of reliable experiments, only the temperature was varied in a limited way.	C

Data table Np/2: REF: Barney and Anderson (1979) JAEA-SDB version 4 – DATA:Np/Granitic rocks, #44268-44273 GUIDELINE: Revision 4b (May 19, 2005)			
Checkpoint		Evaluation	Rating
I-a.1	SDB	All mandatory information is completed.	Yes
I-a.2	SDB	All mandatory information is completed.	Yes
I-b	SDB	A table with K_d values is provided.	class 1
II-a	SDB REF	Mineralogy is not indicated. Specific surface area is provided. No further information is available.	C/D
II-b	SDB	Initial pH value is 8.2. It is reported that final pH is constant for 91 days.	B
II-c	SDB REF	There is no information about redox condition. The experimental system is estimated to be aerated condition, then the oxidation number of Np is V.	A/B
II-d	SDB	The concentration of major ions (Na, K, Ca, Mg, Al and Si) in the final solutions is given in figure.	C/D
II-e	SDB	A temperature was carried out at room temperature ($23\pm 2^\circ\text{C}$).	A/B
II-f	SDB REF	A L/S ratio of 6 mL/g is indicated. 5g solid were added to 30 mL solution. Particle size of granite was not indicated.	C/D
II-g	REF	Based on the information given in the SDB, sorption values between 84~98% sorbed can be calculated. • datapoint 44268, 44269, 44271, 44272, 44273 • datapoint 44270	A B
II-h	SDB REF	The initial Np concentration is indicated as $9.2 \times 10^{-7} \sim 7.0 \times 10^{-4}$ M. Based on thermodynamic calculation with PHREEQC (database : JNC-TDB_011213c2.tdb), solubility of Np(V) is 7.4×10^{-5} mol/L. • datapoint 44268 = 9.0×10^{-5} M • datapoint 44269 = 7.0×10^{-4} M • datapoint 44270 = 9.2×10^{-7} M • datapoint 44271 = 7.8×10^{-6} M • datapoint 44272, 44273 = $4.71 \sim 5.46 \times 10^{-5}$ M	unreliable unreliable A A B
II-i	SDB	Filtration (0.3 μm) is indicated.	C/D
II-j	SDB	It is indicated that contact time was 14 and 35 days. In this experiment, kinetics sorption reaction was studied. Np concentration was indicated as a function of reaction time in figure.	A/B
II-k	REF	Samples were shaken. Kinetic information was indicated.	A/B

II-l	SDB	Only initial Np concentration is varied.	C/D
II-m	REF	The experiments were carried out in polycarbonate centrifuge tube. No correction for sorption on vessel walls is reported.	B
II-n	SDB	No information is reported.	D
II-o	SDB	The initial Np concentration is indicated as $9.2 \times 10^{-7} \sim 8.0 \times 10^{-5}$ M.	C

Data table Np/3: REF:Barney and Brown (1979)			
JAEA-SDB version 4 – DATA:Np/Granitic rocks, #44337-44339			
GUIDELINE: Revision 4b (May 19, 2005)			
Checkpoint	Evaluation		Rating
I-a.1	SDB	All mandatory fields are completed.	Yes
I-a.2	SDB	All mandatory information is completed.	Yes
I-b	SDB	A table with K_d values is provided.	class 1
II-a	SDB	CEC and surface area are indicated. Chemical composition is provided as well.	A
II-b	SDB REF	Final pH value is given. The synthetic groundwater used in the experiment was conditioned with 620 mg/L of $\text{CaSO}_4 \cdot 2\text{H}_2\text{O}$ and 302 mg/L of NaHCO_3 . The pH was reported to be constant for each groundwater over the 154 days.	A
II-c	SDB	All experiments were carried out with Np(V) under aerobic conditions.	A/B
II-d	SDB	The concentrations of major ions (Na, Ca, K, Mg, Si) in the final synthetic solutions are given as figure.	A/B
II-e	SDB	A temperature was carried out at room temperature ($23 \pm 2^\circ\text{C}$).	A/B
II-f	SDB REF	A L/S ratio of 6mL/g is indicated. 5 g solid were added to 30 mL solution. Particle size of granite was given “< 1.0 mm”.	A/B
II-g	REF	Based on the information given in the SDB, sorption values between 36~88% sorbed can be calculated.	A
II-h	SDB REF	The initial Np concentration is indicated as 6.8×10^{-5} M. Based on thermodynamic calculation with PHREEQC (database : JNC-TDB_011213c2.tdb), solubility of Np(V) is 7.3×10^{-5} mol/L. The initial concentration is lower than the solubility limit. However, initial Np concentration is less than a factor of 5.	B
II-i	SDB	Phase separation was carried out by centrifugation. But no information of rpm and time is given.	C/D
II-j	SDB	It is indicated that contact time was 14 days. In this experiment, kinetics sorption reaction was studied. Np concentration was indicated as a function of reaction time in figure.	A/B
II-k	REF	Samples were shaken. Kinetic information was indicated.	A/B
II-l	SDB	No variation in L/S or initial Np concentration is indicated.	C/D
II-m	REF	The experiments were carried out in polycarbonate centrifuge tube. No correction for sorption on vessel walls is reported.	B
II-n	SDB	No information is reported.	D
II-o	SDB	Changed parameters were reaction time and solid type (fresh solid and weathered solid)	D

Data table Np/4: REF: Baston et al. (1997)* and Berry et al. (2007)* JAEA-SDB version 4 – DATA: Np/Granitic rocks; granodiorite, #46824-46827, #46938, #46939 GUIDELINE: Revision 4b (May 19, 2005) *REMARK: Update of SDB required for checkpoints II-a, II-c, II-d and II-i.		
Checkpoint	Evaluation	Rating
I-a.1 SDB	All mandatory fields are completed.	Yes
I-a.2 SDB	All mandatory information is provided.	Yes
I-b SDB	A table with K_d values is given.	class 1
II-a SDB	As solid phase, granodiorite is indicated. Major mineral composition is reported.	B
II-b SDB REF	Final pH values are reported. No use of any pH buffer is reported.	A
II-c SDB REF	The oxidation state of Np is not reported. It is indicated that experiments had been performed under nitrogen atmosphere with dithionite as reducing agent. Final Eh values are indicated. It is reported that Np(V) was reduced to Np(IV) with sodium dithionite prior to the adsorption experiments. O_2 levels were reportedly < 1 ppm. All solutions had been de-oxygenated before experimentation. Levels of dithionite were monitored during the experiments, and were corrected where needed.	C/D (update SDB)
II-d SDB REF	As water type, distilled water equilibrated with granodiorite is indicated. Only for datapoints # 46938 and 46939 the final solution composition of equilibration at 60°C and at room temperature is provided. The final solution compositions for datapoints # 46824-46827 are identical to the compositions of datapoints # 46938 and 46939.	A/B (update SDB)
II-e SDB	It is indicated that experiments had been done at 25°C and 60°C.	A/B
II-f SDB	It is indicated that an L/S ratio of 5 with 300 mL solution and 6 g of solid phase had been used for the experiments.	A/B
II-g SDB	Sorption values are calculated from K_d and L/S ratios: Sorption values are either >98% or <2%, and rating C/D is applied.	C/D
II-h SDB REF	Initial [Np] concentration of 6.0×10^{-9} M is indicated. Based on speciation calculations with Phreeqi 2.14.3 using the thermodynamic data in the NAGRA-PSI thermodynamic database (Hummel et al., 2002). The initial Np concentration may have been at, or slightly above, the solubility limit. The solutions were pre-filtered (0.45 μ m) before being equilibrated with the solid. Presumably, Np-precipitate would have been removed in this way.	C/D

II-i	SDB	Filtration through 10000 MWCO or 0.45 µm membranes, or centrifugation at 1100 g for 3 h is indicated.	
	REF	Three liquid/solid separation techniques were employed: 1. Centrifugation at 1100 g for 15 minutes with aliquots being removed from near the surface of the supernatant liquid 2. Centrifugation followed by filtration through a 0.45 µm filter 3. Centrifugation followed by filtration first through a 0.45 µm filter, and then through a 10000 MWCO filter Rising K_d values with the more efficient separation technique are indicating colloid formation. Due to consistency with other data only datapoints where filtration over 10000 MWCO filter is indicated are considered as reliable (expert decision): • # 46824/46826 • # 46825/46827/46938/46939	(revise SDB) B unreliable
II-j	SDB	A contact time of 120 days is indicated.	C/D
II-k	REF	Gentle agitation on a shaker is reported.	A/B
II-l	SDB	No variation in L/S or [Np] had been performed.	C/D
II-m	REF	The experiments had been carried out in polypropylene centrifuge tubes. Sorption on vessel walls was not tested in case of Np. However, tests with Cm suggest that sorption on vessel walls can be neglected.	B
II-n	SDB	Error estimates are given, but it is indicated that no replicate measurements are available.	(revise SDB)
	REF	Error estimates are given which are based on counting statistics only. Neptunium experiments were carried out in duplicate.	B
II-o	SDB	Temperature had been varied (and as a result of the temperature change also the pH varied).	C

Data table Np/5: REF: Bondietti and Francis(1979)

JAEA-SDB version 4 – DATA:Np/Granitic rocks, #49008, 49009

GUIDELINE: Revision 4b (May 19, 2005)

Checkpoint	Evaluation	Rating
I-a.1 SDB	All mandatory fields are completed.	Yes
I-a.2 SDB	Not all mandatory information is provided: it is indicated that no information on phase separation is given in the original REF.	No
REF	No further information is available.	unreliable

Data table Np/6: REF: Kaukonen et al.(1993)

JAEA-SDB version 4 – DATA:Np/Granitic rocks, #53874, #53875

GUIDELINE: Revision 4b (May 19, 2005)

Checkpoint	Evaluation	Rating
I-a.1 SDB	All mandatory fields are completed.	Yes
I-a.2 SDB	Initial Np concentration information is not completed.	No

Data table Np/7: REF: Koskinen et al.(1985)

JAEA-SDB version 4 – DATA:Np/Granitic rocks, #54025-54032

GUIDELINE: Revision 4b (May 19, 2005)

Checkpoint	Evaluation	Rating
I-a.1 SDB	All mandatory fields are completed.	Yes

I-a.2	SDB	All mandatory information are completed.	Yes
I-b	SDB	The K_d is given in tabular form.	class 1
II-a	SDB REF	CEC and specific surface area are not reported. Information about mineral composition is given.	C/D
II-b	SDB	Initial as well as final pH are given.	A
II-c	SDB REF	Information about Eh values is not given. Experiments were done under air; i.e., under oxidizing conditions. All data was considered as Np(V).	A/B
II-d	REF	The initial solution composition is reported.	A/B
II-e	SDB	Temperatures of $20 \pm 2^\circ\text{C}$ are reported.	A/B
II-f	SDB REF	Solution/solid ratios are 10 mL/g. Solid masses and liquid volumes are not reported.	C/D
II-g	REF	The %-sorbed can be calculated with K_d and L/S ratio: The %-sorbed of all datapoints are 41.2~51.9%	A
II-h	SDB REF	An initial [Np] of 6.07×10^{-7} M is indicated. Based on thermodynamic calculation with PHREEQC (database : JNC-TDB_011213c2.tdb), solubility of Np(V) is 8.7×10^{-4} mol/L. The initial concentration is clearly lower than the solubility limit.	A
II-i	SDB REF	The phase separation is carried out by centrifugation (8000 rpm, 60min) and 0.45 μm Millipore membrane filter. • Datapoints #54025, 54027, 54030, 54032 • Datapoints #54026, 54028, 54029, 54031	B A
II-j	SDB	A reaction time of 7 days is indicated.	C/D
II-k	REF	Samples were shaken for 7 days.	A/B
II-l	REF	No variation is indicated for either L/S or initial [Np] concentration.	C/D
II-m	REF	Information about reactant vessel is not reported.	C/D
II-n	SDB	Error of K_d is not reported.	D
II-o	SDB	No parameter variation is indicated.	C

Data table Np/8: REF: Nakayama et al. (1986)			
JAEA-SDB version 4 – DATA:Np/Granitic rocks, #56827-56832			
GUIDELINE: Revision 4b (May 19, 2005)			
Checkpoint	Evaluation		Rating
I-a.1	SDB	All mandatory fields are completed.	Yes
I-a.2	SDB	All mandatory information is completed.	Yes
I-b	SDB	A table with K_d values is provided.	class 1
II-a	SDB	The solid phase is indicated surface area and particle size. But chemical composition is not given.	C/D
II-b	SDB REF	Final pH value is given. The pH was adjusted at about 7 by using a solution of NaOH. Approximate pH values are reported (e.g. pH ~7).	B
II-c	SDB REF	It is indicated that experiments had been performed under aerobic conditions. Eh values are not reported. It is reported that Np(V) was used for the experiments.	A/B
II-d	SDB REF	As water type, pre-equilibrated water and distilled water are indicated. Final solution compositions are not given. The final solution composition of the equilibrated groundwater is not provided, but it is assumed that no essential changes take	C/D

		place by equilibration with granodiorite.	
II-e	SDB	Experiments were carried out at room temperature.	A/B
II-f	SDB REF	A L/S ratio of 30 mL/g is indicated. 1 g solid were added to 30 mL solution. Particle size of granite was given “32~60 and < 60 mesh”.	A/B
II-g	REF	Based on the information given in the SDB, sorption values between 4.2~11.0% sorbed can be calculated.	A
II-h	SDB REF	The initial Np concentration is indicated 1.0×10^{-4} M. Based on thermodynamic calculation with PHREEQC (database : JNC-TDB_011213c2.tdb), solubility of Np(V) is 6.1×10^{-5} mol/L. The initial concentration is higher than the solubility limit.	unreliable

Data table Np/9: REF: Nakayama et al.(1994)

JAEA-SDB version 4 – DATA:Np/Granitic rocks, #56863-56865

GUIDELINE: Revision 4b (May 19, 2005)

Checkpoint	Evaluation	Rating
I-a.1 SDB	All mandatory fields are completed.	Yes
I-a.1 SDB	Information about separation method is not reported.	No

Data table Np/10: REF: Suksi et al.(1989)

JAEA-SDB version 4 – DATA:Np/Granitic rocks, #59376, 59377

GUIDELINE: Revision 4b (May 19, 2005)

Checkpoint	Evaluation	Rating
I-a.1 SDB	All mandatory fields are completed.	Yes
I-a.2 SDB	All mandatory information is completed.	Yes
I-b SDB	%-sorb is given in tabular form.	class 3
II-a SDB REF	CEC and specific surface area are not reported. Information about mineral composition is given.	C/D
II-b SDB	Only initial pH is given.	D
II-c SDB REF	Information about Eh values is not given. Datapoint #59376 as Np(V) was carried out under oxidizing condition. Datapoint #59377 as Np(IV) was carried out under N ₂ atmosphere. But reducing agent was not used. • Datapoints #59376 = oxidizing condition • Datapoints #59377 = reducing condition	A/B C/D
II-d REF	The initial solution composition is reported.	A/B
II-e SDB	Information about temperature is not reported.	C/D
II-f SDB	Information about solid/solution ratio is not reported.	C/D
II-g REF	The %-sorbed can not be calculated. Because of no L/S ratio.	C/D
II-h SDB REF	An initial [Np] of 6.7×10^{-5} M(#56376) and 7.8×10^{-5} M(#56377) is indicated. Based on thermodynamic calculation with PHREEQC (database : JNC-TDB_011213c2.tdb), solubility of Np(V) and Np(IV) are 8.7×10^{-4} mol/L and 3.4×10^{-9} mol/L. The initial Np(V) concentration is clearly lower than the solubility limit, The initial Np(IV) concentration is clearly higher than the solubility limit. • Datapoints #59376 = oxidizing condition • Datapoints #59377 = reducing condition	A unreliable

II-i	SDB REF	The phase separation is carried out by centrifugation and 0.22 µm Millipore filter.	A
II-j	SDB	Experiment was carried out from 0 to 480 days.	A/B
II-k	REF	Information about agitation is not reported.	C/D
II-l	REF	No variation is indicated for either L/S or initial [Np] concentration.	C/D
II-m	REF	Information about reactant vessel is not reported.	C/D
II-n	SDB	Error of K_d is not reported.	D
II-o	SDB	Only reaction time is varied.	C

Data table Np/11: REF: Tachi et al.(2010) JAEA-SDB version 4 – DATA:Np/Granitic rocks, #59834-59863 GUIDELINE: Revision 4b (May 19, 2005)			
Checkpoint		Evaluation	Rating
I-a.1	SDB	All mandatory fields are completed.	Yes
I-a.2	SDB	All mandatory information is completed.	Yes
I-b	SDB	The K_d is given in tabular form.	class 1
II-a	SDB REF	Specific surface area is reported. Information about mineral composition and chemical composition is given.	C/D
II-b	SDB	Initial as well as final pH is given.	A
II-c	SDB	Information about Eh values is given. Experiment was carried out under Ar atmosphere.	A/B
II-d	REF	The concentrations of some ions in the equilibrated solutions are provided.	C/D
II-e	SDB	Experiment was carried out at room temperature.	A/B
II-f	SDB REF	Solution/solid ratio is 50 mL/g. Solid masses and liquid volume are not reported.	A/B
II-g	REF	The %-sorbed can be calculated with K_d and L/S ratio: • Datapoints # 59834-59842, 59849-59851 • Datapoints #59843-59848, 59852-59863	A B
II-h	SDB REF	An initial [Np] of 8.50×10^{-10} M is indicated. Based on thermodynamic calculation with PHREEQC (database : JNC-TDB_011213c2.tdb), solubility of Np(IV) are 3.2×10^{-9} mol/L. The initial Np(IV) concentration is clearly lower than the solubility limit. However, initial Np concentration is less than a factor of 5.	B
II-i	SDB	The phase separation is carried out by using 10,000 MWCO filter.	B
II-j	SDB REF	A reaction time of 1, 7, 14, 21, 35 days is indicated. • Datapoints # 59834-59836, 59849-59851 • Datapoints #59837-59848, 59852-59863	C/D A/B
II-k	REF	Information about agitation is not reported.	C/D
II-l	REF	No variation is indicated for either L/S or initial [Np] concentration.	C/D
II-m	REF	Information about reactant vessel is not reported.	C/D
II-n	SDB	Error of K_d is not reported.	D
II-o	SDB	Only reaction time is varied.	C

Data table Np/12: REF:Torstenfelt et al. (1988) JAEA-SDB version 4 – DATA:Np/Granitic rocks, #61441-61457 GUIDELINE: Revision 4b (May 19, 2005)		
Checkpoint	Evaluation	Rating
I-a.1 SDB	All mandatory fields are completed.	Yes
I-a.2 SDB	All mandatory information is completed.	Yes
I-b SDB REF	The K_d values are scanned from graphs. The graphs are a linear representation of K_d .	class 3
II-a SDB REF	The granites studied were Finnsjö granite, Stripa granite and Westerly granite. Main minerals and CEC is not given. No additional information is available.	C/D
II-b SDB	The final pH values are indicated. The pH had been adjusted with HCl or NaOH.	A
II-c SDB REF	It is indicated that all experiments were done under air. O_2 levels of the reference groundwater are provided. It is reported that Np(V) was used for the experiments.	A/B
II-d SDB REF	The initial solution composition is given (in the separate file “solution composition”). No additional information is available.	C/D
II-e SDB	Room temperature is indicated.	A/B
II-f SDB REF	A L/S of 50 mL/g is indicated. 0.5 g solid and 25 mL solution were used.	C/D
II-g REF	Based on the information given in the SDB, all sorption values are calculated to lie in the range 28.6~81.5% sorbed.	A
II-h SDB REF	An initial Np concentration of 1×10^{-7} M is indicated. Based on the data by Yamaguchi et al. (1991) in the presence of air, rating A is given.	A
II-i SDB REF	Centrifugation at 20,000~60,000 rpm is indicated. Torstenfelt et al.(1988) note that the sorption of Np does not vary significantly as a function of centrifugation speed. • datapoint:61442-61446, 61448-61452, 61454-61456 • datapoint:61441, 61447, 61453, 61457 (no phase separation)	A unreliable
II-j SDB REF	Reaction times of 1, 7 and 30 days are indicated, but K_d values are not given for individual reaction times. It is not clear which reaction time corresponds to the reported K_d values. Therefore, rating C/D is given.	C/D
II-k REF	No information is given.	A/B
II-l SDB	No variation in L/S or initial Np concentration is indicated.	C/D
II-m REF	The experiments were done in centrifugation tubes; the respective material is not specified. No information regarding sorption on vessel walls or corrections is given. Assuming that corrections would have been reported, rating B is given.	B
II-n SDB REF	No information is given with regard to error. Experiments were done in duplicates, but no errors are given, It is further not clear, whether the reported values represent sample means.	D
II-o SDB	Only pH had been varied.	C

Data table Np/13: REF: Meijer et al.(1990)		
JAEA-SDB version 4 – DATA:Np/Other minerals (Oxide or Hydroxide), #62110, #62111		
GUIDELINE: Revision 4b (May 19, 2005)		
Checkpoint	Evaluation	Rating
I-a.1 SDB	All mandatory fields are completed.	Yes
I-a.2 SDB	Separation method information is not completed.	No

Data table Np/14: REF: Nakayama and Sakamoto(1991)		
JAEA-SDB version 4 – DATA:Np/ Other minerals (Oxide or Hydroxide), #56661-56680, #56703-56794		
GUIDELINE: Revision 4b (May 19, 2005)		
Checkpoint	Evaluation	Rating
I-a.1 SDB	All mandatory fields are completed.	Yes
I-a.2 SDB	All mandatory information is completed.	Yes
I-b SDB	Linear graph % sorbed is given.	class 4
II-a SDB	Specific surface area is reported. But CEC is not reported.	B
II-b SDB	Final pH is given. This study was carried out adjusting pH by HNO ₃ or NaOH.	A
II-c SDB REF	Information about Eh values is not given. Experiments were done under air; i.e., under oxidizing conditions. Np in this study is considered as Np(V).	A/B
II-d REF	The solution of this study is 0.1 M NaNO ₃ . It can be calculated solution composition, because mineral composition is reported.	C/D
II-e SDB	This study was carried out at 30°C	A/B
II-f SDB REF	Solution/solid ratio is 1,000 mL/g. Solid masses of 100mg are added to a liquid volume of 100 mL.	A/B
II-g REF	The %-sorbed can be calculated with K _d and L/S ratio: • Datapoints # 56678, 56680, 56720, 56749, 56750, 56785 • Except above datapoints	C/D A
II-h SDB REF	An initial [Np] of 6.0×10^{-6} M is indicated. It was confirmed by filtration that neptunium was present as soluble species.	A
II-i SDB	The phase separation is carried out by 0.45 µm membrane filter.	A
II-j SDB REF	A reaction time is reported at two to three hours for hematite, magnetite and alumina and two days for goethite. This study carried out sorption kinetics. So it was considered that this experimental condition reached to equilibrium.	A/B
II-k REF	Information about agitation method is not given.	C/D
II-l REF	No variation is indicated for either L/S or initial [Np] concentration.	C/D
II-m REF	Reactant vessel is reported as glass flask. From the blank test, it was found that the sorption onto the vessel walls was negligibly small.	A
II-n SDB	Error of K _d is not reported.	D
II-o SDB	It is changed pH (oxidizing or reducing condition).	C

Data table Np/15: REF: Ticknor(1993) JAEA-SDB version 4 – DATA:Np/ Other minerals (Oxide or Hydroxide), #60842-60847, #60854-60859 GUIDELINE: Revision 4b (May 19, 2005)		
Checkpoint	Evaluation	Rating
I-a.1 SDB	All mandatory fields are completed.	Yes
I-a.2 SDB	All mandatory information is completed.	Yes
I-b SDB	The K_d is given in tabular form.	class 1
II-a SDB	CEC and specific surface area are reported.	A
II-b SDB	Initial as well as final pH is given.	B
II-c SDB REF	Information about Eh values is not given. This study was carried out under normal O ₂ condition and low O ₂ condition. • Datapoints #60842, 60844, 60846, 60854-60856 = normal O ₂ condition • Datapoints #60843, 60845, 60847, 60857-60859 = low O ₂ condition	A/B C/D
II-d REF	The initial solution composition is reported.	A/B
II-e SDB	Information about temperature is not reported.	C/D
II-f SDB REF	Solution/solid ratios are 4 mL/g. Solid masses of 1.0 g are added to a liquid volume of 4 mL.	A/B
II-g REF	The %-sorbed can be calculated with K_d and L/S ratio: • Datapoints # 60842-60857 = 80.0~94.7% • Datapoints #60858, 60859 = 95.2~95.5%	A C/D
II-h SDB REF	An initial [Np] of 8.84×10^{-6} M for low TDS and mid TDS, 9.05×10^{-6} M for High TDS is indicated. (TDS = total dissolved solid) It was confirmed that aliquots were taken from the bulk solutions for radiometric analyses at times corresponding to the sorption period used in experiments.	A
II-i SDB	The phase separation is carried out by centrifugation (2800 g, 15~20min).	A
II-j SDB	Reaction times of 27 and 30 days are indicated.	A/B
II-k REF	Information about agitation method is not reported.	C/D
II-l REF	No variation is indicated for either L/S or initial [Np] concentration.	C/D
II-m REF	Polypropylene bottles are used in this study.	B
II-n SDB	Error of K_d is reported. Three replicates of each solution-radionuclide-mineral-redox/ph combination were used.	A
II-o SDB	Experimental conditions such as O ₂ condition and TDS had been varied.	C

Data table Np/16: REF: Allard et al.(1982) JAEA-SDB version 4 – DATA:Np/Bentonite (Clay minerals), #63692, #63693 GUIDELINE: Revision 4b (May 19, 2005)		
Checkpoint	Evaluation	Rating
I-a.1 SDB	All mandatory fields are completed.	Yes
I-a.2 SDB	All mandatory information is completed.	Yes
I-b SDB	The K_d is given with logarithmic values.	class 1
II-a REF	This study used Wyoming bentonite MX-80.	A

II-b	SDB	Initial as well as final pH are given.	A
II-c	SDB REF	Information about Eh values is not given. This study was carried out as Np(V)	A/B
II-d	REF	The initial solution composition is not reported. But it was reported total salt and total carbonates.	C/D
II-e	SDB	This study was carried out at 25±1°C.	A/B
II-f	SDB REF	Solution/solid ratios are 100 mL/g. Solid masses of 0.2 g are added to a liquid volume of 20 mL.	A/B
II-g	REF	The %-sorbed can be calculated with K_d and L/S ratio: • Datapoints #63692 = 32.9% • Datapoints #63693 = 53.5%	A
II-h	SDB REF	An initial [Np] concentration is reported 1.9×10^{-7} M for datapoint #63692 and 1.9×10^{-9} M for datapoint #63693. Based on thermodynamic calculation with PHREEQC (database : JNC-TDB_011213c2.tdb), solubility of Np(V) are 1.1×10^{-3} mol/L. The initial Np(V) concentration is clearly lower than the solubility limit.	A
II-i	SDB	The phase separation is carried out by centrifugation (27,000 g, 1.0 hour).	B
II-j	SDB REF	Reaction times of 6 hour, 1 day, 6 days, 1 week are indicated. Only data for 6 days given in this paper.	A/B
II-k	REF	Information about agitation method was not reported.	C/D
II-l	REF	No variation is indicated for L/S. But this study was carried out at two initial [Np] concentrations.	B
II-m	REF	Reactant vessel used is polypropylene vessel. It was reported that the surface area of the exposed fine grained solids are several orders of magnitude larger than the surface of the vessel.	A
II-n	SDB	Error of K_d is not reported.	D
II-o	SDB	Only initial [Np] concentration had been varied.	C

Data table Np/17: REF: Morgan et al.(1988)			
JAEA-SDB version 4 – DATA:Np/Bentonite (Clay minerals), #63962-64004			
GUIDELINE: Revision 4b (May 19, 2005)			
Checkpoint	Evaluation		Rating
I-a.1	SDB	All mandatory fields are completed.	Yes
I-a.2	SDB	All mandatory information is completed.	Yes
I-b	SDB	The K_d is given with average value in tabular form.	class 1
II-a	REF	This study used Wyoming bentonite clay.	A
II-b	SDB	Only final pH is given.	B
II-c	SDB REF	Information about Eh values is not given. This study was carried out as Np(V) under air-saturated condition.	A/B
II-d	REF	The initial solution composition is not reported. But liquid of this study used demineralised water. Solid used is Wyoming bentonite clay. So solution composition can be calculated.	C/D
II-e	SDB	Information about temperature is not reported.	C/D
II-f	SDB REF	A L/S ratios are 200, 100 and 50 mL/g. Solid masses of 0.25, 0.5 and 1.0 g are added to a liquid volume of 50 mL.	A/B
II-g	REF	The %-sorbed can be calculated with K_d and L/S ratio:	

		<ul style="list-style-type: none"> • Datapoints #63980, 63993, 63998 = 97.0~98.2% • Datapoints else = 22.5~90.9% 	B A
II-h	SDB	An initial [Np] concentration is reported 1.0×10^{-6} , 1.0×10^{-7} , 1.0×10^{-8} , 1.0×10^{-9} , 1.0×10^{-10} M.	A
	REF	This study was carried out based on the solubility and sorption measurements reported previously.	
II-i	SDB	The phase separation is carried out by centrifugation (2000 g, 1.0 min).	B
II-j	SDB	Reaction times of 1, 2, 10 days are indicated.	A/B
II-k	REF	Agitation method was reported as “shaking”.	A/B
II-l	REF	Sorption isotherms have been measured at each solution/solid ratio.	A
II-m	REF	Reactant vessel used is polypropylene centrifuge tube.	A
II-n	SDB	Error of K_d is not reported.	D
II-o	SDB	Initial [Np] concentration, reaction time and solution/solid ratio are varied.	C

3.1.4 Selenium

Data table Se/1: REF: Fujikawa and Fukui (1997b)* JAEA-SDB version 4 – DATA: Se/Granitic rocks; granodiorite, #51967-51978 GUIDELINE: Revision 4b (May 19, 2005) * REMARK: Data in SDB do not correspond to the given reference (Part I), they are from Part II, Radiochimica Acta 76, 163-172 (1997).		
Checkpoint	Evaluation	Rating
I-a.1 SDB	All mandatory fields are completed	Yes
I-a.2 SDB REF	Information about mineralogy and surface characteristics (e.g. BET or CEC) and atmosphere/redox conditions are missing. The chemical composition of the granodiorite is available in a cited reference. However, surface characteristics are not described. It is reported that a mixture of Se(IV)/(VI) was measured in the supernatant solution. Therefore the given K_d values are considered to be unreliable.	No, unreliable

Data table Se/2: REF: Sato et al. (1997)* JAEA-SDB version 4 –DATA: Se/Granitic rocks; granodiorite, #58965-58973 GUIDELINE: Revision 4b (May 19, 2005) * REMARK: Update of SDB required for checkpoints I-a.2, II-a, and II-n.		
Checkpoint	Evaluation	Rating
I-a.1 SDB	All mandatory fields are completed.	Yes
I-a.2 SDB REF	Redox state of Se and redox conditions (Eh values are not reported). All experiments were carried out in an N ₂ -atmospheric glove box (O ₂ < 1ppm) and experimental solutions were degassed. A SeO ₂ powder was added to the solutions.	(update SDB) Yes (tentative)
I-b REF	A table with K_d values is provided.	class 1
II-a SDB REF	Three granodiorite samples are reported as solid phases (intact granodiorite, altered granodiorite and fracture fillings). CEC values (2.0, 1.9 and 17.3 meq/100 g) are provided. Kurihashi granodiorite of the Kamaishi In Situ Test Site had been used for the experiments. It is assumed that mineralogy and detailed composition of the granodiorite samples are known. BET values are reported in the reference.	A (tentative) (update SDB if applicable)
II-b SDB	Final pH values are reported (after a contact time of 66 days, which can be assumed to be enough to reach equilibrium).	A
II-c SDB	It is indicated that experiments had been performed under N ₂ -atmosphere and experimental solutions were degassed. Eh values are not reported. Due to the kinetic stability of added Se(IV) under ambient conditions, rating C/D is applied.	C/D
II-d SDB REF	The final solution composition of the equilibrated groundwater is provided. In situ groundwater sampled from the Kamaishi In Situ Test Site was used for the sorption experiments.	A/B
II-e SDB	Experiments had been conducted at room temperature.	A/B
II-f SDB	A liquid/solid ratio of 20 mL/g is reported: for the experiments 1.5 g of solid and 30 mL of solution were used. With BET values of 0.7 m ² /g (intact granodiorite) and 1.9 m ² /g (altered granodiorite or fracture fillings), rating C/D is applied.	C/D

II-g	SDB	The sorption value (calculated from K_d and L/S ratios) ranges between 0% and 7%: <ul style="list-style-type: none"> • # 58965, 58968, 58969 (7%, 6%, 7%) • # 58967, 58970, 58972, 58973 (4%, 3%, 3%, 4%) • # 58966, 58971 (1%, 0%) 	A B C/D
II-h	SDB	Initial [Se] is reported as 1.0×10^{-4} M. According to Phreeqc-calculations using the thermodynamic data in the NAGRA-PSI thermodynamic database (Hummel et al., 2002) supplemented with the thermodynamic equilibrium of CaSeO_3 (taken from NEA, 2005), the reported Se concentration is a factor of two below the solubility limit.	B
II-i	SDB	It is reported that reaction mixtures were filtered with a 10,000 MWCO (Molecular Weight Cut-Off) ultrafilter.	B
II-j	SDB	A contact time of 36 days is indicated. This reaction time is considered to be reasonably long.	C/D
II-k	REF	There is no information about the agitation method.	C/D
II-l	SDB	No variation in L/S or initial Cs concentration is indicated.	C/D
II-m	REF	The experiments were carried out in glass bottles. Corrections for sorption on the vessel wall had been performed by measurement of tracer concentration in the blank solution. This may have led to overcorrection.	C/D
II-n	SDB REF	No error estimates are reported. Only one replicate is indicated. Three replicates are indicated but no error estimates are reported.	C (update SDB)
II-o	SDB	No parameter variation was performed.	D

Data table Se/3: REF: Shibutani et al. (1994)*

JAEA-SDB version 4 – DATA: Se/Granitic rocks; granodiorite, #59136-59141

GUIDELINE: Revision 4b (May 19, 2005)

* REMARK: Since information about the oxidation state of Se is not given in the SDB or reference translation, it was assumed that Se is in the oxidation state +IV. The classification is based on this assumption.

All K_d values although measured at different pH are indicated to be zero. It is assumed that a calculation mistake occurred. K_d values in the SDB need to be revised. Update of SDB required for checkpoints I-a.2, II-d, II-f and II-h.

Checkpoint	Evaluation	Rating
I-a.1 SDB	All mandatory fields are completed.	Yes
I-a.2 SDB	Redox state of Se and redox conditions (Eh values are not reported).	(update SDB)
REF	All experiments were carried out in an N_2 -atmospheric glove box ($\text{O}_2 < 1$ ppm). Redox state of Se not mentioned in the translation.	Yes (tentative)
I-b SDB	It is indicated that K_d values are provided as % sorbed.	class 2
II-a SDB	Granodiorite is indicated as solid phase. Mineralogy is not indicated. Specific surface area is provided.	C/D
II-b SDB	Final pH values are reported (after a contact time of 14 days, which can be assumed to be enough to reach equilibrium).	A
II-c SDB	It is indicated that experiments had been performed in an atmosphere with <1 ppm of oxygen.	C/D
REF	It is reported that experiments had been performed under N_2 -atmosphere with <1 ppm of oxygen present. Eh values are not reported. Due to the kinetic stability of added Se(IV) under	

		ambient conditions, rating C/D is applied.	
II-d	SDB	As water type 0.01 M NaCl solution is indicated. The final solution composition of the equilibrated groundwater is not provided, but it is assumed that no essential changes take place by equilibration with granodiorite.	A/B
	REF	As water type 0.1 M NaCl solution is reported.	(revise SDB)
II-e	SDB	Experiments had been conducted at room temperature.	A/B
II-f	SD	A liquid/solid ratio of 20 mL/g is reported	A/B
	REF	The L/S ratio is indicated to be 25 mL/g. With the indicated specific surface area of 9 m ² /g rating A/B is applied.	(revise SDB)
II-g	SDB	The sorption values are calculated from K _d and L/S ratios. The sorption value is 0% for all datapoints.	C/D
II-h	SDB	Initial [Se] is indicated as 1.0×10^{-4} M. According to Phreeqci-calculations using the thermodynamic data in the NAGRA-PSI thermodynamic database (Hummel et al., 2002), the reported Se concentration is clearly below the solubility limit (also in case of [Se]= 1.0×10^{-3} M).	A
	REF	Initial [Se] is reported to be 1.0×10^{-3} M.	(revise SDB)
II-i	SDB	It is reported that reaction mixtures were filtered with a 10,000 MWCO (Molecular Weight Cut-Off) ultrafilter.	B
II-j	SDB	A contact time of 14 days is indicated. This reaction time is considered to be reasonably long.	C/D
II-k	REF	There is no information about the agitation method.	C/D
II-l	SDB	No variation in L/S or initial Se concentration is indicated.	C/D
II-m	REF	There is no information about the vessel type used for experimentation. It is indicated that blank measurements had been made, but it is not reported if corrections for sorption on the vessel walls had been performed.	C/D
II-n	SDB	No error estimates are reported. Only one replicate is indicated.	D
II-o	SDB	pH had been varied systematically.	C

Data table Se/4: REF: Ticknor and McMurry(1996)*		
JAEA-SDB version 4 –DATA: Se/granitic rocks, granite, #60586-60605		
GUIDELINE: Revision 4b (May 19, 2005)		
* REMARK: Update required for checkpoints II-a, II-c, II-i		
Checkpoint	Evaluation	Rating
I-a.1 SDB	All mandatory fields are completed.	Yes
I-a.2 SDB	It is indicated that Eh, atmosphere/redox conditions and temperature are not reported.	Yes
	REF It is reported, that solutions at lower pH were prepared and used in air. The solutions at higher pH were prepared and used under a N ₂ atmosphere to avoid dissolution of CO ₂ of the atmosphere.	(update SDB)
I-b SDB	A table with log K _d values is provided.	class 1
II-a SDB	As solid phase granite is reported. Elemental composition and specific surface area is given.	B (update SDB)
	REF Granite is from Lac de Bonnet batholith; albite, K-feldspar, biotite, quartz identified by XRD. It was crushed/sieved to 106~180 μm	
II-b SDB	Final pH values are reported.	A
II-c SDB	It is indicated that redox conditions such as Eh values are not reported.	A/B (update

	REF	It is reported that oxygen was present in the atmosphere surrounding the experimental solutions. An Eh value of 400 mV is indicated for the experiments conducted under ambient conditions and an Eh value of 150 mV for experiments performed under N ₂ atmosphere. Due to the redox stability of selenite under ambient conditions, rating A/B is given.	SDB)								
II-d	SDB	As water type, 1%, 10% and 100% synthetic groundwater WN-1M is indicated. The solutions contain different concentrations of fulvic acid and were pre-equilibrated before the sorption experiments.	A/B								
II-e	SDB	It is not specified at which temperature experiments had been performed. It is assumed that experiments had been made at ambient temperature.	C/D								
II-f	SDB	20 mL of solution and 0.5 g of solid are indicated, giving 40 mL/g. This corresponds to a solid surface of 1.2 m ² .	C/D								
II-g	SDB	For datapoints #60586-60592, zero sorption is indicated (formally C/D, not rated). For the other datapoints, the sorption values (calculated from K _d and L/S ratios)give the following rating. <table><tr><td>datapoint #</td><td>rating</td></tr><tr><td>60595, 60598, 60599, 60600, 60601, 60603, 60604, 60605</td><td>A</td></tr><tr><td>60593, 60594, 60596</td><td>B</td></tr><tr><td>60597, 60602</td><td>C/D</td></tr></table>	datapoint #	rating	60595, 60598, 60599, 60600, 60601, 60603, 60604, 60605	A	60593, 60594, 60596	B	60597, 60602	C/D	see table
datapoint #	rating										
60595, 60598, 60599, 60600, 60601, 60603, 60604, 60605	A										
60593, 60594, 60596	B										
60597, 60602	C/D										
II-h	SDB	Initial Se concentrations between 1.0×10 ⁻⁸ M and 1.0×10 ⁻⁴ M are given. Based on speciation calculations (for 25°C) using the thermodynamic data in NAGRA-PSI thermodynamic database (Hummel et al., 2002) supplemented with the solubility product of CaSeO ₃ (taken from NEA, 2005), the initial Se concentrations are below the solubility limit. Fulvic acid has not been taken into account in these calculations. <ul style="list-style-type: none">• # 60586, 60587, 60589, 60590, 60591, 60592, 60597, 60602• all others	B A								
II-i	SDB REF	Centrifugation of the samples is indicated as phase separation. Solid and liquid phases had been separated by centrifugation at 30,000 g prior to analysis.	C/D (update SDB)								
II-j	SDB	A reaction time of 28 days is indicated.	A/B								
II-k	REF	No information about the agitation of the samples is provided.	C/D								
II-l	SDB	K _d values were obtained for three different initial Se concentrations.	B								
II-m	REF	The experiments were carried out in polycarbonate centrifuge tubes. Radioisotope concentration in the blank was measured and defined as initial radionuclide concentration. This could have led to a possible overcorrection and rating C/D is applied.	C/D								
II-n	SDB	No error information is available.	D								
II-o	SDB	Experiments had been performed at two [RN] and with 1%, 10% and 100% WN-1M synthetic solutions.	B								

Data table Se/5: REF: Ticknor et al. (1988)* JAEA-SDB version 4 – DATA: Se/Granitic rocks: GRANITE, #60688-60696 GUIDELINE: Revision 4b (June 2, 2006) * REMARK: Update of SDB required for checkpoints I-a.2 and II-i.		
Checkpoint	Evaluation	Rating
I-a.1 SDB	All mandatory fields are completed.	Yes
I-a.2 SDB REF	Separation of the samples is not reported. It is reported, that aliquots of the aqueous phases were taken for the radiometric analysis. Phase separation was performed by high-speed centrifugation (personal communication with T. T. Vandergraaf).	Yes (update SDB)
I-b REF	A table with log K_d values is provided.	class 1
II-a SDB	As solid phases granite, purchased from the Cold Spring Quarry on the Lac du Bonnet pluton in Manitoba are reported. A detailed chemical composition of the minerals and their specific surface areas and CEC are available.	A
II-b SDB REF	Initial as well as final pH are indicated. The solution pH was determined with litmus paper (assumed range < 1 pH). No pH correction by addition of buffer was performed after hydrazine addition.	A
II-c SDB	Redox conditions are reported for each experiment. Experiments are performed under aerobic conditions, under nitrogen and under reducing conditions with addition of hydrazine under nitrogen atmosphere. All experiments were conducted in pre-equilibrated systems. Initial and final Eh values are given. • # 60691/93/94 (aerobic conditions, Se(IV)) • # 60689/90/92 (nitrogen atmosphere, Se(IV)) • # 60688/95/96 (hydrazine, nitrogen atmosphere, Se(– II), only one reducing agent is indicated)	A/B A/B C/D
II-d SDB	As water type, 1%, 10% and 100% SCSSS (standard Canadian Shield saline solution, synthetic brine) is indicated. Under reducing conditions, the solutions are 0.08 M in hydrazine. Final solution compositions are not given, but it is supposed that no essential changes take place with 10% and 100% SCSSS. It is supposed that final solution compositions with 1% SCSSS with goethite or hematite can be estimated.	A/B C/D
II-e SDB	A temperature of 22°C is indicated.	A/B
II-f SDB	It is reported that standard-scale experiments used 10 mL of solution and 0.4 g of solid. This corresponds to a liquid/solid ratio of 25 mL/g.	A/B
II-g SDB	The sorption values (calculated from K_d and L/S ratios) range between 12% and 63%.	A
II-h SDB	Initial Se concentrations between 4.43×10^{-11} M ~ 8.84×10^{-11} M are given. Based on speciation calculations (for 25°C) using the thermodynamic data in JNC-TDB_011213c2 the initial Se concentrations are below the solubility limit.	A
II-i REF	Phase separation was performed by high-speed centrifugation (personal communication with T. T. Vandergraaf).	C/D (update SDB)
II-j SDB	A reaction time of 14 days is indicated.	C/D

	REF	No further (kinetic) information is provided.	
II-k	REF	The samples were intermittently agitated.	A/B
II-l	SDB	No variation in L/S or initial Se concentration is indicated.	C/D
II-m	REF	The experiments were carried out in polypropylene centrifuge tubes. Sorption on vessel walls was not tested and no corrections had been done.	C/D
II-n	SDB	No error information is available.	D
II-o	SDB	Only the SCSSS salinity is varied.	C

Data table Se/6: REF: Davis and Leckie (1980)*

JAEA-SDB version 4 – DATA: Se/Other minerals: iron oxyhydroxide, #50201-50229

GUIDELINE: Revision 4b (May 19, 2005)

*REMARK: Update of SDB required for checkpoints II-a and II-i.

Checkpoint	Evaluation	Rating
I-a.1	SDB All mandatory fields are completed.	Yes
I-a.2	SDB All mandatory information is provided. REF Information about the separation was obtained by personal communication with James A. Davis.	Yes
I-b	SDB A graph with % sorbed Se(VI) as a function of pH is provided.	class 4
II-a	SDB As solid phase, iron oxyhydroxide is reported. It is indicated that specific surface area and CEC are not reported. REF The BET is reported in the cited publication (Davis and Leckie, 1978).	A (update SDB)
II-b	SDB Final pH values are reported.	A
II-c	SDB All experiments had been performed under nitrogen atmosphere. No reducing reactant was added to the solutions. Eh values are not reported, however selenate is not redox sensitive under the reported conditions.	A/B
II-d	SDB As water type, 0.1 M NaNO ₃ is indicated. Final solution composition is not given, but it is supposed that no essential changes take place with 0.1 M NaNO ₃ .	A/B
II-e	SDB A temperature of 25°C is indicated.	A/B
II-f	SDB A liquid/solid ratio of 5,555 mL/g is indicated. REF It is reported that 1.0×10^{-3} M Fe(OH) ₃ was used in the experiments. Specific solid and solution data are not given.	C/D
II-g	SDB The sorption value (calculated from K _d and L/S ratios) ranges between 8% and 90%.	A
II-h	SDB Initial SeO ₄ ²⁻ concentrations between 1.0×10^{-3} and 2.0×10^{-7} are given. Selenate is not solubility limited in a NaNO ₃ -solution with iron oxyhydroxide as substrate.	A
II-i	REF According to personal communication with James A. Davis, the samples had been centrifuged for phase separation.	C/D (tentative)
II-j	SDB A reaction time of 0.017 days is indicated (25 minutes). REF Iron oxyhydroxide is not a stable solid phase, therefore relatively short contact times were chosen. However uptake of selenate was fast and within 25 minutes a metastable equilibrium state was reached and results were reproducible.	A/B
II-k	REF No agitation method is reported, but experimental results indicate that equilibrium had been reached.	A/B
II-l	SDB No isotherm is available, but initial [SeO ₄ ²⁻] had been varied.	B

II-m	REF	No information about the reaction vessel is given.	C/D
II-n	REF	No error information is available.	D
II-o	SDB	Initial $[\text{SeO}_4^{2-}]$ and pH had been varied systematically.	B

Data table Se/7: REF: Fujikawa and Fukui (1997b)* JAEA-SDB version 4 – DATA: Se/Other minerals: magnetite, hematite, #52015-52038 GUIDELINE: Revision 4b (May 19, 2005) * REMARK: Data in SDB do not correspond to the given reference (Part I), they are from Part II, Radiochimica Acta 76, 163-172 (1997).			
Checkpoint		Evaluation	Rating
I-a.1	SDB	All mandatory fields are completed.	Yes
I-a.2	SDB	All mandatory information is provided.	Yes
I-b	SDB	A table with log K_d values is provided.	class 1
II-a	SDB	Magnetite and hematite are reported as mineral phases. Mineralogy and characteristics of these compounds are determined.	A
	REF	The solid phases were purchased from Nihon-Hikagaku Co.	
II-b	SDB	Final pH values are indicated.	A
II-c	SDB REF	It is indicated that Eh values are not reported. It is reported that experimental systems were oxic with Eh values ranging from 100 to 300 mV in NaCl and Na_2SO_4 solutions and from 80 to 200 mV in Na_2CO_3 and NaHCO_3 solutions. The solid substrate magnetite is not stable under the reported Eh values. The oxidation states of Se in all supernatant solutions are reported to be +IV and +VI. It is unclear in which state of the experiments selenate had been generated. Therefore the given K_d values are considered to be unreliable.	unreliable

Data table Se/8: REF: Hayes et al. (1988)* JAEA-SDB version 4 – DATA: Se/Other minerals: goethite, hydrous ferric oxide (HFO) #52828-52974 GUIDELINE: Revision 4b (May 19, 2005) * REMARK: Update of SDB required for checkpoints I-a.2 and II-c.			
Checkpoint		Evaluation	Rating
I-a.1	SDB	All mandatory fields are completed.	Yes
I-a.2	SDB REF	It is indicated that atmosphere/redox conditions are not reported. See annotations of criteria II-c.	Yes (tentative)
I-b	SDB	Graphs with % sorbed SeO_3^{2-} and SeO_4^{2-} are provided.	class 4
II-a	SDB	As solid phases goethite and hydrous ferric oxide (HFO) are indicated. The specific surface area of goethite is reported to be 52 m^2/g , the one of HFO is 600 m^2/g .	A
II-b	SDB	Final pH values are reported and NaNO_3 was used as electrolyte solution.	A
II-c	SDB REF	Redox conditions or Eh values are not reported. It is reported that no change of the redox status of selenate or selenite was observed over the equilibration time of the adsorption experiments. Assuming that no redox active agents were added to the experiments and reactions were performed under ambient conditions, rating A/B is given.	A/B (update SDB)

II-d	SDB	As water types, 0.001 M, 0.005 M, 0.01M, 0.1 M and 1.0 M NaNO ₃ are indicated.	A/B
	REF	Final solution compositions are not given, but it is supposed that no essential changes take place with solutions of concentrations equal or higher than 0.01 M in NaNO ₃ .	
II-e	SDB	It is indicated that reaction temperature is not reported.	C/D
II-f	SDB	Liquid/solid ratios of 33 mL/g (goethite) and of 11,236 mL/g (HFO) are indicated.	C/D
	REF	It is reported that for experiments 3 mL polypropylene vessels had been used. In case of goethite (# 52828 to 52905) this corresponds to 90 mg of solid phase and a sorbent surface of 4.7 m ² . In case of HFO, 0.27 mg of solid in the experiment correspond to a sorbent surface of 0.16 m ² with the reported L/S.	
II-g	SDB	The sorption values (calculated from K _d and L/S ratios) range between 1% and 99%:	B
		• # 52828/29/43/46, # 52832 to 52836, # 52896 to 52898, # 52938, # 52942-52944, # 52951/52, # 52959 to 52963	C/D
		• # 52867-52873, # 52892/93, # 52908-52914, # 52928 to 52932, # 52955 to 52957	A
		• others	
II-h	SDB	Initial selenite or selenate concentrations of 1.0×10^{-4} M are indicated. In sodium nitrate solution selenite and selenate are not solubility limited.	A
II-i	SDB	Centrifugation is indicated as separation method.	C/D
	REF	Samples were centrifuged at 22,000 g for one hour.	
II-j	SDB	A reaction time of 0.27 days is indicated for experiments with goethite, and 0.05 days for experiments with HFO.	C/D
	REF	It is mentioned that kinetic studies over longer periods of equilibration (7 days) had shown no apparent oxidation/reduction of selenium in goethite suspensions.	
II-k	REF	The samples were agitated by end-over-end rotation at 8 rpm.	A/B
II-l	SDB	No variation in L/S or initial Se concentration is indicated.	C/D
II-m	REF	The experiments were carried out in polypropylene centrifuge tubes. Correction for sorption on vessel walls had not been performed.	B
II-n	SDB	No error information is available.	D
II-o	SDB	Electrolyte concentration and pH had been varied systematically.	B

Data table Se/9: REF: Shibutani et al. (1994)*

JAEA-SDB version 4 – DATA: Se/Other minerals: goethite, #59142-59169

GUIDELINE: Revision 4b (May 19, 2005)

* REMARK: Since information about the oxidation state of Se is not given in the SDB or reference translation, it was assumed that Se is in the oxidation state +IV. The classification is based on this assumption.

The K_d values of datapoints # 59142-59159 are precisely identical although measured at different pH. It is assumed that these datapoints were measured at the detection limit and are therefore considered as unreliable. Update of SDB required for checkpoints I-a.2, II-d, II-f and II-h.

Checkpoint	Evaluation	Rating
I-a.1	SDB	All mandatory fields are completed.
I-a.2	SDB	Redox state of Se and redox conditions (Eh values) are not
		(update)

	REF	reported. All experiments were carried out in an N ₂ -atmospheric glove box (O ₂ < 1ppm).	SDB) Yes (tentative)
I-b	SDB	It is indicated that K _d values are provided as % sorbed.	class 2
II-a	SDB	Goethite (α -FeOOH) is indicated as solid phase. Specific surface area is provided.	B
II-b	SDB	Final pH values are reported (after a contact time of 14 days, which can be assumed to be enough to reach equilibrium).	A
II-c	SDB REF	It is indicated that experiments had been performed in an atmosphere with <1 ppm of oxygen. It is reported that experiments had been performed under N ₂ -atmosphere with <1 ppm of oxygen present. Eh values are not reported. Due to the kinetic stability of added Se(IV) under ambient conditions, rating C/D is applied.	C/D
II-d	SDB REF	As water type 0.01 M NaCl solution is indicated. The final solution composition of the equilibrated groundwater is not provided, but can be estimated, due to the use of goethite as pure mineral. As water type 0.1 M NaCl solution is reported.	A/B (revise SDB)
II-e	SDB	Experiments had been conducted at room temperature.	A/B
II-f	SDB REF	A liquid/solid ratio of 20 mL/g is reported The L/S ratio is indicated to be 25 mL/g. With the indicated specific surface area of 9 m ² /g rating A/B is applied.	A/B (revise SDB)
II-g	SDB	The sorption values are calculated from K _d and L/S ratios: • # 59160~59169 (7~81% sorption)	A
II-h	SDB REF	Initial [Se] is indicated as 1.0×10^{-4} M. According to Phreeqci-calculations using the thermodynamic data in the NAGRA-PSI thermodynamic database (Hummel et al., 2002), the reported Se concentration is clearly below the solubility limit (also in case of [Se]= 1.0×10^{-3} M). Initial [Se] is reported to be 1.0×10^{-3} M.	A (revise SDB)
II-i	SDB	It is reported that reaction mixtures were filtered with a 10,000 MWCO (Molecular Weight Cut-Off) ultrafilter.	B
II-j	SDB	A contact time of 14 days is indicated. This reaction time is considered to be reasonably long.	C/D
II-k	REF	There is no information about the agitation method.	C/D
II-l	SDB	No variation in L/S or initial Se concentration is indicated.	C/D
II-m	REF	There is no information about the vessel type used for experimentation. It is indicated that blank measurements had been made, but it is not reported if corrections for sorption on the vessel walls had been performed.	C/D
II-n	SDB	No error estimates are reported. Only one replicate is indicated.	D
II-o	SDB	pH had been varied systematically.	C

Data table Se/10: REF: Shibutani et al. (1994)* JAEA-SDB version 4 – DATA: Se/Other minerals; Al-oxide/-hydroxide, #59170-59178 GUIDELINE: Revision 4b (May 19, 2005) * REMARK: Since information about the oxidation state of Se is not given in the SDB or reference translation, it was assumed that Se is in the oxidation state +IV. The classification is based on this assumption. The K _a values of datapoints # 59173-59175 and # 59177/59178 are precisely identical although measured at different pH. It is assumed that these datapoints were measured at the detection limit and are therefore classified as unreliable. Update of SDB required for checkpoints I-a.2, II-d, II-f and II-h.			
Checkpoint		Evaluation	Rating
I-a.1	SDB	All mandatory fields are completed.	Yes
I-a.2	SDB	Redox state of Se and redox conditions (Eh values) are not reported.	(update SDB)
	REF	All experiments were carried out in an N ₂ -atmospheric glove box (O ₂ < 1ppm). Redox state of Se not mentioned in the translation.	Yes (tentative)
I-b	SDB	It is indicated that K _a values are provided as % sorbed.	class 2
II-a	SDB	Al(OH) ₃ is indicated as solid phase. Specific surface area is provided.	B
II-b	SDB	Final pH values are reported (after a contact time of 14 days, which can be assumed to be enough to reach equilibrium).	A
II-c	SDB	It is indicated that experiments had been performed in an atmosphere with <1 ppm of oxygen.	C/D
	REF	It is reported that experiments had been performed under N ₂ -atmosphere with <1 ppm of oxygen present. Eh values are not reported. Due to the kinetic stability of added Se(IV) under ambient conditions, rating C/D is applied.	
II-d	SDB	As water type 0.01 M NaCl solution is indicated. The final solution composition of the equilibrated groundwater is not provided, but can be estimated, due to the use of Al(OH) ₃ as pure mineral.	A/B (revise SDB)
	REF	As water type 0.1 M NaCl solution is reported.	
II-e	SDB	Experiments had been conducted at room temperature.	A/B
II-f	SDB	A liquid/solid ratio of 20 mL/g is reported, but the L/S ratio is indicated to be 100 mL/g. With the indicated specific surface area of 23 m ² /g rating A/B is applied.	A/B (revise SDB)
II-g	SDB	The sorption values are calculated from K _a and L/S ratios: • # 59176 (76% sorption) • # 59172 (3% sorption) • # 59171 (<1% sorption) • # 59170 (0% sorption; assumed calculation mistake)	A B C/D unreliable
II-h	SDB	Initial [Se] is indicated as 1.0 × 10 ⁻⁴ M. According to Phreeqci-calculations using the thermodynamic data in the NAGRA-PSI thermodynamic database (Hummel et al., 2002), the reported Se concentration is clearly below the solubility limit (also in case of [Se]=1.0 × 10 ⁻³ M).	A (revise SDB)
	REF	Initial [Se] is reported to be 1.0 × 10 ⁻³ M.	
II-i	SDB	It is reported that reaction mixtures were filtered with a 10,000 MWCO (Molecular Weight Cut-Off) ultrafilter.	B
II-j	SDB	A contact time of 14 days is indicated. This reaction time is considered to be reasonably long.	C/D

II-k	REF	There is no information about the agitation method.	C/D
II-l	SDB	No variation in L/S or initial Se concentration is indicated.	C/D
II-m	REF	There is no information about the vessel type used for experimentation. It is indicated that blank measurements had been made, but it is not reported if corrections for sorption on the vessel walls had been performed.	C/D
II-n	SDB	No error estimates are reported. Only one replicate is indicated.	D
II-o	SDB	pH had been varied systematically.	C

Data table Se/11: REF: Ticknor and McMurry (1996)* JAEA-SDB version 4 – DATA: Se/Other minerals; goethite, #60606-60621 GUIDELINE: Revision 4b (May 19, 2005) * REMARK: Update required for checkpoints I-a.2 and II-c			
Checkpoint		Evaluation	Rating
I-a.1	SDB	All mandatory fields are completed.	Yes
I-a.2	SDB REF	It is indicated that reaction atmosphere/redox conditions and the reaction temperature are not reported. It is reported, that solutions at lower pH were prepared and used in air. The solutions at higher pH were prepared and used under a N ₂ atmosphere to avoid dissolution of CO ₂ of the atmosphere.	Yes (update SDB)
I-b	SDB	A table with log K _a values is provided.	class 1
II-a	SDB	As solid phase goethite with up to 25% quartz obtained from Biwabik, Minnesota is reported. The solid was crushed and wet sieved (details described). There is a detailed chemical composition of the mineral available and its specific surface area is given.	A
II-b	SDB	Final pH values are reported.	A
II-c	SDB REF	It is indicated that redox conditions such as Eh values are not reported. It is reported that oxygen was present in the atmosphere surrounding the experimental solutions. An Eh value of 400 mV is indicated for the experiments conducted under ambient conditions and an Eh value of 150 mV for experiments performed under N ₂ atmosphere. Due to the redox stability of selenite under ambient conditions, rating A/B is given.	A/B (update SDB)
II-d	SDB	As water type, 1%, 10% and 100% synthetic groundwater WN-1M is indicated. The solutions contain different concentrations of fulvic acid and were pre-equilibrated before the sorption experiments.	A/B
II-e	SDB	It is not specified at which temperature experiments had been performed. It is assumed that experiments had been made at ambient temperature.	C/D
II-f	SDB	It is reported that standard-scale experiments used 20 mL of solution and 0.5 g of solid. This corresponds to a liquid/solid ratio of 40 mL/g and a solid surface of 1.2 m ² .	C/D
II-g	SDB	The sorption value (calculated from K _a and L/S ratios) ranges between 22% and 92%.	A
II-h	SDB	Initial Se concentrations between 1.0×10^{-8} M and 1.0×10^{-4} M are given. Based on speciation calculations (for 25°C) using the thermodynamic data in NAGRA-PSI thermodynamic database (Hummel et al., 2002) supplemented with the thermodynamic equilibrium of CaSeO ₃ (taken from NEA, 2005)), the initial Se	

		concentrations are below the solubility limit. • # 60606/07, # 60610 to 60613, # 60615/17 • all others	B A
II-i	SDB REF	Centrifugation of the samples is indicated as phase separation. Solid and liquid phases had been separated by centrifugation at 30,000 g prior to analysis.	C/D
II-j	SDB	A reaction time of 28 days is indicated.	A/B
II-k	REF	No information about the agitation of the samples is provided.	C/D
II-l	SDB	Two different Se concentrations are indicated and similar K_d values were obtained.	B
II-m	REF	The experiments were carried out in polycarbonate centrifuge tubes. Radioisotope concentration in the blank was measured and defined as initial radionuclide concentration. This could have led to a possible overcorrection and rating C/D is applied.	C/D
II-n	SDB	No error information is available.	D
II-o	SDB	Experiments had been performed at two [RN] and with 1%, 10% and 100% WN-1M synthetic solutions.	B

Data table Se/12: REF: Ticknor et al. (1988)* JAEA-SDB version 4 – DATA: Se/Other Minerals; goethite, hematite, #60724-60732, # 60742-60750 GUIDELINE: Revision 4b (May 19, 2005) * REMARK: Update of SDB required for checkpoints I-a.2 and II-i.			
Checkpoint		Evaluation	Rating
I-a.1	SDB	All mandatory fields are completed.	Yes
I-a.2	SDB REF	Separation of the samples is not reported. It is reported, that aliquots of the aqueous phases were taken for the radiometric analysis. Phase separation was performed by high-speed centrifugation (personal communication with T. T. Vandergraaf).	Yes (update SDB)
I-b	REF	A table with log K_d values is provided.	class 1
II-a	SDB	As solid phases goethite and hematite, purchased from Wards Natural Science Limited are reported. A detailed chemical composition of the minerals and their specific surface areas and CEC are available. The hematite was used as received from the supplier. The goethite was further treated, the sample was crushed and wet sieved. It contains 15% of quartz.	A
II-b	SDB REF	Initial as well as final pH are indicated. The solution pH was determined with litmus paper (assumed range < 1 pH). No pH correction by addition of buffer was performed after hydrazine addition.	A
II-c	SDB	Redox conditions are reported for each experiment. Experiments are performed under aerobic conditions, under nitrogen and under reducing conditions with addition of hydrazine under nitrogen atmosphere. All experiments were conducted in pre-equilibrated systems. Initial and final Eh values are given. • # 60727/28/30 and # 60744/45/48 (aerobic conditions, Se(VI)) • # 60729/31/32 and # 60746/47/50 (nitrogen atmosphere, Se(IV)) • #60724/25/26 and #60742/43/49 (hydrazine, nitrogen atmosphere, Se(–II), only one reducing agent is indicated)	A/B A/B C/D

II-d	SDB	As water type, 1%, 10% and 100% SCSSS (standard Canadian Shield saline solution, synthetic brine) is indicated. Under reducing conditions, the solutions are 0.08 M in hydrazine. Final solution compositions are not given, but it is supposed that no essential changes take place with 10% and 100% SCSSS. It is supposed that final solution compositions with 1% SCSSS with goethite or hematite can be estimated.	A/B C/D
II-e	SDB	A temperature of 22°C is indicated.	A/B
II-f	SDB	It is reported that standard-scale experiments used 10 mL of solution and 0.4 g of solid. This corresponds to a liquid/solid ratio of 25 mL/g.	A/B
II-g	SDB	The sorption values (calculated from K_d and L/S ratios) range between 40% and 85%.	A
II-h	SDB	Initial Se concentrations between 4.34×10^{-11} M and 1.21×10^{-10} M are given. Based on speciation calculations (for 25°C) using the thermodynamic data in JNC-TDB_011213c2 the initial Se concentrations are below the solubility limit.	A
II-i	REF	Phase separation was performed by high-speed centrifugation (personal communication with T. T. Vandergraaf).	C/D (update SDB)
II-j	SDB REF	A reaction time of 14 days is indicated. No further (kinetic) information is provided.	C/D
II-k	REF	The samples were intermittently agitated.	A/B
II-l	SDB	No variation in L/S or initial Se concentration is indicated.	C/D
II-m	REF	The experiments were carried out in polypropylene centrifuge tubes. Sorption on vessel walls was not tested and no corrections had been done.	C/D
II-n	SDB	No error information is available.	D
II-o	SDB	Only the SCSSS salinity is varied.	C

3.1.5 Thorium

Data table Th/1: REF: Allard et al. (1979b) JAEA-SDB version 4 - DATA: Th/Granitic rocks; granite #42459-42470 GUIDELINE: Revision 4b (May 19, 2005)		
Checkpoint	Evaluation	Rating
I-a.1 SDB	All mandatory fields are completed.	Yes
I-a.2 SDB	All mandatory information is provided.	Yes
I-b REF	A table with log K_d values is given.	class 1
II-a SDB	As solid phase granite is indicated. Mineralogy and surface characteristics are not reported.	C/D
II-b SDB	Initial pH values are reported.	C
II-c SDB REF	Redox state of Th is not indicated. Experiments had been performed under aerobic conditions. Eh values not reported. Th is not redox sensitive.	A/B
II-d SDB	Detailed compositions of two different water types are indicated.	A/B
II-e SDB	A reaction temperature of 25°C and 65°C is indicated.	A/B
II-f SDB REF	A liquid/solid ratio of 30~50 mL/g is reported. A surface to mass ratio of <10 m ² /kg is reported. Assumed that this is the specific surface of granite, with 1~3 g of solid phase per reaction vial the total surface is 0.01~0.03 m ² /vial.	C/D
II-g SDB REF	The following sorption values were calculated from K_d and L/S ratios: #42461 (98%), 42467 (96%), 42468 (96%), 42469 (96%) #42460 (100%), 42464 (99%)	B C/D
II-h SDB REF	Initial [Th] is reported as 1.0×10^{-5} M and $<1.0 \times 10^{-8}$ M. According to the data from Rai et al.(1999a) and based on speciation calculations with Phreeqi 2.14.3 using the thermodynamic data in the NAGRA-PSI thermodynamic database (Hummel et al., 2002) the initial [Th] of 1.0×10^{-5} M was clearly above the respective solubility limit for the reported data at pH 8.2. These datapoints are considered as unreliable and are excluded from further evaluation. The initial [Th] of $<1.0 \times 10^{-8}$ M is clearly below the solubility limit and for these datapoints rating A is applied. #42459, 42462, 42463, 42465, 42466 and 42470 #42460, 42461, 42464, 42467, 42468 and 42469	unreliable A
II-i SDB REF	It is indicated that samples had been centrifuged during 50 minutes at 7,000 rpm and filtered through a 0.2 µm membrane filter. It is reported that filtration did not change the sorption values.	A
II-j SDB	A contact time of 7 to 180 is indicated. The log K_d values of equal experiments but different reaction times differ by a factor of about 10. Since there is only the initial pH vales provided and the reaction time of 7 days is considered to be reasonable long, the data with a reaction time of 180 days are assessed as unreliable: #42460 and 42464 #42461, 42467-42469	unreliable C/D

		The natural groundwaters contain 0.5 and 20 mL/g of iron. Reported K_d values of Th and Am show a significant increase at a contact time of 180 days, whereas K_d values of Cs do not differ much from the values measured after 7 days. On the basis of this information, sorption of Am and Th onto iron oxides is very likely during a contact time of 180 days.	
II-k	REF	The samples were shaken.	A/B
II-l	REF	No variation in L/S is indicated. There are two initial Th concentrations indicated, but datapoints of higher [Th] were considered as unreliable in checkpoint No. II-h.	C/D
II-m	REF	The experiments were carried out in glass bottles. Corrections for sorption on vessel wall have not been done.	C/D
II-n	REF	No error estimates are indicated. Number of replicates is not reported.	D
II-o	REF	Sorption was measured at two different temperatures.	C

Data table Th/2: REF: Allard et al. (1978)* JAEA-SDB version 4 - DATA: Th/Granitic rocks; granite #42230, 42231 GUIDELINE: Revision 4b (May 19, 2005) *REMARK: The solid/liquid ratio needs to be verified. Update of SDB required for checkpoints I-b, II-b, II-C, II-d, II-h and II-i			
Checkpoint		Evaluation	Rating
I-a.1	SDB	All mandatory fields are completed.	Yes
I-a.2	SDB	All mandatory information is provided.	Yes
I-b	SDB REF	K_d values are provided in [m ³ /kg]. Only two of nine available K_d values from the reference are transferred to the SDB. The K_d values in SDB do not correspond to the reported values in the reference.	class 1 (update SDB)
II-a	SDB	As solid phase granite is indicated. Major mineralogy and surface characteristics are not reported.	C/D
II-b	SDB REF	Initial and final pH values are reported. Apparently for experiments concerning complex formation and solubility a pH of 7 to 9 was applied. Seemingly no pH values are reported for the sorption experiments, but it is assumed that experiments had been performed at a pH of 7 to 9.	(update SDB) D (tentative)
II-c	SDB REF	Redox state of Th is indicated as +IV. Experiments had been performed under aerobic and under reducing conditions with Fe(II/III) present in solution. Eh values are reported to be -0.15 to -0.21 V for experiment #42230. Th is not redox sensitive. Eh values in a pH range of 7~9 are reported to be -0.15 to -0.27 V.	(update SDB) A/B
II-d	SDB	It is indicated that experiments had been performed in synthetic groundwater aq293. Final solution composition is reported. There are datapoints of experiments with another synthetic groundwater aq1105 available. For datapoint #42230 the concentration of reducing agent Fe(II/III) in solution is not reported.	A/B (update SDB) unreliable
II-e	SDB	A temperature of 25°C is indicated.	A/B
II-f	REF	Due to lacking surface characteristics and the applied amount of solid phase for the experiments, rating C/D is applied.	C/D

II-g	SDB	An L/S ratio of 11 mL/g is indicated in the SDB. However there was no information found in the reference concerning the L/S. Sorption values need to be validated after update of the SDB, since listed K_d values do not correspond to the information found in the reference.	C/D (tentative)
II-h	SDB REF	An initial Th concentration of 1.0×10^{-11} is indicated. Sorption measurements had been performed at a [Th] of 1.0×10^{-8} M (K_d values >4.0 and 3.6 (180d), and 2.9 and 3.1 (7d)). Based on speciation calculations with Phreeqi 2.14.3 using the thermodynamic data in the NAGRA-PSI thermodynamic database (Hummel et al., 2002) the initial Th concentration of 1.0×10^{-8} M is clearly below the solubility limit for the data at pH 7 to 9. The [Th] of 1.0×10^{-5} M is clearly above the solubility limit, therefore datapoints with K_d values 3.3, 3.7, 2.9 and 3.1 are considered as unreliable.	(update SDB) A unreliable
II-i	SDB REF	It is indicated that samples had been centrifuged for 50 min. at 4,000 rpm. It is assumed that for sorption experiments the samples were treated similar as described for sorption experiments of americium: Centrifugation for 1h at 7,000 rpm and eventually filtration over 0.2 μ m membrane.	(update SDB) C/D (tentative)
II-j	SDB REF	A contact time of 180 days is indicated. Additional datapoints are available with a contact time of 7 days (K_d values three times 2.9 and 3.1 m ³ /kg).	C/D
II-k	REF	There was no information found concerning the agitation of the samples.	C/D
II-l	REF	No variation in L/S or initial Th of reliable datapoints had been performed.	C/D
II-m	REF	Information about the type of reaction vial was found in the reference.	C/D
II-n	REF	No error information is available.	D
II-o	REF	No parameter variation is indicated.	D

Data table Th/3: REF: Koskinen et al. (1985)*		
JAEA-SDB version 4 - DATA: Th/Granitic rocks; mica gneiss and tonalite #54053-54056		
GUIDELINE: Revision 4b (May 19, 2005)		
*REMARK: Update of SDB required for checkpoints II-a and II-j		
Checkpoint	Evaluation	Rating
I-a.1 SDB	All mandatory fields are completed.	Yes
I-a.2 SDB	All mandatory information is provided.	Yes
I-b REF	K_d values are provided in [mL/g].	class 1
II-a SDB	As solid phase mica gneiss and tonalite are indicated. It is indicated that surface characteristics are not reported.	(update SDB)
REF	The main minerals of the crushed rocks are reported for both, tonalite and mica gneiss. Grain size and surface characteristics are not reported.	C/D
II-b SDB	Initial and final discrete pH values are reported.	A
II-c SDB	Thorium with the oxidation state (+IV) and oxic conditions are indicated. This is not redox sensitive.	A/B
REF	²³⁴ Th was separated from dilute HNO ₃ -solution of uranyl nitrate by	

		TTA-extraction and was added as $\text{Th}(\text{NO}_3)_4$.	
II-d	SDB	It is indicated that synthetic groundwater was used for experiments and a detailed solution composition is given.	A/B
II-e	SDB	A temperature of 20°C is indicated.	A/B
II-f	REF	Due to lacking surface characteristics and the applied amount of solid phase for the experiments, rating C/D is applied.	C/D
II-g	SDB	The sorption value is calculated from K_d and L/S ratios and is for all datapoints 99%.	C/D
II-h	SDB	An initial Th concentration of 1.0×10^{-13} to 1.0×10^{-15} is reported. According to the data in Rai et al. (1999a) the [Th] is at a pH of 8 to 9 clearly below the solubility limit.	A
II-i	SDB	It is indicated that samples had been centrifuged for 60 min. at 8,000 rpm. Samples of datapoints #54054 and #54055 had additionally been filtered over a 0.45 μm membrane. There is no effect of filtration on the K_d -values.	B
II-j	SDB REF	A contact time of 14 days is indicated. The radionuclide was added after one week of pre-equilibration with synthetic groundwater and was allowed to react for 7 days.	C/D (update SDB)
II-k	REF	The samples were shaken.	A/B
II-l	REF	No variation in L/S or initial Th concentration is indicated.	C/D
II-m	REF	Reactions had been done in plastic centrifuge tubes and no corrections for the sorption on the vessel walls had been performed.	B
II-n	REF	No error information is available.	D
II-o	REF	No parameter variation is indicated.	D

Data table Th/4: REF: Ueta (1998)*			
JAEA-SDB version 4 – DATA: Th/Granitic rocks; granodiorite #61613-61620			
GUIDELINE: Revision 4b (May 19, 2005)			
*REMAEK: Update of SDB required for checkpoints II-a and II-d.			
Checkpoint		Evaluation	Rating
I-a.1	SDB	All mandatory fields are completed.	Yes
I-a.2	SDB	All mandatory information is provided.	Yes
I-b	SDB	K_d values are provided in [m^3/kg].	class 1
II-a	SDB	As solid phase granodiorite from Gunnma-ken Souri is indicated. Major mineralogy and surface characteristics of the granodiorite are not reported.	C/D
	REF	A surface area of 0.7 m^2/g is reported.	update SDB
II-b	SDB	Initial and final pH values are reported.	A
II-c	SDB	Redox state of Th is not indicated. Experiments had been performed under aerobic conditions. Eh values are not reported. Th is not redox sensitive.	A/B
II-d	SDB	Experiments had been performed in seawater and distilled water. Final solution compositions are not reported: • # 61613-61616: due to lacking mineralogy the solution composition after equilibration with distilled water cannot be estimated. • # 61617-61620: it is supposed that no essential changes take place with seawater.	update SDB unreliable, no further evaluation
	REF	Carbonate concentrations of the solutions are reported. Solutions	A/B

		had been analysed after pre-equilibration.	
II-e	SDB	A temperature of 25°C is indicated.	A/B
II-f	SDB	It is indicated that 1 g of solid per reaction vial was used. With the indicated BET the total solid surface is 0.7 m ² /vial.	C/D
II-g	REF	The sorption values are calculated from K _d and L/S ratios. It is 91% for datapoints # 61617-616120.	A
II-h	SDB	An initial Th concentration of 5.0 × 10 ⁻⁹ M is indicated. Based on speciation calculations with Phreeqci 2.14.3 using the thermodynamic data in the NAGRA-PSI thermodynamic database (Hummel et al., 2002) the initial Th concentration was just below the respective solubility limit for the reported data around pH 8 (supported by checkpoint II-i).	C/D
II-i	SDB	Similar results were obtained by filtration over 0.45 µm membranes and filtration over a 10,000 MWCO (molecular weight cut-off) filter.	A
II-j	SDB	A contact time of 30 days is indicated.	C/D
II-k	REF	The samples were shaken.	A/B
II-l	SDB	No variation in L/S or initial Th concentration is indicated.	C/D
II-m	REF	Type of reaction vial is not reported. Corrections for sorption on vessel wall have been done. Sorbed Th was extracted by acid leaching. Further information about correction procedure is not available.	C/D
II-n	SDB	No error information is available.	D
II-o	SDB	No parameter variation is indicated.	D

Data table Th/5: REF: Hunter et al. (1988)*

JAEA-SDB version 4 – DATA: Th/Other minerals; Fe-oxide/-hydroxide #53524-53526

GUIDELINE: Revision 4b (May 19, 2005)

* REMARK: Only three datapoints out of several data sets are listed in the SDB (Points should be entered into SDB or a remark in SDB is required). Update of SDB required for checkpoints I-a.2.

Checkpoint		Evaluation	Rating
I-a.1	SDB	All mandatory fields are completed.	Yes
I-a.2	SDB	All mandatory information is provided. It is indicated that the redox state of Th is not reported.	Yes (update SDB)
	REF	Oxidation state of Th is reported. Th is not redox sensitive.	
I-b	REF	A linear graph with % sorbed Th is provided.	class 4
II-a	SDB	As solid phase goethite with its CEC is indicated.	A
II-b	SDB	Final pH values are reported.	A
II-c	SDB	No redox conditions are indicated. Th is not redox sensitive.	A/B
II-d	SDB	UV irradiated seawater is indicated.	A/B
	REF	The salinity of the natural seawater is reported to be 3.42% (~0.1 M). A detailed solution composition is not given. It is indicated/suggested that the effects of carbonate and bicarbonate ions on Th adsorption by goethite can be neglected at seawater alkalinities.	
II-e	SDB	A reaction temperature of 20°C is indicated.	A/B
II-f	SDB	A liquid/solid ratio of 1,852 mL/g is reported.	A/B
	REF	A typical specific surface area of FeOOH reported in the literature is found to be 18 to 40 m ² /g. For the experiments 0.54 g of solid	

		and 1 L of solution were used for experiments. With a BET value of 18 m ² /g rating A/B is applied.	
II-g	REF	The sorption values (calculated from K _d and L/S ratios) are 26, 54 and 91%.	A
II-h	SDB	Initial [Th] is reported as 9.0 × 10 ⁻⁶ M. According to the data from Rai et al. (1999a) the given [Th] is at a pH of 4.0 to 5.0 clearly below the solubility limit.	A
II-i	SDB	It is indicated that samples had been centrifuged during 15 minutes at 4,500 g.	C/D
II-j	SDB REF	A contact time of 0.1 day is indicated. Despite the short contact time of 3 hrs rating C/D is applied, since it is reported that separate kinetic measurements established the completeness of Th-uptake by the oxide after 3 hours.	C/D
II-k	REF	Samples were not agitated during the adsorption period, since separate experiments showed that this had no effect on the measured uptake of Th.	A/B (tentative)
II-l	SDB	No variation in L/S or initial Th concentration is indicated.	C/D
II-m	REF	The experiments were carried out in pyrex glass vessels. Adsorption to the flask walls was measured in separate experiments by nitric acid leaching of the vessel walls. Losses were less than 10%. No further information about correction procedures available.	C/D
II-n	SDB	No error estimates are indicated. Number of replicates is not reported.	D
II-o	SDB	Sorption was measured at different pH values (sorption edge).	C

Data table Th/6: REF: Righetto et al. (1988)*		
JAEA-SDB version 4 – DATA: Th/Other minerals; Al-oxide/-hydroxide #58545-58547		
GUIDELINE: Revision 4b (May 19, 2005)		
* REMARK: Only three datapoints are listed in the SDB, due to the original selection of data in context of sorption onto bentonite. Additional information about sorption of Th on aluminum oxide e.g. in presence of carbonate in solution is provided in the reference. Update of SDB required for checkpoints II-c, II-f, II-e and maybe II-o.		
Checkpoint	Evaluation	Rating
I-a.1 SDB	All mandatory fields are completed.	Yes
I-a.2 SDB	All mandatory information is provided.	Yes
I-b REF	A linear graph with % sorbed Th is indicated.	class 4
II-a SDB	As solid phase aluminum oxide with BET and CEC is indicated.	A
II-b SDB	Final discrete pH values are reported and 0.1 M NaClO ₄ solution was used for the experiments.	A
II-c SDB	Thorium with the oxidation state (+IV) is indicated. No further redox conditions are given. Th is not redox sensitive.	A/B
REF	It is reported that experiments had been made under oxic conditions.	update SDB
II-d SDB	It is indicated that the solution was 0.1 M in NaClO ₄ (post equilibration).	A/B
II-e SDB	Temperature is not specified.	C/D
II-f REF	Rating is done based on the indicated L/S ratio (100 L/g). With a BET of 130 m ² /g and assumed that 0.01 g per reaction vial were used, a surface of 1.3 m ² /vial is obtained at best.	C/D

II-g	REF	The sorption values are calculated from K_d and L/S ratios and are 51%, 8% and 91%.	A
II-h	SDB	An initial Th concentration of 1.0×10^{-11} M is reported. According to the data in Rai et al. (1999a) the [Th] is at a pH of 1.8 to 3.6 clearly below the solubility limit.	A
II-i	SDB	It is indicated that samples had been centrifuged for 60 min. at 55,000 rpm (ultracentrifugation).	B
II-j	SDB REF	A contact time of 7 days is indicated. The radionuclide was added after one month of pre-equilibration and was allowed to react for 7 days. It is reported that reaction time was determined by preliminary kinetic runs.	A/B
II-k	REF	The samples were mechanically shaken.	A/B
II-l	SDB	No variation in L/S or initial Th concentration is indicated.	C/D
II-m	REF	Reactions had been done in polyallomer ultracentrifuge tubes “quick seal” of Beckman. Parallel experiments without centrifugation were performed to quantify the nuclide adsorption on the tube walls. Apparently no corrections had been done.	B
II-n	SDB	No error information is available.	D
II-o	SDB REF	pH had been varied. Additional experiments are reported (datapoints not in SDB) where sorption on aluminum oxide in presence of carbonate in solution had been studied.	C maybe update SDB

3.2 Criteria III

Only the entries for Am, Np, Se and Th classified as reliable are being considered for criteria III. All unreliable entries, or entries where classification according to criteria I and II could not be completed, are excluded. Entries for Cs are not included in this analysis because the final cation concentration would have to be estimated or calculated in most cases before a meaningful comparison can be done.

3.2.1 Evaluation of data for americium

The following entries are evaluated in this section; the respective data are shown in Figure 3.2.1-1.

Reference	Data table	Solid phase (group/solids)
Allard & Beall (1979)	Am/16	other minerals / corundum, gibbsite
Allard & Beall (1979)	Am/17	other minerals / hematite, magnetite
Degueldre et al. (1994)	Am/18	other minerals / hematite
Higgo et al. (1983)	Am/19	other minerals / am. Fe- and Mn-oxides
Righetto et al. (1988)	Am/20	other minerals / Al-oxide
Allard et al. (1979b)	Am/3	granitic rocks / granite
Berry et al. (2007)	Am/8	granitic rocks / granodiorite
Ikeda & Amaya. (1998)	Am/11	granitic rocks / granodiorite
Kitamura et al. (1999a)	Am/12	granitic rocks / granite

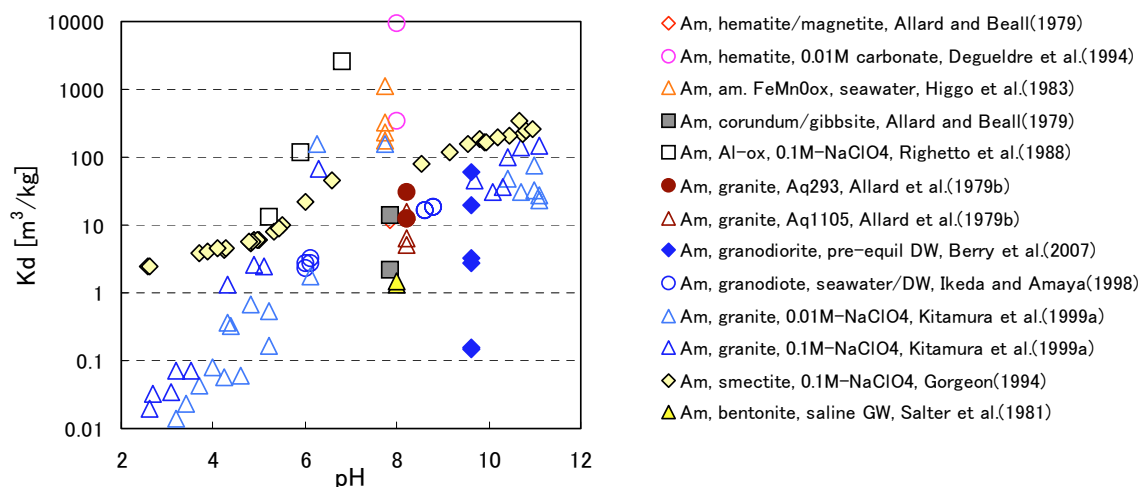


Figure 3.2.1-1 Overview of sorption data for Am on metal oxide minerals and granitic rocks. For comparison, sorption data for Am on smectite and bentonite are also shown. DW = distilled water, GW = ground water.

Overall, the data of Am sorption on a variety of minerals plotted in Figure 3.2.1-1 show a fairly clear trend of increasing K_d with increasing pH. Considering further the differences in conditions, the deviations from this trend are surprisingly small for a large portion of the pH range considered.

With the exception of a few data obtained on (mostly amorphous) metal oxides, the data

in Figure 3.2.1-1 indicate a roughly linearly rising sorption envelope between pH 2~9, followed by a nearly level part up to pH > 12. Even at very high pH, there is no indication of a downward curving sorption edge. This general picture is consistent with the hydrolysis behavior of Am, where the uncharged $\text{Am}(\text{OH})_3(\text{aq})$ forms already at slightly alkaline pH and is the highest hydrolytic species (no further hydrolysis occurs with increasing pH, see Guillaumont et al., 2003).

In order to facilitate a comparison within the three mineral/solid groups considered, the respective data are shown in separate plots below. The data for smectite and bentonite are always included for reference.

Figure 3.2.1-2 shows that the sorption of Am on metal oxides is generally stronger than on clays. This is consistent with the strong tendency of Am to form surface complexes and the high concentration of SOH-groups on Fe- and Al-oxides. The trend of K_d vs. pH is similar for clays and metal oxides, which would also be expected based on the assumed sorption mechanism. The samples used in the experiments by Higgo et al. (1983) contain Mn-oxides, which are known to be even more efficient sorbents than Fe-oxides. This explains the high K_d values even in the presence of seawater. The difference in the values by Degueldre under identical chemical conditions may be due to difference in L/S (see data table Am/18).

The K_d values measured by Allard and Beall (1979) are significantly lower than the other data discussed here. The reason is not clear: Lowering of K_d due to the formation of dissolved complexes should not be more significant than in case of the other studies considered. Allard and Beall (1979) did not use a very effective phase separation method, but carried out corrections for sorption on vessel walls, on the other hand. However, it would require examination of the underlying raw data to decide whether these issues led to erroneously low values. On the other hand, Allard and Beall (1979) used commercial samples of crystalline phases; such solids may have significantly smaller surface areas than natural samples. Considering all issues, the data by Allard and Beall (1979) are evaluated as being not representative for Am sorption on metal oxides.

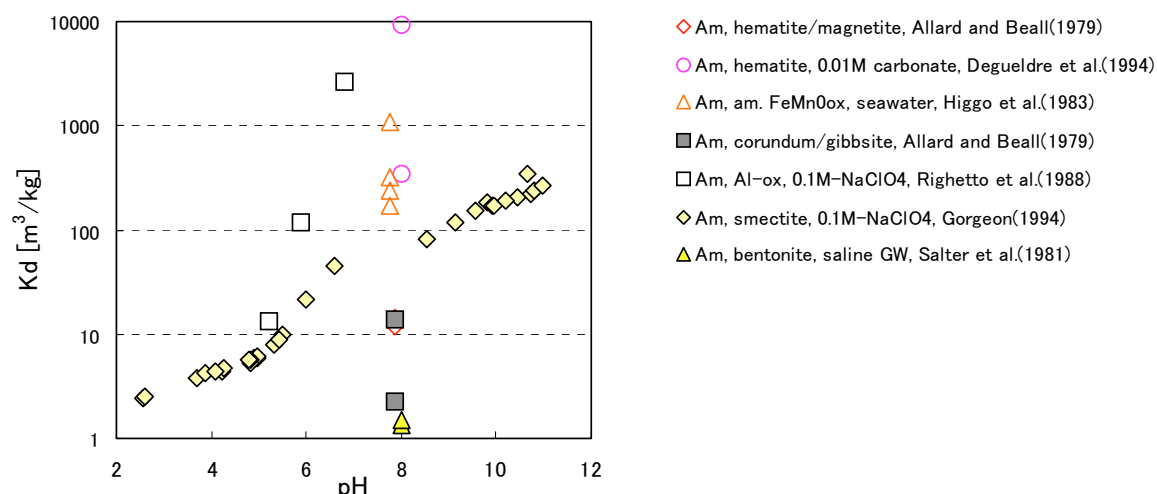


Figure 3.2.1-2 Overview of sorption data for Am on metal oxide minerals. For comparison, sorption data for Am on smectite and bentonite are also shown. DW = distilled water, GW = ground water.

The data for Am sorption on granitic rocks are given in Figure 3.2.1-3. On average, it appears that sorption of Am on granitic rocks is identical to sorption on smectite in terms of trend as a function of pH as well as in terms of magnitude. While the same trend would be expected, it is surprising that sorption on samples of granite and granodiorite is identical to sorption on pure smectite. Granitic rocks typically contain quartz, feldspar, and mica minerals. Based on crystal structure and experience, it can be assumed as a first approximation that sorption of Am will take place primarily on the mica edge surfaces. Modeling results of a simple sorption model based on this assumption (Lothenbach and Ochs, 1999) show that the sorption of Am on edge-type surfaces is so strong, that equally high K_d values may be obtained for granitic rocks and bentonite, depending on solution composition. All data for Am sorption on granitic rocks shown in Figure 3.2.1-3 are evaluated as consistent with independent data. The data from Allard et al. (1979b) are compared with other data for various granite samples (classified earlier, see Ochs and Kunze, 2008), as well as with selected data for clays, reflecting conditions of intermediate to high ionic strength. While the data by Allard et al. (1979b) refer to only one pH, it is evident that they are consistent with other reliable data.

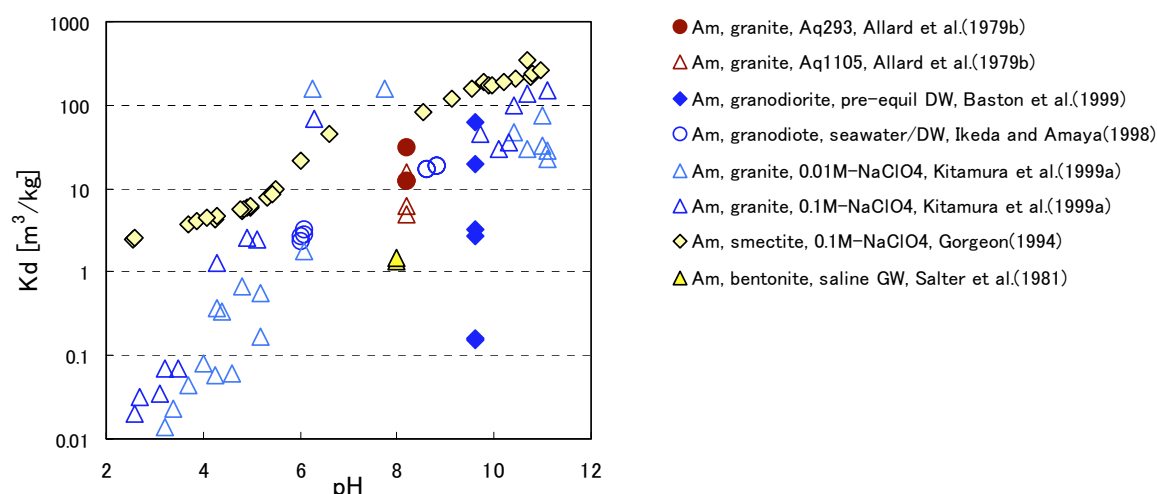


Figure 3.2.1-3 Overview of sorption data for Am on granitic rocks. For comparison, sorption data for Am on smectite and bentonite are also shown. DW = distilled water, GW = ground water.

3.2.2 Evaluation of data for selenium

The following entries are evaluated in this section; the respective data are shown in Figure 3.2.2-1.

Reference	Data table	Solid phase (group/solids)
Davis and Leckie (1980)	Se/6	other minerals / iron oxyhydroxide
Hayes et al. (1988)	Se/8	other minerals / goethite, HFO
Shibutani et al. (1994)	Se/9	other minerals / goethite
Shibutani et al. (1994)	Se/10	other minerals / Al-oxide/-hydroxide
Ticknor and McMurtry (1996)	Se/11	other minerals / goethite
Ticknor et al. (1988)	Se/12	other minerals / goethite, hematite
Sato et al. (1997)	Se/2	granitic rocks / granodiorite

Figure 3.2.2-2 shows a separate plot of the data obtained by Hayes et al. (1988) and by Davis and Leckie (1980) in simple electrolyte solutions. This plot shows the different behavior of selenate and selenite, which can be expected on the basis of, and is consistent with, spectroscopic information as well as insights from modeling exercises (NEA, 2005). The following patterns become apparent from Figure 3.2.2-2:

- K_d values for both Se(VI) and Se(IV) show the same trend as a function of pH, this trend is typical for ligand-exchange of anionic species on oxide-type mineral surfaces;
- the sorption of Se(VI) is weaker than the sorption of Se(IV), which is consistent with the different stability of selenate⁻ and selenite⁻ metal complexes;
- the sorption behavior of Se(IV) is independent of the concentration of the background electrolyte, which is typical for inner-sphere ligand exchange;

- K_d for Se(VI) changes as function of the concentration of the background electrolyte, which indicates competition between selenate and the electrolyte anions and is typical for outer-sphere interaction.

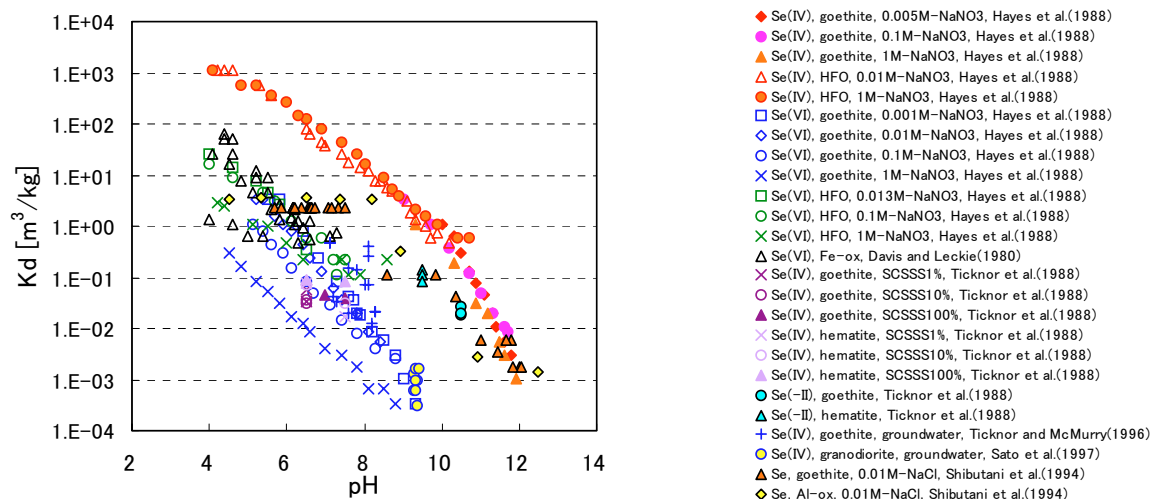


Figure 3.2.2-1 Overview of sorption data for Se on Fe-oxide minerals and granitic rocks. HFO = hydrous ferric oxide, SCSSS = standard Canadian shield saline solution, DW = distilled water, (S)GW = (synthetic) groundwater.

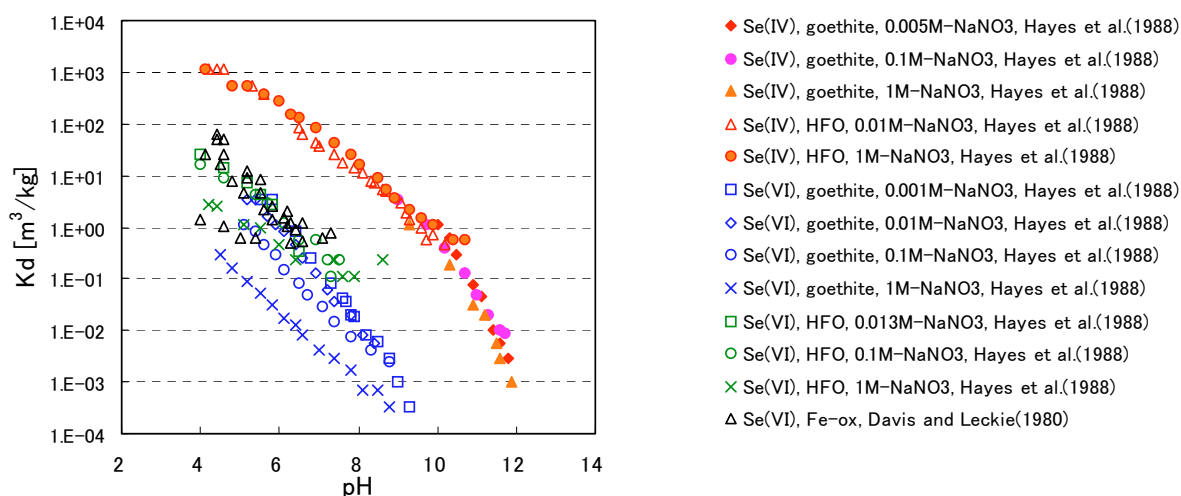


Figure 3.2.2-2 Overview of sorption data for Se on Fe-oxides and -hydroxides. HFO = hydrous ferric oxide.

Figure 3.2.2-3 summarizes the data by Ticknor et al. (1988), Ticknor and McMurray (1996) and Shibutani et al.(1994) on goethite and hematite. The data by Ticknor and co-workers all refer to Se(IV), the respective K_d values appear to be more representative for Se(VI) than for Se(IV), however. In case of the data by Ticknor, the relatively low sorption may be explained with the presence of fulvic acid in the groundwater used for the experiments. However, no direct comparison with any other data is possible.

Therefore, these data are regarded as being not inconsistent with the available independent data.

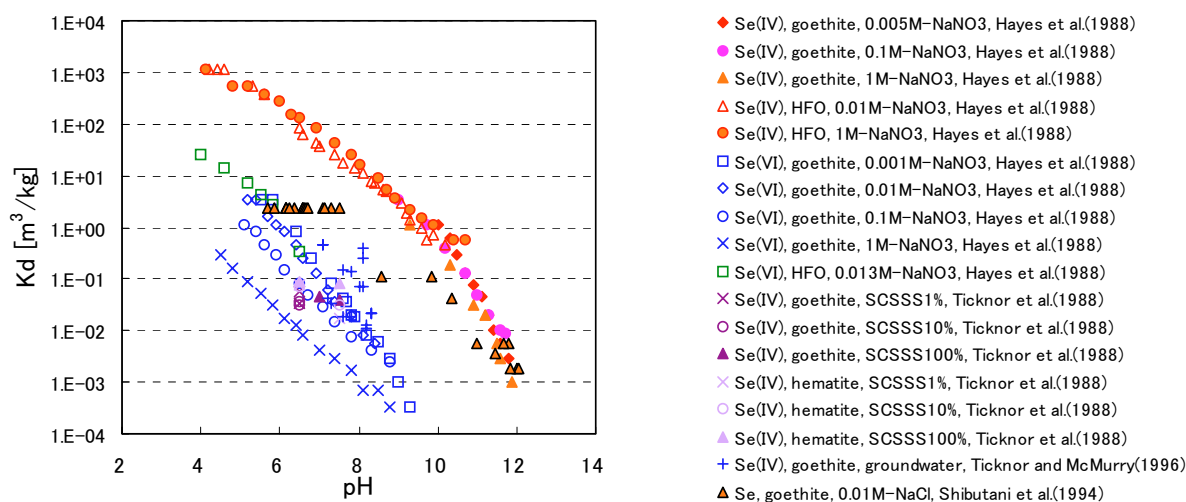


Figure 3.2.2-3 Overview of sorption data for Se on goethite and hematite by Ticknor et al. (1988), Ticknor and McMurray (1996) and Shibutani et al.(1994). Data by Hayes et al. (1988) are given for comparison. HFO = hydrous ferric oxide, SCSSS = standard Canadian Shield saline solution.

In the case of the data by Ticknor et al. (1988), it may also be possible that competition by the high chloride concentration in the SCSSS lead to the observed low sorption, which appears to more representative for Se(VI) than for Se(IV). However, there seems to be little systematic difference between the various chloride concentrations used. It is also not clear why the effect of chloride would be stronger than the effect of fulvic acid. On the other hand, there is no evidence that an oxidation of Se(IV) occurred (there is no difference between experiments in the presence and absence of oxygen). Based on this discussion, the data for Se(IV) by Ticknor et al. (1988) are evaluated as being not conclusive regarding consistency with other data.

In the case of the data by Ticknor and McMurray (1996), the dataset shown for goethite have been obtained within a limited range of pH and do not show a significant trend as a function of pH, but they are approximately consistent with each other. Note that the data by Ticknor and McMurray (1996) for goethite refer to several different conditions in terms of chloride and fulvic acid concentrations, which is the reason for the apparent scatter.

Figure 3.2.2-4 focuses on the data for Se on goethite and Al-oxide by Shibutani et al. (1994), and for Se(−II) on goethite and hematite by Ticknor et al. (1988). The data by Shibutani et al. (1994) show a pH-dependency that is different from any other dataset. While the data at higher pH appear to be approximately consistent with the data for

Se(IV) by Hayes et al. (1988), the data below $\text{pH} \approx 8$ show a constant K_d over a wide range of pH. This behavior is inconsistent with all other observations as well as with the expected behavior of selenite (or selenate). Tentatively, these data are evaluated as unreliable. From tables Se/9 and Se/10, it appears that these data correspond to conditions where nearly all of the Se present had been removed from solution. Thus, it may be that the flat part of the sorption curve represents an analytical detection limit. The data of Ticknor et al. (1988) shown in Figure 3.2.2-4 are the only data for selenide, to our knowledge. Therefore, no comparison with other data is possible. Based on the general chemical behavior of the different oxidation states of Se, intermediate sorption between Se(IV) and Se(VI) appears to be reasonable.

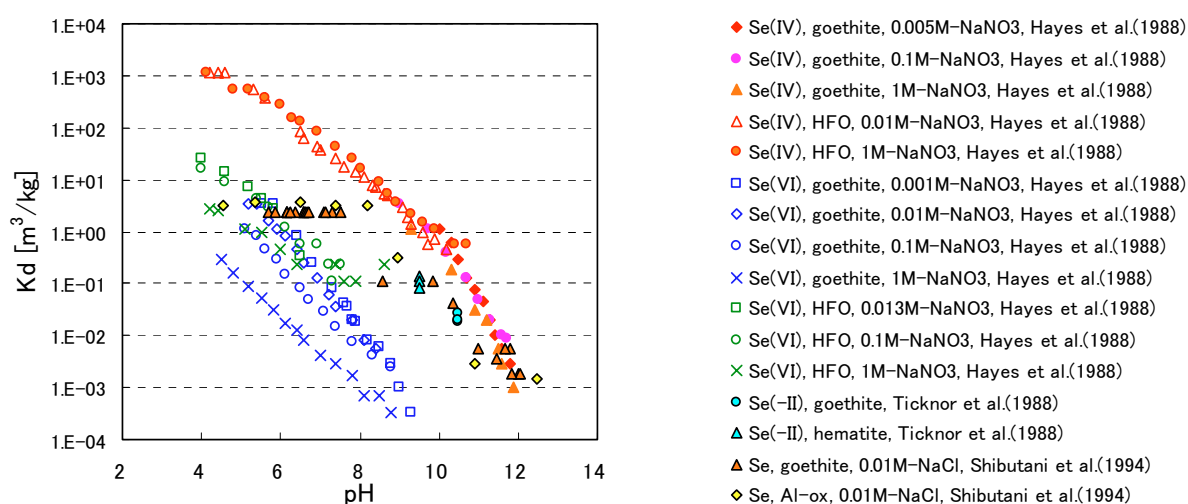


Figure 3.2.2-4 Overview of sorption data for Se on goethite and Al-oxide by Shibutani et al. (1994), and for Se(-II) on goethite and hematite by Ticknor et al. (1988). Data by Hayes et al. (1988) are given for comparison. HFO = hydrous ferric oxide.

Figure 3.2.2-5 shows the available data for granodiorite. Assuming that the data for granodiorite by Sato et al. (1997) refer to Se(IV), it would seem reasonable that the minerals in granodiorite have a lower sorption capacity for anions than goethite or HFO.

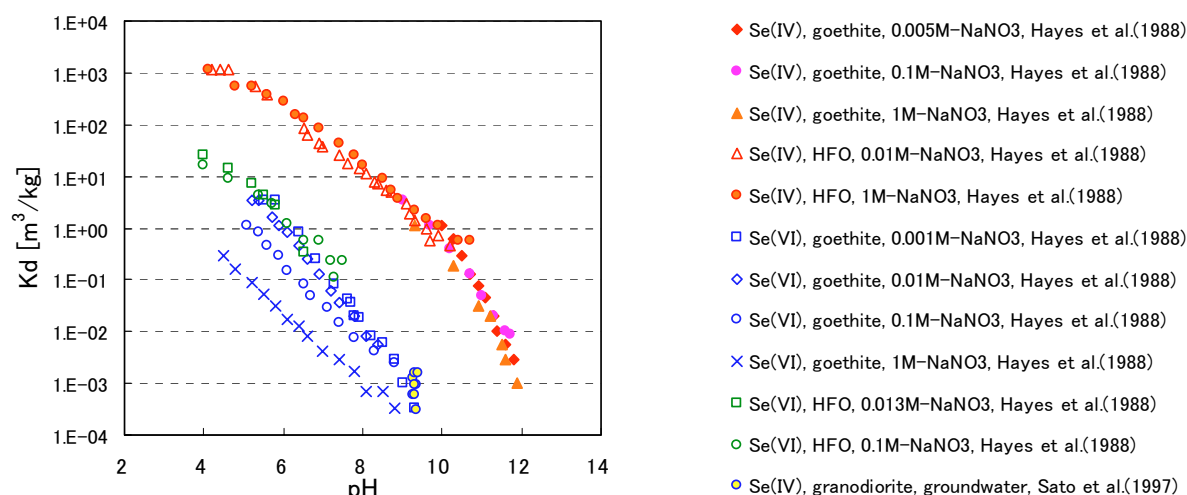


Figure 3.2.2-5 Overview of sorption data for Se on granodiorite. Data by Hayes et al. (1988) are given for comparison. HFO = hydrous ferric oxide.

3.2.3 Evaluation of data for thorium and Neptunium

The following entries are evaluated in this section; the respective data are shown in Figure 3.2.3.

Reference	Data table	Solid phase (group/solids)
Allard et al. (1979b)	Th/1	granitic rock / granite
Allard et al. (1978)	Th/2	granitic rock / granite
Koskinen et al. (1985)	Th/3	granitic rock / mica gneiss, tonalite
Ueta (1998)	Th/4	granitic rock / granodiorite
Hunter et al. (1988)	Th/5	other minerals / goethite
Righetto et al. (1988)	Th/6	other minerals / Al-oxide
Baston et al. (1997)/ Berry et al. (2007)	Np/4	granitic rocks / granodiorite

Considering the difference in mineralogy and solution composition, the data obtained on the various metal oxide phases are consistent with each other as well as with the data for different clay systems by Bradbury and Baeyens (2003a; 2003b).

The data for Th sorption in the seawater on granodiorite by Ueta (1998) and on tuff by Ueta et al. (1999) can be compared with the data for goethite by Hunter (1988), also obtained in the seawater. Considering the nearly level trend of sorption vs. pH observed for Th and the (presumed) difference in sorption capacity between goethite on one hand and granodiorite/tuff on the other hand, the observed level of sorption is estimated as reasonable.

It can be seen that the data by Allard et al. (1978; 1979b) are fairly consistent with other data for Th sorption on roughly similar substrates in the presence of non-inert solutions.

The same holds for the data obtained with Np(IV): in comparison with the data for Th on similar substrates and with the data for Np(IV) on Kunigel-V1 by Baston et al.

(1997), the observed level of sorption is estimated as reasonable.

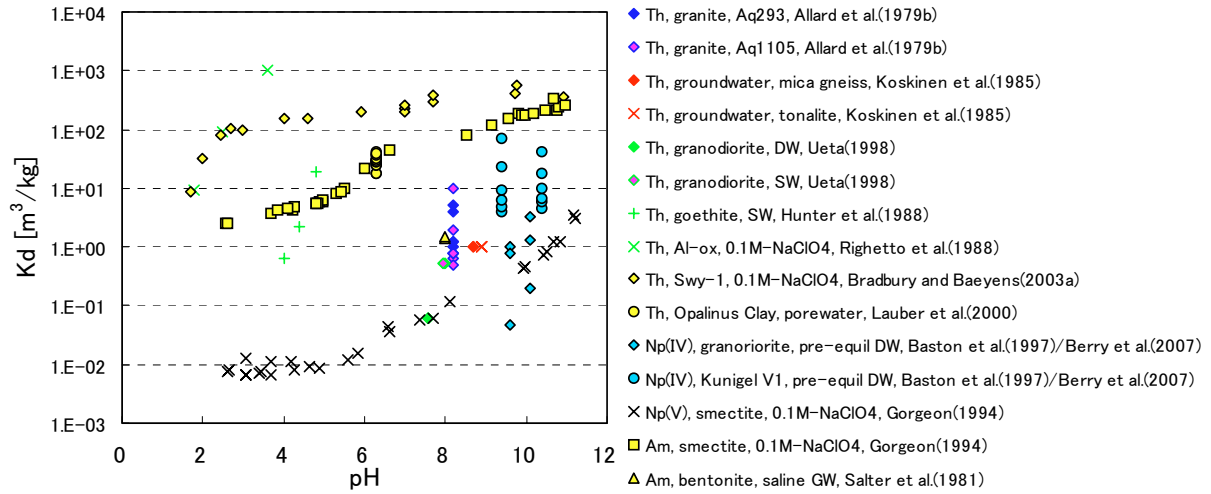


Figure 3.2.3 Overview of sorption data for Th and Np(IV) on metal oxide minerals, granitic rocks. For comparison, sorption data for Th and Np(IV), as well as for Am on various clays and clay minerals are also shown. DW = distilled water, GW = ground water.

4. Summary

The QA/classification of selected entries in the JAEA-SDB, focusing granite rocks which are related to reference systems in H12 PA and possible applications in the context of URL activities, and Fe-oxide/hydroxide, Al-oxide/hydroxide existing widely in geological environment, was done following the approach/guideline defined in our previous report. As a result, the reliability of 1,373 K_d values was evaluated and classified.

Based on the results of the third application of classification guideline to K_d data for granite systems, and Fe-oxide/hydroxide and Al-oxide/hydroxide systems in the chapter 3, some conclusions can be drawn:

- The classification guideline allows a suitable classification of the K_d values on the basis of the completeness of documented key information and the quality of the underlying experimental methods and conditions.
- The classification scheme made it possible to obtain quick overview of the available data, and to provide suitable access to the respective K_d values for the PA-related K_d -setting.
- Finally, JAEA-SDB including QA information should be repeatedly tested through the application to granite systems, and various rocks and geochemical conditions.

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The notation of reference is according to JAEA-SDB reference, considering relation with JAEA-SDB.

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Appendix

Summary tables for K_d classification

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I – Completeness of documentation and type of Kd		II – Technical and scientific quality of reported data																			III – Consistency		Operator	Data	Classification Guideline	
Rating ⇒ I-a: Yes/No, I-b: class 1–6		Checkpoints ⇒ level: A–D (numerical value: 3–0)/unreliable Rating ⇒ class1–6/unreliable																								
Datapoint	Reference	I-a.1	I-a.2	Rating I-a	Rating I-b	II-a	II-b	II-c	II-d	II-e	II-f	II-g	II-h	II-i	II-j	II-k	II-l	II-m	II-n	II-o	Rating II	comment/rating				
42188	Allard and Beall (1979)	yes	yes	unreliable (predicted datapoint)		solid phase	pH	redox condition	solution composition	temperature	S/W	sortive value	initial [RN]	phase separation	reaction time	agitation	RN loading	reaction vessels	error estimates	parameter variation						
42222	Allard et al. (1978)	yes	yes	yes (can be used)	class 1	C/D	D	A/B	unreliable		A/B	C/D	N.E.	A	C/D	C/D	C/D	C/D	C/D	D	D	unreliable N.E.	N.E.	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)
42223	Allard et al. (1978)	yes	yes	yes (can be used)	class 1	C/D	D	A/B	A/B		A/B	C/D	N.E.	A	C/D	C/D	C/D	C/D	C/D	D	D	N.E.	N.E.	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)
42259	Allard et al. (1979b)	yes	yes	yes (can be used)	class 1	C/D	C	A/B	A/B	A/B	C/D	C/D	A	C/D	A/B	A/B	C/D	C/D	D	C	class 3	consistent with independent data	S. Kunze/M. Ochs, BMG	May 2009	Revision 4b (May 19, 2005)	
42260	Allard et al. (1979b)	yes	yes	yes (can be used)	class 1	C/D	C	A/B	A/B	A/B	C/D	C/D	A	C/D	A/B	A/B	C/D	C/D	D	C	class 3	consistent with independent data	S. Kunze/M. Ochs, BMG	May 2009	Revision 4b (May 19, 2005)	
42261	Allard et al. (1979b)	yes	yes	yes (can be used)	class 1	C/D	C	A/B	A/B	A/B	C/D	C/D	A	C/D	A/B	A/B					unreliable		S. Kunze/M. Ochs, BMG	May 2009	Revision 4b (May 19, 2005)	
42262	Allard et al. (1979b)	yes	yes	yes (can be used)	class 1	C/D	C	A/B	A/B	A/B	C/D	C/D	A	C/D	A/B	A/B	C/D	C/D	D	C	class 3	consistent with independent data	S. Kunze/M. Ochs, BMG	May 2009	Revision 4b (May 19, 2005)	
42263	Allard et al. (1979b)	yes	yes	yes (can be used)	class 1	C/D	C	A/B	A/B	A/B	C/D	C/D	A	C/D	A/B	A/B	C/D	C/D	D	C	class 3	consistent with independent data	S. Kunze/M. Ochs, BMG	May 2009	Revision 4b (May 19, 2005)	
42264	Allard et al. (1979b)	yes	yes	yes (can be used)	class 1	C/D	C	A/B	A/B	A/B	C/D	C/D	A	C/D	A/B	A/B	C/D	C/D	D	C	class 3	consistent with independent data	S. Kunze/M. Ochs, BMG	May 2009	Revision 4b (May 19, 2005)	
42525	Allard et al. (1980)	yes	update SDB	yes (can be used)	class 5	A	A	A/B	A/B	A/B	A/B	N.E.	A	C/D	C/D	C/D	C/D	C/D	D	D	N.E.	N.E.	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
42526	Allard et al. (1980)	yes	update SDB	yes (can be used)	class 5	A	A	A/B	A/B	A/B	A/B	N.E.	A	C/D	C/D	C/D	C/D	C/D	D	D	N.E.	N.E.	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
42527	Allard et al. (1980)	yes	update SDB	yes (can be used)	class 5	A	A	A/B	A/B	A/B	A/B	N.E.	A	C/D	C/D	C/D	C/D	C/D	D	D	N.E.	N.E.	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
42528	Allard et al. (1980)	yes	update SDB	yes (can be used)	class 5	A	A	A/B	A/B	A/B	A/B	N.E.	A	C/D	C/D	C/D	C/D	C/D	D	D	N.E.	N.E.	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
44233	Barney and Anderson (1979)	yes	no	can be used tentatively	class 1	C/D	B	A/B	unreliable												unreliable	N.E.	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
44234	Barney and Anderson (1979)	yes	no	can be used tentatively	class 1	C/D	B	A/B	unreliable												unreliable	N.E.	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
44235	Barney and Anderson (1979)	yes	no	can be used tentatively	class 1	C/D	B	A/B	unreliable												unreliable	N.E.	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
44236	Barney and Anderson (1979)	yes	no	can be used tentatively	class 1	C/D	B	A/B	unreliable												unreliable	N.E.	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
44237	Barney and Anderson (1979)	yes	no	can be used tentatively	class 1	C/D	B	A/B	unreliable												unreliable	N.E.	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
44319	Barney and Brown (1979)	yes	no	can be used tentatively	class 1	C/D			unreliable												unreliable	N.E.	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
44320	Barney and Brown (1979)	yes	no	can be used tentatively	class 1	C/D			unreliable												unreliable	N.E.	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
44321	Barney and Brown (1979)	yes	no	can be used tentatively	class 1	C/D			unreliable												unreliable	N.E.	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
65946	Baston et al.(1998)	Yes	Yes	yes (can be used)	class 1	A)	A)	A/B)	A/B)	A/B)	A/B)	B)	B)	A)	C/D)	A/B)	C/D)	A)	A)	D)	class 2		T. Suyama/Y. Tachi(JAEA)	June 2008	Revision 4b (May 19, 2005)	
65947	Baston et al.(1998)	Yes	Yes	yes (can be used)	class 1	A)	A)	A/B)	A/B)	A/B)	A/B)	B)	B)	A)	C/D)	A/B)	C/D)	A)	A)	D)	class 2		T. Suyama/Y. Tachi(JAEA)	June 2008	Revision 4b (May 19, 2005)	
65948	Baston et al.(1998)	Yes	Yes	yes (can be used)	class 1	A)	A)	A/B)	A/B)	A/B)	A/B)	C/D)	B)	A)	C/D)	A/B)	C/D)	A)	A)	D)	class 2		T. Suyama/Y. Tachi(JAEA)	June 2008	Revision 4b (May 19, 2005)	
65949	Baston et al.(1998)	Yes	Yes	yes (can be used)	class 1	A)	A)	A/B)	A/B)	A/B)	A/B)	C/D)	B)	A)	C/D)	A/B)	C/D)	A)	A)	D)	class 2		T. Suyama/Y. Tachi(JAEA)	June 2008	Revision 4b (May 19, 2005)	
65950	Baston et al.(1998)	Yes	Yes	yes (can be used)	class 1	A)	A)	A/B)	A/B)	A/B)	A/B)	C/D)	B)	A)	C/D)	A/B)	C/D)	A)	A)	D)	class 2		T. Suyama/Y. Tachi(JAEA)	June 2008	Revision 4b (May 19, 2005)	
65951	Baston et al.(1998)	Yes	Yes	yes (can be used)	class 1	A)	A)	A/B)	A/B)	A/B)	A/B)	C/D)	B)	A)	C/D)	A/B)	C/D)	A)	A)	D)	class 2		T. Suyama/Y. Tachi(JAEA)	June 2008	Revision 4b (May 19, 2005)	
46906	Baston et al. (1999)	yes	yes	yes (can be used)	class 1	C/D	A	C/D	A/B	A/B	A/B	B	A	unreliable	C/D	A/B	C/D	A	C	D	unreliable	N.E.	S. Kunze/M. Ochs, BMG	February 2008	Revision 4b (May 19, 2005)	
46907	Baston et al. (1999)	yes	yes	yes (can be used)	class 1	C/D	A	C/D	A/B	A/B	A/B	B	A	unreliable	C/D	A/B	C/D	A	C	D	unreliable	N.E.	S. Kunze/M. Ochs, BMG	February 2008	Revision 4b (May 19, 2005)	
46908	Baston et al. (1999)	yes	yes	yes (can be used)	class 1	C/D	A	C/D	A/B	A/B	A/B	C/D	A	B	C/D	A/B	C/D	A	C	D	unreliable	consistent with independent data	S. Kunze/M. Ochs, BMG	February 2008	Revision 4b (May 19, 2005)	
46909	Baston et al. (1999)	yes	yes	yes (can be used)	class 1	C/D	A	C/D	A/B	A/B	A/B	C/D	A	unreliable	C/D	A/B	C/D	A	C	D	unreliable		S. Kunze/M. Ochs, BMG	February 2008	Revision 4b (May 19, 2005)	
46910	Baston et al. (1999)	yes	yes	yes (can be used)	class 1	C/D	A	C/D	A/B	A/B	A/B	C/D	A	unreliable	C/D	A/B	C/D	A	C	D	unreliable		S. Kunze/M. Ochs, BMG	February 2008	Revision 4b (May 19, 2005)	
46911	Baston et al. (1999)	yes	yes	yes (can be used)	class 1	C/D	A	C/D	A/B	A/B	A/B	C/D	A	B	C/D	A/B	C/D	A	C	D	unreliable	consistent with independent data	S. Kunze/M. Ochs, BMG	February 2008	Revision 4b (May 19, 2005)	
49978	Daniels et al. (1981)	yes	no (update SDB)	yes (can be used)	class 1	C/D	A	A/B	unreliable												unreliable	N.E.	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
49979	Daniels et al. (1981)	yes	no (update SDB)	yes (can be used)	class 1	C/D	A	A/B	unreliable												unreliable	N.E.	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
49980	Daniels et al. (1981)	yes	no (update SDB)	yes (can be used)	class 1	C/D	A	A/B	unreliable												unreliable	N.E.	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
49981	Daniels et al. (1981)	yes	no (update SDB)	yes (can be used)	class 1	C/D	A	A/B	unreliable												unreliable	N.E.	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
49982	Daniels et al. (1981)	yes	no (update SDB)	yes (can be used)	class 1	C/D	A	A/B	unreliable												unreliable	N.E.	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
49983	Daniels et al. (1981)	yes	no (update SDB)	yes (can be used)	class 1	C/D	A	A/B	unreliable												unreliable	N.E.	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
49984	Daniels et al. (1981)	yes	no (update SDB)	yes (can be used)	class 1	C/D	A	A/B	unreliable												unreliable	N.E.	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
49985	Daniels et al. (1981)	yes	no (update SDB)	yes (can be used)	class 1	C/D	A	A/B	unreliable												unreliable	N.E.	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
49986	Daniels et al. (1981)	yes	no (update SDB)	yes (can be used)	class 1	C/D	A	A/B	unreliable												unreliable	N.E.	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
49987	Daniels et al. (1981)	yes	no (update SDB)	yes (can be used)	class 1	C/D	A	A/B	unreliable												unreliable	N.E.	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
49988	Daniels et al. (1981)	yes	no (update SDB)	yes (can be used)	class 1	C/D	A	A/B	unreliable												unreliable	N.E.	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
49989	Daniels et al. (1981)	yes	no (update SDB)	yes (can be used)	class 1	C/D	A	A/B	unreliable												unreliable	N.E.	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
49990	Daniels et al. (1981)	yes	no (update SDB)	yes (can be used)	class 1	C/D	A	A/B	unreliable												unreliable	N.E.	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
49991	Daniels et al. (1981)	yes	no (update SDB)	yes (can be used)	class 1	C/D	A	A/B	unreliable												unreliable	N.E.	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
49992	Daniels et al. (1981)	yes	no (update SDB)	yes (can be used)	class 1	C/D	A	A/B	unreliable												unreliable	N.E.	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
49993	Daniels et al. (1981)	yes	no (update SDB)	yes (can be used)	class 1	C/D	A	A/B	unreliable												unreliable	N.E.	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
49994	Daniels et al. (1981)	yes	no (update SDB)	yes (can be used)	class 1	C/D	A	A/B	unreliable												unreliable	N.E.	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
49995	Daniels et al. (1981)	yes	no (update SDB)	yes (can be used)	class 1	C/D	A	A/B	unreliable												unreliable	N.E.	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
49996	Daniels et al. (1981)	yes	no (update SDB)	yes (can be used)	class 1	C/D	A	A/B	unreliable												unreliable	N.E.	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
49997	Daniels et al. (1981)	yes	no (update SDB)	yes (can be used)	class 1	C/D	A	A/B	unreliable												unreliable	N.E.	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
49998	Daniels et al. (1981)	yes	no (update SDB)	yes (can be used)	class 1	C/D	A	A/B	unreliable												unreliable	N.E.	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
49999	Daniels et al. (1981)	yes	no (update SDB)	yes (can be used)	class 1	C/D	A	A/B	unreliable												unreliable	N.E.	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
50000	Daniels et al. (1981)	yes	no (update SDB)	yes (can be used)	class 1	C/D	A	A/B	unreliable												unreliable	N.E.	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
50001	Daniels et al. (1981)	yes	no (update SDB)	yes (can be used)	class 1	C/D	A	A/B	unreliable												unreliable	N.E.	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
50897	Erdal et al. (1979c)	yes	yes	yes (can be used)	class 1	B	A	A/B	A/B	A/B	C/D	C/D	A	B	unreliable						unreliable	N.E.	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
50898	Erdal et al. (1979c)	yes	yes	yes (can be used)	class 1	B	A	A/B	A/B	A/B	C/D	C/D	A	B	unreliable						unreliable	N.E.	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
50899	Erdal et al. (1979c)	yes	yes	yes (can be used)	class 1	B	A	A/B	A/B	A/B	C/D	C/D	A	B	unreliable						unreliable	N.E.	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
50900	Erdal et al. (1979c)	yes	yes	yes (can be used)	class 1	B	A	A/B	A/B	A/B	C/D	C/D	A	B	unreliable						unreliable	N.E.	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
50901	Erdal et al. (1979c)	yes	yes	yes (can be used)	class 1	B	A	A/B	A/B	A/B	C/D	C/D	A													

An		I – Completeness of documentation and type of Kd										II – Technical and scientific quality of reported data														III – Consistency		Operator	Data	Classification Guideline
		Rating ⇒ I-a: Yes/No, I-b: class 1–6										Checkpoints ⇒ level: A–D (numerical value: 3–0)/unreliable Rating ⇒ class1–6/unreliable																		
Datapoint	Reference	I-a.1	I-a.2	Rating I-a	Rating I-b	II-a solid phase	II-b pH	II-c redox condition	II-d solution composition	II-e temperature	II-f S/W	II-g sorptive value	II-h initial [RN]	II-i phase separation	II-j reaction time	II-k agitation	II-l RN loading	II-m reaction vessels	II-n error estimates	II-o parameter variation	Rating II	comment/rating								
56797	Nakayama et al. (1986)	yes	yes	yes (can be used)	class 1	C/D	B	A/B	unreliable												unreliable	N.E.	S. Kunze/M. Ochs, BMG	March 2008	Revision 4b (May 19, 2005)					
56798	Nakayama et al. (1986)	yes	yes	yes (can be used)	class 1	C/D	B	A/B	unreliable												unreliable	N.E.	S. Kunze/M. Ochs, BMG	March 2008	Revision 4b (May 19, 2005)					
56799	Nakayama et al. (1986)	yes	yes	yes (can be used)	class 1	C/D	B	A/B	unreliable												unreliable	N.E.	S. Kunze/M. Ochs, BMG	March 2008	Revision 4b (May 19, 2005)					
56800	Nakayama et al. (1986)	yes	yes	yes (can be used)	class 1	C/D	B	A/B	unreliable												unreliable	N.E.	S. Kunze/M. Ochs, BMG	March 2008	Revision 4b (May 19, 2005)					
56801	Nakayama et al. (1986)	yes	yes	yes (can be used)	class 1	C/D	B	A/B	unreliable												unreliable	N.E.	S. Kunze/M. Ochs, BMG	March 2008	Revision 4b (May 19, 2005)					
56802	Nakayama et al. (1986)	yes	yes	yes (can be used)	class 1	C/D	B	A/B	unreliable												unreliable	N.E.	S. Kunze/M. Ochs, BMG	March 2008	Revision 4b (May 19, 2005)					
56803	Nakayama et al. (1986)	yes	yes	yes (can be used)	class 1	C/D	B	A/B	unreliable												unreliable	N.E.	S. Kunze/M. Ochs, BMG	March 2008	Revision 4b (May 19, 2005)					
56804	Nakayama et al. (1986)	yes	yes	yes (can be used)	class 1	C/D	B	A/B	unreliable												unreliable	N.E.	S. Kunze/M. Ochs, BMG	March 2008	Revision 4b (May 19, 2005)					
56805	Nakayama et al. (1986)	yes	yes	yes (can be used)	class 1	C/D	B	A/B	unreliable												unreliable	N.E.	S. Kunze/M. Ochs, BMG	March 2008	Revision 4b (May 19, 2005)					
56806	Nakayama et al. (1986)	yes	yes	yes (can be used)	class 1	C/D	B	A/B	unreliable												unreliable	N.E.	S. Kunze/M. Ochs, BMG	March 2008	Revision 4b (May 19, 2005)					
57264	Pinnioja et al. (1984)	yes	yes	yes (can be used)	class 1	A	C	A/B	A/B	A/B	C/D	C/D	A	C/D	C/D	A/B	C/D	C/D	A	D	class 3	N.E.	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)					
57265	Pinnioja et al. (1984)	yes	yes	yes (can be used)	class 1	A	C	A/B	A/B	A/B	A/B	C/D	A	C/D	C/D	A/B	C/D	C/D	A	D	class 3	N.E.	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)					
59374	Suksi et al. (1987)			cannot be used (no batch Kd)																	unreliable	N.E.	S. Kunze/M. Ochs, BMG	April 2009	Revision 4b (May 19, 2005)					
59375	Suksi et al. (1987)			cannot be used (no batch Kd)																	unreliable	N.E.	S. Kunze/M. Ochs, BMG	April 2009	Revision 4b (May 19, 2005)					
42201	Allard and Beall (1979)	yes	yes	yes (can be used)	class 5	B	B	A/B	A/B	A/B	C/D	A	A	C/D	C/D	C/D	C/D	C/D	D	D	class 3	not conclusive, may not be representative	S. Kunze/M. Ochs, BMG	November 2007	Revision 4b (May 19, 2005)					
42205	Allard and Beall (1979)	yes	yes	yes (can be used)	class 5	B	B	A/B	A/B	A/B	C/D	B	A	C/D	C/D	C/D	C/D	C/D	D	D	class 3	not conclusive, may not be representative	S. Kunze/M. Ochs, BMG	November 2007	Revision 4b (May 19, 2005)					
42207	Allard and Beall (1979)	yes	yes	yes (can be used)	class 5	A	B	A/B	A/B	A/B	A/B	B	A	C/D	C/D	C/D	C/D	C/D	D	D	class 3	not conclusive, may not be representative	S. Kunze/M. Ochs, BMG	November 2007	Revision 4b (May 19, 2005)					
42210	Allard and Beall (1979)	yes	yes	yes (can be used)	class 5	A	B	A/B	A/B	A/B	A/B	B	A	C/D	C/D	C/D	C/D	C/D	D	D	class 3	not conclusive, may not be representative	S. Kunze/M. Ochs, BMG	November 2007	Revision 4b (May 19, 2005)					
50234	Degueldre et al. (1994)	yes	yes	yes (can be used)	class 5	B	A	A/B	A/B	C/D	C/D	A	A/B	C/D	C/D	A/B	B	C/D	A	B	class 2	consistent with independent data	S. Kunze/M. Ochs, BMG	November 2007	Revision 4b (May 19, 2005)					
50235	Degueldre et al. (1994)	yes	yes	yes (can be used)	class 5	B	A	A/B	A/B	C/D	C/D	C/D	A/B	C/D	C/D	A/B	B	C/D	A	B	class 2	consistent with independent data	S. Kunze/M. Ochs, BMG	November 2007	Revision 4b (May 19, 2005)					
53056	Higgo et al. (1983)	yes	yes	yes (can be used)	class 1	C/D	B	A/B	C/D	A/B	C/D	C/D	B	C/D	C/D	A/B	C/D	B	C	D	class 4	consistent with independent data	S. Kunze/M. Ochs, BMG	November 2007	Revision 4b (May 19, 2005)					
53057	Higgo et al. (1983)	yes	yes	yes (can be used)	class 1	C/D	B	A/B	C/D	A/B	C/D	C/D	B	C/D	C/D	A/B	C/D	B	C	D	class 4	consistent with independent data	S. Kunze/M. Ochs, BMG	November 2007	Revision 4b (May 19, 2005)					
53058	Higgo et al. (1983)	yes	yes	yes (can be used)	class 1	C/D	B	A/B	C/D	A/B	C/D	C/D	B	C/D	C/D	A/B	C/D	B	C	D	class 4	consistent with independent data	S. Kunze/M. Ochs, BMG	November 2007	Revision 4b (May 19, 2005)					
53059	Higgo et al. (1983)	yes	yes	yes (can be used)	class 1	C/D	B	A/B	C/D	A/B	C/D	C/D	B	C/D	C/D	A/B	C/D	B	C	D	class 4	consistent with independent data	S. Kunze/M. Ochs, BMG	November 2007	Revision 4b (May 19, 2005)					
53060	Higgo et al. (1983)	yes	yes	yes (can be used)	class 1	C/D	B	A/B	C/D	A/B	C/D	C/D	B	C/D	C/D	A/B	C/D	B	C	D	class 4	consistent with independent data	S. Kunze/M. Ochs, BMG	November 2007	Revision 4b (May 19, 2005)					
58542	Righetto et al. (1988)	yes	yes	yes (can be used)	class 4	A	A	A/B	A/B	C/D	C/D	A	A	B	A/B	A/B	B	B	D	C	class 2	consistent with independent data	S. Kunze/M. Ochs, BMG	November 2007	Revision 4b (May 19, 2005)					
58543	Righetto et al. (1988)	yes	yes	yes (can be used)	class 4	A	A	A/B	A/B	C/D	C/D	A	A	B	A/B	A/B	B	B	D	C	class 2	consistent with independent data	S. Kunze/M. Ochs, BMG	November 2007	Revision 4b (May 19, 2005)					
58544	Righetto et al. (1988)	yes	yes	yes (can be used)	class 4	A	A	A/B	A/B	C/D	C/D	B	A	B	A/B	A/B	B	B	D	C	class 2	consistent with independent data	S. Kunze/M. Ochs, BMG	November 2007	Revision 4b (May 19, 2005)					

Cs	I – Completeness of documentation and type of Kd	II – Technical and scientific quality of reported data																				III – Consistency	Operator	Data	Classification Guideline
	Rating ⇒ I-a: Yes/No, I-b: class 1-6	Checkpoints ⇒ level: A-D (numerical value: 3-0)/unreliable Rating ⇒ class1-6/unreliable																							
Datapoint	Reference	I-a.1	I-a.2	Rating I-a	Rating I-b	II-a solid phase	II-b pH	II-c redox condition	II-d solution composition	II-e temperature	II-f S/W	II-g sorptive value	II-h initial [RN]	II-i phase separation	II-j reaction time	II-k agitation	II-l RN loading	II-m reaction vessels	II-n error estimates	II-o parameter variation	Rating II	comment/rating			
42301	Allard et al. (1979b)	yes	yes	yes (can be used)	class 1	C/D	C	A/B	C/D	A/B	C/D	A	A	A	A/B	C/D	B	C/D	D	B	class 3	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
42302	Allard et al. (1979b)	yes	yes	yes (can be used)	class 1	C/D	C	A/B	C/D	A/B	C/D	A	A	A	A/B	C/D	B	C/D	D	B	class 3	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
42303	Allard et al. (1979b)	yes	yes	yes (can be used)	class 1	C/D	C	A/B	C/D	A/B	C/D	B	A	A	A/B	C/D	B	C/D	D	B	class 3	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
42304	Allard et al. (1979b)	yes	yes	yes (can be used)	class 1	C/D	C	A/B	C/D	A/B	C/D	B	A	A	A/B	C/D	B	C/D	D	B	class 3	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
42305	Allard et al. (1979b)	yes	yes	yes (can be used)	class 1	C/D	C	A/B	C/D	A/B	C/D	A	A	A	A/B	C/D	B	C/D	D	B	class 3	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
42306	Allard et al. (1979b)	yes	yes	yes (can be used)	class 1	C/D	C	A/B	C/D	A/B	C/D	A	A	A	A/B	C/D	B	C/D	D	B	class 3	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
42307	Allard et al. (1979b)	yes	yes	yes (can be used)	class 1	C/D	C	A/B	C/D	A/B	C/D	A	A	A	A/B	C/D	B	C/D	D	B	class 3	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
42308	Allard et al. (1979b)	yes	yes	yes (can be used)	class 1	C/D	C	A/B	C/D	A/B	C/D	A	A	A	A/B	C/D	B	C/D	D	B	class 3	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
42309	Allard et al. (1979b)	yes	yes	yes (can be used)	class 1	C/D	C	A/B	C/D	A/B	C/D	A	A	A	A/B	C/D	B	C/D	D	B	class 3	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
42310	Allard et al. (1979b)	yes	yes	yes (can be used)	class 1	C/D	C	A/B	C/D	A/B	C/D	A	A	A	A/B	C/D	B	C/D	D	B	class 3	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
42311	Allard et al. (1979b)	yes	yes	yes (can be used)	class 1	C/D	C	A/B	C/D	A/B	C/D	A	A	A	A/B	C/D	B	C/D	D	B	class 3	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
42312	Allard et al. (1979b)	yes	yes	yes (can be used)	class 1	C/D	C	A/B	C/D	A/B	C/D	A	A	A	A/B	C/D	B	C/D	D	B	class 3	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
43989	Andersson et al. (1983b)	yes	yes	yes (can be used)	class 1	C/D	unreliable														unreliable	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
43990	Andersson et al. (1983b)	yes	yes	yes (can be used)	class 1	C/D	unreliable														unreliable	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
43991	Andersson et al. (1983b)	yes	no	no (can not be used)																	unreliable	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
43992	Andersson et al. (1983b)	yes	no	no (can not be used)																	unreliable	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
43993	Andersson et al. (1983b)	yes	yes	yes (can be used)	class 1	C/D	unreliable														unreliable	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
43994	Andersson et al. (1983b)	yes	yes	yes (can be used)																	unreliable	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
43995	Andersson et al. (1983b)	yes	no	no (can not be used)																	unreliable	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
43996	Andersson et al. (1983b)	yes	yes	yes (can be used)	class 1	C/D	unreliable														unreliable	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
43997	Andersson et al. (1983b)	yes	no	no (can not be used)																	unreliable	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
43998	Andersson et al. (1983b)	yes	yes	yes (can be used)	class 1	C/D	unreliable														unreliable	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
43999	Andersson et al. (1983b)	yes	no	no (can not be used)																	unreliable	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
44000	Andersson et al. (1983b)	yes	yes	yes (can be used)	class 1	C/D	unreliable														unreliable	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
44001	Andersson et al. (1983b)	yes	no	no (can not be used)																	unreliable	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
44002	Andersson et al. (1983b)	yes	yes	yes (can be used)	class 1	C/D	unreliable														unreliable	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
44003	Andersson et al. (1983b)	yes	yes	yes (can be used)	class 1	C/D	unreliable														unreliable	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
44004	Andersson et al. (1983b)	yes	no	no (can not be used)																	unreliable	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
44005	Andersson et al. (1983b)	yes	no	no (can not be used)																	unreliable	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
44006	Andersson et al. (1983b)	yes	yes	yes (can be used)	class 1	C/D	unreliable														unreliable	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
44007	Andersson et al. (1983b)	yes	yes	yes (can be used)	class 1	C/D	D	A/B	C/D	A/B	C/D	A	A	C/D	A/B	C/D	C/D	A	D	—	unreliable	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
44008	Andersson et al. (1983b)	yes	yes	yes (can be used)	class 1	C/D	D	A/B	C/D	A/B	C/D	C/D	A	C/D	A/B	C/D	C/D	A	D	—	class 5	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
44009	Andersson et al. (1983b)	yes	yes	yes (can be used)	class 1	C/D	D	A/B	C/D	A/B	C/D	C/D	A	C/D	A/B	C/D	C/D	A	D	—	class 5	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
44010	Andersson et al. (1983b)	yes	yes	yes (can be used)	class 1	C/D	D	A/B	C/D	A/B	C/D	C/D	A	C/D	A/B	C/D	C/D	A	D	—	class 5	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
44250	Barney and Anderson (1979)	yes	no	yes (can be used)	class 1	C/D	B	A/B	unreliable												unreliable	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
44251	Barney and Anderson (1979)	yes	no	yes (can be used)	class 1	C/D	B	A/B	unreliable												unreliable	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
44252	Barney and Anderson (1979)	yes	no	yes (can be used)	class 1	C/D	B	A/B	unreliable												unreliable	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
44253	Barney and Anderson (1979)	yes	no	yes (can be used)	class 1	C/D	B	A/B	unreliable												unreliable	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
44254	Barney and Anderson (1979)	yes	no	yes (can be used)	class 1	C/D	B	A/B	unreliable												unreliable	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
44255	Barney and Anderson (1979)	yes	no	yes (can be used)	class 1	C/D	B	A/B	unreliable												unreliable	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
44328	Barney and Brown (1979)	yes	no	yes (can be used)	class 1	C/D	B	A/B	unreliable												unreliable	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
44329	Barney and Brown (1979)	yes	no	yes (can be used)	class 1	C/D	B	A/B	unreliable												unreliable	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
44330	Barney and Brown (1979)	yes	no	yes (can be used)	class 1	C/D	B	A/B	unreliable												unreliable	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
47310	Benischek et al. (1992a)	yes	no																		unreliable	S. Kunze/M. Ochs, BMG	March 2009	Revision 4b (May 19, 2005)	
47311	Benischek et al. (1992a)	yes	no																		unreliable	S. Kunze/M. Ochs, BMG	March 2009	Revision 4b (May 19, 2005)	
47312	Benischek et al. (1992a)	yes	no																		unreliable	S. Kunze/M. Ochs, BMG	March 2009	Revision 4b (May 19, 2005)	
47313	Benischek et al. (1992a)	yes	no																		unreliable	S. Kunze/M. Ochs, BMG	March 2009	Revision 4b (May 19, 2005)	
47314	Benischek et al. (1992a)	yes	no																		unreliable	S. Kunze/M. Ochs, BMG	March 2009	Revision 4b (May 19, 2005)	
47315	Benischek et al. (1992a)	yes	no																		unreliable	S. Kunze/M. Ochs, BMG	March 2009	Revision 4b (May 19, 2005)	
47316	Benischek et al. (1992a)	yes	no																		unreliable	S. Kunze/M. Ochs, BMG	March 2009	Revision 4b (May 19, 2005)	
47317	Benischek et al. (1992a)	yes	no																		unreliable	S. Kunze/M. Ochs, BMG	March 2009	Revision 4b (May 19, 2005)	
47318	Benischek et al. (1992a)	yes	no																		unreliable	S. Kunze/M. Ochs, BMG	March 2009	Revision 4b (May 19, 2005)	
47319	Benischek et al. (1992a)	yes	no																		unreliable	S. Kunze/M. Ochs, BMG	March 2009	Revision 4b (May 19, 2005)	
47320	Benischek et al. (1992a)	yes	no																		unreliable	S. Kunze/M. Ochs, BMG	March 2009	Revision 4b (May 19, 2005)	
47321	Benischek et al. (1992a)	yes	no																		unreliable	S. Kunze/M. Ochs, BMG	March 2009	Revision 4b (May 19, 2005)	
47322	Benischek et al. (1992a)	yes	no																		unreliable	S. Kunze/M. Ochs, BMG	March 2009	Revision 4b (May 19, 2005)	
47323	Benischek et al. (1992a)	yes	no																		unreliable	S. Kunze/M. Ochs, BMG	March 2009	Revision 4b (May 19, 2005)	
47324	Benischek et al. (1992a)	yes	no																		unreliable	S. Kunze/M. Ochs, BMG	March 2009	Revision 4b (May 19, 2005)	
47325	Benischek et al. (1992a)	yes	no																		unreliable	S. Kunze/M. Ochs, BMG	March 2009	Revision 4b (May 19, 2005)	
47326	Benischek et al. (1992a)	yes	no																		unreliable	S. Kunze/M. Ochs, BMG	March 2009	Revision 4b (May 19, 2005)	
47327	Benischek et al. (1992a)	yes	no																		unreliable	S. Kunze/M. Ochs, BMG	March 2009	Revision 4b (May 19, 2005)	
47328	Benischek et al. (1992a)	yes	no																		unreliable	S. Kunze/M. Ochs, BMG	March 2009	Revision 4b (May 19, 2005)	
47329	Benischek et al. (1992a)	yes	no																		unreliable	S. Kunze/M. Ochs, BMG	March 2009	Revision 4b (May 19, 2005)	
47330	Benischek et al. (1992a)	yes	no																		unreliable	S. Kunze/M. Ochs, BMG	March 2009	Revision 4b (May 19, 2005)	
47331	Benischek et al. (1992a)	yes	no																		unreliable	S. Kunze/M. Ochs, BMG	March 2009	Revision 4b (May 19, 2005)	
47332	Benischek et al. (1992a)	yes	no																		unreliable	S. Kunze/M. Ochs, BMG	March 2009	Revision 4b (May 19, 2005)	
47333	Benischek et al. (1992a)	yes	no																		unreliable	S. Kunze/M. Ochs, BMG	March 2009	Revision 4b (May 19, 2005)	
47334	Benischek et al. (199																								

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I – Completeness of documentation and type of Kd				II – Technical and scientific quality of reported data																	III – Consistency		Operator	Data	Classification Guideline
Rating ⇒ I-a: Yes/No, I-b: class 1–6				Checkpoints ⇒ level: A–D (numerical value: 3–0)/unreliable Rating ⇒ class1–6/unreliable																					
Datapoint	Reference	I–a.1	I–a.2	Rating I–a	Rating I–b	II–a solid phase	II–b pH	II–c redox condition	II–d solution composition	II–e temperature	II–f S/W	II–g sorption value	II–h initial [RN]	II–i phase separation	II–j reaction time	II–k agitation	II–l RN loading	II–m reaction vessels	II–n error estimates	II–o parameter variation	Rating II	comment/rating			
62563	Byegard et al. (1998)	yes	no	no (can not be used)																	unreliable	M. Ochs, BMG	May 2009	Revision 4b (May 19, 2005)	
62564	Byegard et al. (1998)	yes	no	no (can not be used)																	unreliable	M. Ochs, BMG	May 2009	Revision 4b (May 19, 2005)	
62565	Byegard et al. (1998)	yes	no	no (can not be used)																	unreliable	M. Ochs, BMG	May 2009	Revision 4b (May 19, 2005)	
62566	Byegard et al. (1998)	yes	no	no (can not be used)																	unreliable	M. Ochs, BMG	May 2009	Revision 4b (May 19, 2005)	
62567	Byegard et al. (1998)	yes	no	no (can not be used)																	unreliable	M. Ochs, BMG	May 2009	Revision 4b (May 19, 2005)	
62568	Byegard et al. (1998)	yes	no	no (can not be used)																	unreliable	M. Ochs, BMG	May 2009	Revision 4b (May 19, 2005)	
62569	Byegard et al. (1998)	yes	no	no (can not be used)																	unreliable	M. Ochs, BMG	May 2009	Revision 4b (May 19, 2005)	
62570	Byegard et al. (1998)	yes	no	no (can not be used)																	unreliable	M. Ochs, BMG	May 2009	Revision 4b (May 19, 2005)	
62571	Byegard et al. (1998)	yes	no	no (can not be used)																	unreliable	M. Ochs, BMG	May 2009	Revision 4b (May 19, 2005)	
62572	Byegard et al. (1998)	yes	no	no (can not be used)																	unreliable	M. Ochs, BMG	May 2009	Revision 4b (May 19, 2005)	
62573	Byegard et al. (1998)	yes	no	no (can not be used)																	unreliable	M. Ochs, BMG	May 2009	Revision 4b (May 19, 2005)	
62586	Byegard et al. (1998)	yes	no	no (can not be used)																	unreliable	M. Ochs, BMG	May 2009	Revision 4b (May 19, 2005)	
62587	Byegard et al. (1998)	yes	no	no (can not be used)																	unreliable	M. Ochs, BMG	May 2009	Revision 4b (May 19, 2005)	
62588	Byegard et al. (1998)	yes	no	no (can not be used)																	unreliable	M. Ochs, BMG	May 2009	Revision 4b (May 19, 2005)	
62589	Byegard et al. (1998)	yes	no	no (can not be used)																	unreliable	M. Ochs, BMG	May 2009	Revision 4b (May 19, 2005)	
62590	Byegard et al. (1998)	yes	no	no (can not be used)																	unreliable	M. Ochs, BMG	May 2009	Revision 4b (May 19, 2005)	
62591	Byegard et al. (1998)	yes	no	no (can not be used)																	unreliable	M. Ochs, BMG	May 2009	Revision 4b (May 19, 2005)	
62592	Byegard et al. (1998)	yes	no	no (can not be used)																	unreliable	M. Ochs, BMG	May 2009	Revision 4b (May 19, 2005)	
62593	Byegard et al. (1998)	yes	no	no (can not be used)																	unreliable	M. Ochs, BMG	May 2009	Revision 4b (May 19, 2005)	
62594	Byegard et al. (1998)	yes	no	no (can not be used)																	unreliable	M. Ochs, BMG	May 2009	Revision 4b (May 19, 2005)	
62595	Byegard et al. (1998)	yes	no	no (can not be used)																	unreliable	M. Ochs, BMG	May 2009	Revision 4b (May 19, 2005)	
62596	Byegard et al. (1998)	yes	no	no (can not be used)																	unreliable	M. Ochs, BMG	May 2009	Revision 4b (May 19, 2005)	
62597	Byegard et al. (1998)	yes	no	no (can not be used)																	unreliable	M. Ochs, BMG	May 2009	Revision 4b (May 19, 2005)	
62598	Byegard et al. (1998)	yes	no	no (can not be used)																	unreliable	M. Ochs, BMG	May 2009	Revision 4b (May 19, 2005)	
62599	Byegard et al. (1998)	yes	no	no (can not be used)																	unreliable	M. Ochs, BMG	May 2009	Revision 4b (May 19, 2005)	
62600	Byegard et al. (1998)	yes	no	no (can not be used)																	unreliable	M. Ochs, BMG	May 2009	Revision 4b (May 19, 2005)	
62601	Byegard et al. (1998)	yes	no	no (can not be used)																	unreliable	M. Ochs, BMG	May 2009	Revision 4b (May 19, 2005)	
62602	Byegard et al. (1998)	yes	no	no (can not be used)																	unreliable	M. Ochs, BMG	May 2009	Revision 4b (May 19, 2005)	
62603	Byegard et al. (1998)	yes	no	no (can not be used)																	unreliable	M. Ochs, BMG	May 2009	Revision 4b (May 19, 2005)	
62616	Byegard et al. (1998)	yes	no	no (can not be used)																	unreliable	M. Ochs, BMG	May 2009	Revision 4b (May 19, 2005)	
62617	Byegard et al. (1998)	yes	no	no (can not be used)																	unreliable	M. Ochs, BMG	May 2009	Revision 4b (May 19, 2005)	
62618	Byegard et al. (1998)	yes	no	no (can not be used)																	unreliable	M. Ochs, BMG	May 2009	Revision 4b (May 19, 2005)	
62619	Byegard et al. (1998)	yes	no	no (can not be used)																	unreliable	M. Ochs, BMG	May 2009	Revision 4b (May 19, 2005)	
62620	Byegard et al. (1998)	yes	no	no (can not be used)																	unreliable	M. Ochs, BMG	May 2009	Revision 4b (May 19, 2005)	
62621	Byegard et al. (1998)	yes	no	no (can not be used)																	unreliable	M. Ochs, BMG	May 2009	Revision 4b (May 19, 2005)	
62622	Byegard et al. (1998)	yes	no	no (can not be used)																	unreliable	M. Ochs, BMG	May 2009	Revision 4b (May 19, 2005)	
62623	Byegard et al. (1998)	yes	no	no (can not be used)																	unreliable	M. Ochs, BMG	May 2009	Revision 4b (May 19, 2005)	
62624	Byegard et al. (1998)	yes	no	no (can not be used)																	unreliable	M. Ochs, BMG	May 2009	Revision 4b (May 19, 2005)	
62625	Byegard et al. (1998)	yes	no	no (can not be used)																	unreliable	M. Ochs, BMG	May 2009	Revision 4b (May 19, 2005)	
62626	Byegard et al. (1998)	yes	no	no (can not be used)																	unreliable	M. Ochs, BMG	May 2009	Revision 4b (May 19, 2005)	
62627	Byegard et al. (1998)	yes	no	no (can not be used)																	unreliable	M. Ochs, BMG	May 2009	Revision 4b (May 19, 2005)	
62628	Byegard et al. (1998)	yes	no	no (can not be used)																	unreliable	M. Ochs, BMG	May 2009	Revision 4b (May 19, 2005)	
62629	Byegard et al. (1998)	yes	no	no (can not be used)																	unreliable	M. Ochs, BMG	May 2009	Revision 4b (May 19, 2005)	
62630	Byegard et al. (1998)	yes	no	no (can not be used)																	unreliable	M. Ochs, BMG	May 2009	Revision 4b (May 19, 2005)	
62631	Byegard et al. (1998)	yes	no	no (can not be used)																	unreliable	M. Ochs, BMG	May 2009	Revision 4b (May 19, 2005)	
62632	Byegard et al. (1998)	yes	no	no (can not be used)																	unreliable	M. Ochs, BMG	May 2009	Revision 4b (May 19, 2005)	
62633	Byegard et al. (1998)	yes	no	no (can not be used)																	unreliable	M. Ochs, BMG	May 2009	Revision 4b (May 19, 2005)	
62634	Byegard et al. (1998)	yes	no	no (can not be used)																	unreliable	M. Ochs, BMG	May 2009	Revision 4b (May 19, 2005)	
62635	Byegard et al. (1998)	yes	no	no (can not be used)																	unreliable	M. Ochs, BMG	May 2009	Revision 4b (May 19, 2005)	
62636	Byegard et al. (1998)	yes	no	no (can not be used)																	unreliable	M. Ochs, BMG	May 2009	Revision 4b (May 19, 2005)	
50041	Daniels et al. (1981)	yes	no	yes (can be used)	class 1	B	D	A/B	C/D	C/D	C/D	C/D	A	B	unreliable						unreliable	S. Kunze, M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
50042	Daniels et al. (1981)	yes	no	yes (can be used)	class 1	B		A/B	C/D	A/B	C/D	B	A	C/D	unreliable						unreliable	S. Kunze, M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
50043	Daniels et al. (1981)	yes	no	yes (can be used)	class 1	B	C	A/B	C/D	A/B	C/D	B	A	C/D	unreliable						unreliable	S. Kunze, M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
50044	Daniels et al. (1981)	yes	no	yes (can be used)	class 1	B	A	A/B	C/D	A/B	C/D	B	unreliable								unreliable	S. Kunze, M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
50045	Daniels et al. (1981)	yes	no	yes (can be used)	class 1	B	A	A/B	C/D	A/B	C/D	B	unreliable	B	unreliable						unreliable	S. Kunze, M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
50046	Daniels et al. (1981)	yes	no	yes (can be used)	class 1	B	D	A/B	C/D	C/D	C/D	C/D	A		unreliable						unreliable	S. Kunze, M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
50047	Daniels et al. (1981)	yes	no	yes (can be used)	class 1	B	A	A/B	C/D	A/B	C/D	A	unreliable								unreliable	S. Kunze, M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
50048	Daniels et al. (1981)	yes	no	yes (can be used)	class 1	B	C	A/B	C/D	A/B	C/D	A		C/D	unreliable						unreliable	S. Kunze, M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
50049	Daniels et al. (1981)	yes	no	yes (can be used)	class 1	B	C	A/B	C/D	A/B	C/D	A	A	C/D	unreliable						unreliable	S. Kunze, M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
50050	Daniels et al. (1981)	yes	no	yes (can be used)	class 1	B	D	A/B	C/D	C/D	C/D	C/D	A	B	unreliable						unreliable	S. Kunze, M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
50051	Daniels et al. (1981)	yes	no	yes (can be used)	class 1	B	C	A/B	C/D	A/B	C/D	A	A	C/D	unreliable						unreliable	S. Kunze, M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
50052	Daniels et al. (1981)	yes	no	yes (can be used)	class 1	B	D	A/B	C/D	C/D	C/D	C/D	A	B	unreliable						unreliable	S. Kunze, M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
50053	Daniels et al. (1981)	yes	no	yes (can be used)	class 1	B	A	A/B	C/D	A/B	C/D	B	unreliable								unreliable	S. Kunze, M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
50054	Daniels et al. (1981)	yes	no	yes (can be used)	class 1	B		A/B	C/D	A/B	C/D	A		C/D	unreliable						unreliable	S. Kunze, M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
50055	Daniels et al. (1981)	yes	no	yes (can be used)	class 1	B	D	A/B	C/D	C/D	C/D	C/D	A	B	unreliable						unreliable	S. Kunze, M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
50056	Daniels et al. (1981)	yes	no	yes (can be used)	class 1	B	C	A/B	C/D	A/B	C/D	A	A	C/D	unreliable						unreliable	S. Kunze, M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
50057	Daniels et al. (1981)	yes	no	yes (can be used)	class 1	B	C	A/B	C/D	A/B	C/D	A	A	C/D	unreliable						unreliable	S. Kunze, M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
50058	Daniels et al. (1981)	yes	no	yes (can be used)	class 1	B	D	A/B	C/D	A/B	C/D	C/D	A	B	unreliable						unreliable	S. Kunze, M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
50059	Daniels et al. (1981)	yes	no	yes (can be used)	class 1	B	A	A/B	C/D	A/B	C/D	A	unreliable								unreliable	S. Kunze, M. Ochs, BMG	November 2008</		

Cs	I – Completeness of documentation and type of Kd				II – Technical and scientific quality of reported data																III – Consistency	Operator	Data	Classification Guideline	
	Rating ⇒ I-a: Yes/No, I-b: class 1-6				Checkpoints ⇒ level: A-D (numerical value: 3-0)/unreliable Rating ⇒ class1-6/unreliable																				
Datapoint	Reference	I-a.1	I-a.2	Rating I-a	Rating I-b	II-a	II-b	II-c	II-d	II-e	II-f	II-g	II-h	II-i	II-j	II-k	II-l	II-m	II-n	II-o	Rating II	comment/rating			
51756	Fujikawa and Fukui (1997)	yes	no	unreliable		solid phase															unreliable	S. Kunze/M. Ochs, BMG	October 2007	Revision 4b (May 19, 2005)	
51757	Fujikawa and Fukui (1997)	yes	no	unreliable																	unreliable	S. Kunze/M. Ochs, BMG	October 2007	Revision 4b (May 19, 2005)	
51758	Fujikawa and Fukui (1997)	yes	no	unreliable																	unreliable	S. Kunze/M. Ochs, BMG	October 2007	Revision 4b (May 19, 2005)	
51759	Fujikawa and Fukui (1997)	yes	no	unreliable																	unreliable	S. Kunze/M. Ochs, BMG	October 2007	Revision 4b (May 19, 2005)	
51760	Fujikawa and Fukui (1997)	yes	no	unreliable																	unreliable	S. Kunze/M. Ochs, BMG	October 2007	Revision 4b (May 19, 2005)	
51761	Fujikawa and Fukui (1997)	yes	no	unreliable																	unreliable	S. Kunze/M. Ochs, BMG	October 2007	Revision 4b (May 19, 2005)	
51762	Fujikawa and Fukui (1997)	yes	no	unreliable																	unreliable	S. Kunze/M. Ochs, BMG	October 2007	Revision 4b (May 19, 2005)	
53346	Huitti et al. (1998)	yes	no	yes (tentative)	class 1	B	A	A/B	A/B	A/B	C/D	A	A	D	A/B	A/B	A	B	A	B	class 2	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
53347	Huitti et al. (1998)	yes	no	yes (tentative)	class 1	B	A	A/B	A/B	A/B	C/D	A	A	D	A/B	A/B	A	B	A	B	class 2	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
53348	Huitti et al. (1998)	yes	no	yes (tentative)	class 1	B	A	A/B	A/B	A/B	C/D	A	A	D	A/B	A/B	A	B	A	B	class 2	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
53349	Huitti et al. (1998)	yes	no	yes (tentative)	class 1	B	A	A/B	A/B	A/B	C/D	A	A	D	A/B	A/B	A	B	A	B	class 2	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
53350	Huitti et al. (1998)	yes	no	yes (tentative)	class 1	B	A	A/B	A/B	A/B	C/D	A	A	D	A/B	A/B	A	B	A	B	class 2	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
53351	Huitti et al. (1998)	yes	no	yes (tentative)	class 1	B	A	A/B	A/B	A/B	C/D	A	A	D	A/B	A/B	A	B	A	B	class 2	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
53352	Huitti et al. (1998)	yes	no	yes (tentative)	class 1	B	A	A/B	A/B	A/B	C/D	A	A	D	A/B	A/B	A	B	A	B	class 2	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
53353	Huitti et al. (1998)	yes	no	yes (tentative)	class 1	B	A	A/B	A/B	A/B	C/D	A	A	D	A/B	A/B	A	B	A	B	class 2	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
53354	Huitti et al. (1998)	yes	no	yes (tentative)	class 1	B	A	A/B	A/B	A/B	C/D	A	A	D	A/B	A/B	A	B	A	B	class 2	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
53355	Huitti et al. (1998)	yes	no	yes (tentative)	class 1	B	A	A/B	A/B	A/B	C/D	A	A	D	A/B	A/B	A	B	A	B	class 2	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
53356	Huitti et al. (1998)	yes	no	yes (tentative)	class 1	B	A	A/B	A/B	A/B	C/D	A	A	D	A/B	A/B	A	B	A	B	class 2	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
53357	Huitti et al. (1998)	yes	no	yes (tentative)	class 1	B	A	A/B	A/B	A/B	C/D	A	A	D	A/B	A/B	A	B	A	B	class 2	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
53358	Huitti et al. (1998)	yes	no	yes (tentative)	class 1	B	A	A/B	A/B	A/B	C/D	A	A	D	A/B	A/B	A	B	A	B	class 2	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
53359	Huitti et al. (1998)	yes	no	yes (tentative)	class 1	B	A	A/B	A/B	A/B	C/D	A	A	D	A/B	A/B	A	B	A	B	class 2	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
53360	Huitti et al. (1998)	yes	no	yes (tentative)	class 1	B	A	A/B	A/B	A/B	C/D	A	A	D	A/B	A/B	A	B	A	B	class 2	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
53361	Huitti et al. (1998)	yes	no	yes (tentative)	class 1	B	A	A/B	A/B	A/B	C/D	A	A	D	A/B	A/B	A	B	A	B	class 2	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
53362	Huitti et al. (1998)	yes	no	yes (tentative)	class 1	B	A	A/B	A/B	A/B	C/D	A	A	D	A/B	A/B	A	B	A	B	class 2	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
53363	Huitti et al. (1998)	yes	no	yes (tentative)	class 1	B	A	A/B	A/B	A/B	C/D	A	A	D	A/B	A/B	A	B	A	B	class 2	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
53364	Huitti et al. (1998)	yes	no	yes (tentative)	class 1	B	A	A/B	A/B	A/B	C/D	A	A	D	A/B	A/B	A	B	A	B	class 2	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
53365	Huitti et al. (1998)	yes	no	yes (tentative)	class 1	B	A	A/B	A/B	A/B	C/D	A	A	D	A/B	A/B	A	B	A	B	class 2	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
53366	Huitti et al. (1998)	yes	no	yes (tentative)	class 1	B	A	A/B	A/B	A/B	C/D	A	A	D	A/B	A/B	A	B	A	B	class 2	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
53367	Huitti et al. (1998)	yes	no	yes (tentative)	class 1	B	A	A/B	A/B	A/B	C/D	A	A	D	A/B	A/B	A	B	A	B	class 2	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
53368	Huitti et al. (1998)	yes	no	yes (tentative)	class 1	B	A	A/B	A/B	A/B	C/D	A	A	D	A/B	A/B	A	B	A	B	class 2	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
53369	Huitti et al. (1998)	yes	no	yes (tentative)	class 1	B	A	A/B	A/B	A/B	C/D	A	A	D	A/B	A/B	A	B	A	B	class 2	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
53370	Huitti et al. (1998)	yes	no	yes (tentative)	class 1	B	A	A/B	A/B	A/B	C/D	A	A	D	A/B	A/B	A	B	A	B	class 2	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
53371	Huitti et al. (1998)	yes	no	yes (tentative)	class 1	B	A	A/B	A/B	A/B	C/D	A	A	D	A/B	A/B	A	B	A	B	class 2	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
53372	Huitti et al. (1998)	yes	no	yes (tentative)	class 1	B	A	A/B	A/B	A/B	C/D	A	A	D	A/B	A/B	A	B	A	B	class 2	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
53373	Huitti et al. (1998)	yes	no	yes (tentative)	class 1	B	A	A/B	A/B	A/B	C/D	A	A	D	A/B	A/B	A	B	A	B	class 2	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
53374	Huitti et al. (1998)	yes	no	yes (tentative)	class 1	B	A	A/B	A/B	A/B	C/D	A	A	D	A/B	A/B	A	B	A	B	class 2	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
53375	Huitti et al. (1998)	yes	no	yes (tentative)	class 1	B	A	A/B	A/B	A/B	C/D	A	A	D	A/B	A/B	A	B	A	B	class 2	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
53376	Huitti et al. (1998)	yes	no	yes (tentative)	class 1	B	A	A/B	A/B	A/B	C/D	A	A	D	A/B	A/B	A	B	A	B	class 2	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
53377	Huitti et al. (1998)	yes	no	yes (tentative)	class 1	B	A	A/B	A/B	A/B	C/D	A	A	D	A/B	A/B	A	B	A	B	class 2	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
53378	Huitti et al. (1998)	yes	no	yes (tentative)	class 1	B	A	A/B	A/B	A/B	C/D	A	A	D	A/B	A/B	A	B	A	B	class 2	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
53379	Huitti et al. (1998)	yes	no	yes (tentative)	class 1	B	A	A/B	A/B	A/B	C/D	C/D	A	D	A/B	A/B	A	B	A	B	class 2	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
53380	Huitti et al. (1998)	yes	no	yes (tentative)	class 1	B	A	A/B	A/B	A/B	C/D	A	A	D	A/B	A/B	A	B	A	B	class 2	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
53381	Huitti et al. (1998)	yes	no	yes (tentative)	class 1	B	A	A/B	A/B	A/B	C/D	A	A	D	A/B	A/B	A	B	A	B	class 2	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
53382	Huitti et al. (1998)	yes	no	yes (tentative)	class 1	B	A	A/B	A/B	A/B	C/D	A	A	D	A/B	A/B	A	B	A	B	class 2	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
53383	Huitti et al. (1998)	yes	no	yes (tentative)	class 1	B	A	A/B	A/B	A/B	C/D	A	A	D	A/B	A/B	A	B	A	B	class 2	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
53384	Huitti et al. (1998)	yes	no	yes (tentative)	class 1	B	A	A/B	A/B	A/B	C/D	C/D	A	D	A/B	A/B	A	B	A	B	class 2	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
53385	Huitti et al. (1998)	yes	no	yes (tentative)	class 1	B	A	A/B	A/B	A/B	C/D	A	A	D	A/B	A/B	A	B	A	B	class 2	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
53386	Huitti et al. (1998)	yes	no	yes (tentative)	class 1	B	A	A/B	A/B	A/B	C/D	A	A	D	A/B	A/B	A	B	A	B	class 2	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
53387	Huitti et al. (1998)	yes	no	yes (tentative)	class 1	B	A	A/B	A/B	A/B	C/D	C/D	A	D	A/B	A/B	A	B	A	B	class 2	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
53388	Huitti et al. (1998)	yes	no	yes (tentative)	class 1	B	A	A/B	A/B	A/B	C/D	C/D	A	D	A/B	A/B	A	B	A	B	class 2	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
53389	Huitti et al. (1998)	yes	no	yes (tentative)	class 1	B	A	A/B	A/B	A/B	C/D	A	A	D	A/B	A/B	A	B	A	B	class 2	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
53390	Huitti et al. (1998)	yes	no	yes (tentative)	class 1	B	A	A/B	A/B	A/B	C/D	A	A	D	A/B	A/B	A	B	A	B	class 2	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
53391	Huitti et al. (1998)	yes	no	yes (tentative)	class 1	B	A	A/B	A/B	A/B	C/D	A	A	D	A/B	A/B	A	B	A	B	class 2	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
53392	Huitti et al. (1998)	yes	no	yes (tentative)	class 1	B	A	A/B	A/B	A/B	C/D	A	A	D	A/B	A/B	A	B	A	B	class 2	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
53393	Huitti et al. (1998)	yes	no	yes (tentative)	class 1	B	A	A/B	A/B	A/B	C/D	A	A	D	A/B	A/B	A	B	A	B	class 2	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
53394	Huitti et al. (1998)	yes	no	yes (tentative)	class 1	B	A	A/B	A/B	A/B	C/D	A	A	D	A/B	A/B	A	B	A	B	class 2	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
53395	Huitti et al. (1998)	yes	no	yes (tentative)	class 1	B	A	A/B	A/B	A/B	C/D	A	A	D	A/B	A/B	A	B	A	B	class 2	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
53396	Huitti et al. (1998)	yes	no	yes (tentative)	class 1	B	A	A/B	A/B	A/B	C/D	A	A	D	A/B	A/B	A	B	A	B	class 2	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
53397	Huitti et al. (1998)	yes	no	yes (tentative)	class 1	B	A	A/B	A/B	A/B	C/D	A	A	D	A/B	A/B	A	B	A	B	class 2	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
53398	Huitti et al. (1998)	yes	no	yes (tentative)	class 1	B	A	A/B	A/B	A/B	C/D	C/D	A	D	A/B	A/B	A	B	A	B	class 2	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
53399	Huitti et al. (1998)	yes	no	yes (tentative)	class 1	B	A	A/B	A/B	A/B	C/D	A	A	D	A/B	A/B	A	B	A	B	class 2	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
53400	Huitti et al. (1998)	yes	no	yes (tentative)	class 1	B	A	A/B	A/B	A/B	C/D	A	A	D	A/B	A/B	A	B	A	B	class 2	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
53401	Huitti et al. (1998)	yes	no	yes (tentative)	class 1	B	A	A/B	A/B	A/B	C/D	A	A	D	A/B	A/B	A	B	A	B	class 2	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
53402	Huitti																								

I - Completeness of documentation and type of Kd	II - Technical and scientific quality of reported data																			III - Consistency	Operator	Data	Classification Guideline		
Rating => I-a: Yes/No, I-b: class 1-6	Checkpoints => II-e: A-D (numerical value: 3-0)/unreliable Rating => class1-6/unreliable																			comment/rating					
Datapoint	Reference	I-a.1	I-a.2	Rating I-a	Rating I-b	II-a solid phase	II-b pH	II-c redox condition	II-d solution composition	II-e temperature	II-f S/W	II-g sorptive value	II-h initial [RN]	II-i phase separation	II-j reaction time	II-k agitation	II-l RN loading	II-m reaction vessels	II-n error estimates	II-o parameter variation	Rating II				
53460	Huitt et al. (1998)	yes	no	yes (tentative)	class 1	B	A	A/B	A/B	A/B	A/B	C/D	A	D	A/B	A/B	A	B	A	B	class 2	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
53461	Huitt et al. (1998)	yes	no	yes (tentative)	class 1	B	A	A/B	A/B	A/B	A/B	A	A	D	A/B	A/B	A	B	A	B	class 1	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
53462	Huitt et al. (1998)	yes	no	yes (tentative)	class 1	B	A	A/B	A/B	A/B	A/B	A	A	D	A/B	A/B	A	B	A	B	class 1	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
53463	Huitt et al. (1998)	yes	no	yes (tentative)	class 1	B	A	A/B	A/B	A/B	A/B	A	A	D	A/B	A/B	A	B	A	B	class 1	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
53464	Huitt et al. (1998)	yes	no	yes (tentative)	class 1	B	A	A/B	A/B	A/B	A/B	C/D	A	D	A/B	A/B	A	B	A	B	class 2	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
53465	Huitt et al. (1998)	yes	no	yes (tentative)	class 1	B	A	A/B	A/B	A/B	C/D	C/D	A	D	A/B	A/B	A	B	A	B	class 2	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
53466	Huitt et al. (1998)	yes	no	yes (tentative)	class 1	B	A	A/B	A/B	A/B	C/D	A	A	D	A/B	A/B	A	B	A	B	class 2	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
53467	Huitt et al. (1998)	yes	no	yes (tentative)	class 1	B	A	A/B	A/B	A/B	C/D	A	A	D	A/B	A/B	A	B	A	B	class 2	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
53468	Huitt et al. (1998)	yes	no	yes (tentative)	class 1	B	A	A/B	A/B	A/B	C/D	A	A	D	A/B	A/B	A	B	A	B	class 2	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
53469	Huitt et al. (1998)	yes	no	yes (tentative)	class 1	B	A	A/B	A/B	A/B	C/D	A	A	D	A/B	A/B	A	B	A	B	class 2	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
53470	Huitt et al. (1998)	yes	no	yes (tentative)	class 1	B	A	A/B	A/B	A/B	C/D	A	A	D	A/B	A/B	A	B	A	B	class 2	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
53471	Huitt et al. (1998)	yes	no	yes (tentative)	class 1	B	A	A/B	A/B	A/B	C/D	A	A	D	A/B	A/B	A	B	A	B	class 2	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
53472	Huitt et al. (1998)	yes	no	yes (tentative)	class 1	B	A	A/B	A/B	A/B	C/D	A	A	D	A/B	A/B	A	B	A	B	class 2	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
53473	Huitt et al. (1998)	yes	no	yes (tentative)	class 1	B	A	A/B	A/B	A/B	C/D	A	A	D	A/B	A/B	A	B	A	B	class 2	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
53474	Huitt et al. (1998)	yes	no	yes (tentative)	class 1	B	A	A/B	A/B	A/B	C/D	A	A	D	A/B	A/B	A	B	A	B	class 2	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
53475	Huitt et al. (1998)	yes	no	yes (tentative)	class 1	B	A	A/B	A/B	A/B	C/D	A	A	D	A/B	A/B	A	B	A	B	class 2	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
53476	Huitt et al. (1998)	yes	no	yes (tentative)	class 1	B	A	A/B	A/B	A/B	C/D	C/D	A	D	A/B	A/B	A	B	A	B	class 2	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
53477	Huitt et al. (1998)	yes	no	yes (tentative)	class 1	B	A	A/B	A/B	A/B	C/D	A	A	D	A/B	A/B	A	B	A	B	class 2	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
53478	Huitt et al. (1998)	yes	no	yes (tentative)	class 1	B	A	A/B	A/B	A/B	C/D	B	A	D	A/B	A/B	A	B	A	B	class 2	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
53479	Huitt et al. (1998)	yes	no	yes (tentative)	class 1	B	A	A/B	A/B	A/B	C/D	C/D	A	D	A/B	A/B	A	B	A	B	class 2	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
53480	Huitt et al. (1998)	yes	no	yes (tentative)	class 1	B	A	A/B	A/B	A/B	C/D	B	A	D	A/B	A/B	A	B	A	B	class 2	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
53481	Huitt et al. (1998)	yes	no	yes (tentative)	class 1	B	A	A/B	A/B	A/B	C/D	B	A	D	A/B	A/B	A	B	A	B	class 2	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
53482	Huitt et al. (1998)	yes	no	yes (tentative)	class 1	B	A	A/B	A/B	A/B	C/D	B	A	D	A/B	A/B	A	B	A	B	class 2	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
53483	Huitt et al. (1998)	yes	no	yes (tentative)	class 1	B	A	A/B	A/B	A/B	C/D	A	A	D	A/B	A/B	A	B	A	B	class 2	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
53484	Huitt et al. (1998)	yes	no	yes (tentative)	class 1	B	A	A/B	A/B	A/B	C/D	A	A	D	A/B	A/B	A	B	A	B	class 2	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
53485	Huitt et al. (1998)	yes	no	yes (tentative)	class 1	B	A	A/B	A/B	A/B	C/D	B	A	D	A/B	A/B	A	B	A	B	class 2	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
53486	Huitt et al. (1998)	yes	no	yes (tentative)	class 1	B	A	A/B	A/B	A/B	C/D	B	A	D	A/B	A/B	A	B	A	B	class 2	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
53487	Huitt et al. (1998)	yes	no	yes (tentative)	class 1	B	A	A/B	A/B	A/B	C/D	B	A	D	A/B	A/B	A	B	A	B	class 2	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
53488	Huitt et al. (1998)	yes	no	yes (tentative)	class 1	B	A	A/B	A/B	A/B	C/D	A	A	D	A/B	A/B	A	B	A	B	class 2	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
53489	Huitt et al. (1998)	yes	no	yes (tentative)	class 1	B	A	A/B	A/B	A/B	C/D	B	A	D	A/B	A/B	A	B	A	B	class 2	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
53490	Huitt et al. (1998)	yes	no	yes (tentative)	class 1	B	A	A/B	A/B	A/B	C/D	A	A	D	A/B	A/B	A	B	A	B	class 2	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
53491	Huitt et al. (1998)	yes	no	yes (tentative)	class 1	B	A	A/B	A/B	A/B	C/D	A	A	D	A/B	A/B	A	B	A	B	class 2	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
53492	Huitt et al. (1998)	yes	no	yes (tentative)	class 1	B	A	A/B	A/B	A/B	C/D	A	A	D	A/B	A/B	A	B	A	B	class 2	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
53493	Huitt et al. (1998)	yes	no	yes (tentative)	class 1	B	A	A/B	A/B	A/B	C/D	A	A	D	A/B	A/B	A	B	A	B	class 2	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
53494	Huitt et al. (1998)	yes	no	yes (tentative)	class 1	B	A	A/B	A/B	A/B	C/D	A	A	D	A/B	A/B	A	B	A	B	class 2	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
53495	Huitt et al. (1998)	yes	no	yes (tentative)	class 1	B	A	A/B	A/B	A/B	C/D	A	A	D	A/B	A/B	A	B	A	B	class 2	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
53496	Huitt et al. (1998)	yes	no	yes (tentative)	class 1	B	A	A/B	A/B	A/B	C/D	A	A	D	A/B	A/B	A	B	A	B	class 2	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
53497	Huitt et al. (1998)	yes	no	yes (tentative)	class 1	B	A	A/B	A/B	A/B	C/D	A	A	D	A/B	A/B	A	B	A	B	class 2	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
53498	Huitt et al. (1998)	yes	no	yes (tentative)	class 1	B	A	A/B	A/B	A/B	C/D	A	A	D	A/B	A/B	A	B	A	B	class 2	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
53499	Huitt et al. (1998)	yes	no	yes (tentative)	class 1	B	A	A/B	A/B	A/B	C/D	A	A	D	A/B	A/B	A	B	A	B	class 2	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
53500	Huitt et al. (1998)	yes	no	yes (tentative)	class 1	B	A	A/B	A/B	A/B	C/D	A	A	D	A/B	A/B	A	B	A	B	class 2	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
53501	Huitt et al. (1998)	yes	no	yes (tentative)	class 1	B	A	A/B	A/B	A/B	C/D	A	A	D	A/B	A/B	A	B	A	B	class 2	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
53502	Huitt et al. (1998)	yes	no	yes (tentative)	class 1	B	A	A/B	A/B	A/B	C/D	A	A	D	A/B	A/B	A	B	A	B	class 2	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
53503	Huitt et al. (1998)	yes	no	yes (tentative)	class 1	B	A	A/B	A/B	A/B	C/D	A	A	D	A/B	A/B	A	B	A	B	class 2	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
53504	Huitt et al. (1998)	yes	no	yes (tentative)	class 1	B	A	A/B	A/B	A/B	C/D	A	A	D	A/B	A/B	A	B	A	B	class 2	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
53505	Huitt et al. (1998)	yes	no	yes (tentative)	class 1	B	A	A/B	A/B	A/B	C/D	B	A	D	A/B	A/B	A	B	A	B	class 2	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
53506	Huitt et al. (1998)	yes	no	yes (tentative)	class 1	B	A	A/B	A/B	A/B	C/D	A	A	D	A/B	A/B	A	B	A	B	class 2	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
53507	Huitt et al. (1998)	yes	no	yes (tentative)	class 1	B	A	A/B	A/B	A/B	C/D	A	A	D	A/B	A/B	A	B	A	B	class 2	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
53508	Huitt et al. (1998)	yes	no	yes (tentative)	class 1	B	A	A/B	A/B	A/B	C/D	A	A	D	A/B	A/B	A	B	A	B	class 2	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
53509	Huitt et al. (1998)	yes	no	yes (tentative)	class 1	B	A	A/B	A/B	A/B	C/D	A	A	D	A/B	A/B	A	B	A	B	class 2	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
53510	Huitt et al. (1998)	yes	no	yes (tentative)	class 1	B	A	A/B	A/B	A/B	C/D	A	A	D	A/B	A/B	A	B	A	B	class 2	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
53511	Huitt et al. (1998)	yes	no	yes (tentative)	class 1	B	A	A/B	A/B	A/B	C/D	A	A	D	A/B	A/B	A	B	A	B	class 2	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
53512	Huitt et al. (1998)	yes	no	yes (tentative)	class 1	B	A	A/B	A/B	A/B	C/D	A	A	D	A/B	A/B	A	B	A	B	class 2	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
53513	Huitt et al. (1998)	yes	no	yes (tentative)	class 1	B	A	A/B	A/B	A/B	C/D	A	A	D	A/B	A/B	A	B	A	B	class 2	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
53514	Huitt et al. (1998)	yes	no	yes (tentative)	class 1	B	A	A/B	A/B	A/B	C/D	A	A	D	A/B	A/B	A	B	A	B	class 2	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
53515	Huitt et al. (1998)	yes	no	yes (tentative)	class 1	B	A	A/B	A/B	A/B	C/D	A	A	D	A/B	A/B	A	B	A	B	class 2	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
53516	Huitt et al. (1998)	yes	no	yes (tentative)	class 1	B	A	A/B	A/B	A/B	C/D	A	A	D	A/B	A/B	A	B	A	B	class 2	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
53517	Huitt et al. (1998)	yes	no	yes (tentative)	class 1	B	A	A/B	A/B	A/B	C/D	A	A	D	A/B	A/B	A	B	A	B	class 2	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
53518	Huitt et al. (1998)	yes	no	yes (tentative)	class 1	B	A	A/B	A/B	A/B	C/D	C/D	A	D	A/B	A/B	A	B	A	B	class 2	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
53519	Huitt et al. (1998)	yes	no	yes (tentative)	class 1	B	A	A/B	A/B	A/B	C/D	A	A	D	A/B	A/B	A	B	A	B	class 2	S. Kunze/M. Ochs, BMG	November 2008	Revision 4b (May 19, 2005)	
53520	Huitt et al. (1998)	yes	no	yes (tentative)	class 1	B	A	A/B	A/B	A/B	C/D	A	A	D	A/B	A/B	A	B	A	B	class 2	S. Kunze/M. Ochs, BMG			

Cs	I – Completeness of documentation and type of Kd				II – Technical and scientific quality of reported data																III – Consistency	Operator	Data	Classification Guideline																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																										
		Rating ⇒ I-a: Yes/No, I-b: class 1-6																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																

Datapoint	Reference	I - Completeness of documentation and type of Kd										II - Technical and scientific quality of reported data															III - Consistency	Operator	Data	Classification Guideline
		Rating => I-a: Yes/No, I-b: class 1-6										Checkpoints => level: A-D (numerical value: 3-0)/unreliable Rating => class1-6/unreliable																		
		I-a.1	I-a.2	Rating I-a	Rating I-b	II-a solid phase	II-b pH	II-c redox condition	II-d solution composition	II-e temperature	II-f S/W	II-g sortive value	II-h initial [RN]	II-i phase separation	II-j reaction time	II-k agitation	II-l RN loading	II-m reaction vessels	II-n error estimates	II-o parameter variation	Rating II	comment/rating								
42381	Allard et al.(1979b)	Yes	Yes	Yes (can be used)	class 1	C/D	B	A/B	C/D	A/B	A/B	A	B	C/D	A/B	A/B	C/D	C/D	D	C	class 4	T. Suyama/Y. Tachi(JAEA)	April 2008	Revision 4b (May 19, 2005)						
42382	Allard et al.(1979b)	Yes	Yes	Yes (can be used)	class 1	C/D	B	A/B	C/D	A/B	A/B	A	B	C/D	A/B	A/B	C/D	C/D	D	C	class 4	T. Suyama/Y. Tachi(JAEA)	April 2008	Revision 4b (May 19, 2005)						
42383	Allard et al.(1979b)	Yes	Yes	Yes (can be used)	class 1	C/D	B	A/B	C/D	A/B	A/B	A	B	C/D	A/B	A/B	C/D	C/D	D	C	class 4	T. Suyama/Y. Tachi(JAEA)	April 2008	Revision 4b (May 19, 2005)						
42384	Allard et al.(1979b)	Yes	Yes	Yes (can be used)	class 1	C/D	B	A/B	C/D	A/B	A/B	A	B	C/D	A/B	A/B	C/D	C/D	D	C	class 4	T. Suyama/Y. Tachi(JAEA)	April 2008	Revision 4b (May 19, 2005)						
42385	Allard et al.(1979b)	Yes	Yes	Yes (can be used)	class 1	C/D	B	A/B	C/D	A/B	A/B	A	B	C/D	A/B	A/B	C/D	C/D	D	C	class 4	T. Suyama/Y. Tachi(JAEA)	April 2008	Revision 4b (May 19, 2005)						
42386	Allard et al.(1979b)	Yes	Yes	Yes (can be used)	class 1	C/D	B	A/B	C/D	A/B	A/B	A	B	C/D	A/B	A/B	C/D	C/D	D	C	class 4	T. Suyama/Y. Tachi(JAEA)	April 2008	Revision 4b (May 19, 2005)						
44268	Barney and Anderson(1979)	Yes	Yes	Yes (can be used)	class 1	C/D	B	A/B	C/D	A/B	C/D	A	unreliable	C/D	A/B	A/B	C/D	B	D	C	unreliable	T. Suyama/Y. Tachi(JAEA)	April 2008	Revision 4b (May 19, 2005)						
44269	Barney and Anderson(1979)	Yes	Yes	Yes (can be used)	class 1	C/D	B	A/B	C/D	A/B	C/D	A	unreliable	C/D	A/B	A/B	C/D	B	D	C	unreliable	T. Suyama/Y. Tachi(JAEA)	April 2008	Revision 4b (May 19, 2005)						
44270	Barney and Anderson(1979)	Yes	Yes	Yes (can be used)	class 1	C/D	B	A/B	C/D	A/B	C/D	B	A	C/D	A/B	A/B	C/D	B	D	C	class 4	T. Suyama/Y. Tachi(JAEA)	April 2008	Revision 4b (May 19, 2005)						
44271	Barney and Anderson(1979)	Yes	Yes	Yes (can be used)	class 1	C/D	B	A/B	C/D	A/B	C/D	A	A	C/D	A/B	A/B	C/D	B	D	C	class 3	T. Suyama/Y. Tachi(JAEA)	April 2008	Revision 4b (May 19, 2005)						
44272	Barney and Anderson(1979)	Yes	Yes	Yes (can be used)	class 1	C/D	B	A/B	C/D	A/B	C/D	A	B	C/D	A/B	A/B	C/D	B	D	C	class 3	T. Suyama/Y. Tachi(JAEA)	April 2008	Revision 4b (May 19, 2005)						
44273	Barney and Anderson(1979)	Yes	Yes	Yes (can be used)	class 1	C/D	B	A/B	C/D	A/B	C/D	A	B	C/D	A/B	A/B	C/D	B	D	C	class 4	T. Suyama/Y. Tachi(JAEA)	April 2008	Revision 4b (May 19, 2005)						
44337	Barney and Brown(1979)	Yes	Yes	Yes (can be used)	class 1	A	A	A/B	A/B	A/B	A/B	A	B	C/D	A/B	A/B	C/D	B	D	D	class 3	T. Suyama/Y. Tachi(JAEA)	April 2008	Revision 4b (May 19, 2005)						
44338	Barney and Brown(1979)	Yes	Yes	Yes (can be used)	class 1	A	A	A/B	A/B	A/B	A/B	A	B	C/D	A/B	A/B	C/D	B	D	D	class 3	T. Suyama/Y. Tachi(JAEA)	April 2008	Revision 4b (May 19, 2005)						
44339	Barney and Brown(1979)	Yes	Yes	Yes (can be used)	class 1	A	A	A/B	A/B	A/B	A/B	A	B	C/D	A/B	A/B	C/D	B	D	D	class 3	T. Suyama/Y. Tachi(JAEA)	April 2008	Revision 4b (May 19, 2005)						
46824	Baston et al.(1997)	Yes	Yes	Yes (can be used)	class 1	B	A	C/D	A/B	A/B	A/B	C/D	C/D	B	C/D	A/B	C/D	B	B	C	class 3	S. Kunze/M. Ochs, BMG	January 2008	Revision 4b (May 19, 2005)						
46825	Baston et al.(1997)	Yes	Yes	Yes (can be used)	class 1	B	A	C/D	A/B	A/B	A/B	C/D	C/D	unreliable	B	C/D	A/B	C/D	B	C	unreliable	S. Kunze/M. Ochs, BMG	January 2008	Revision 4b (May 19, 2005)						
46826	Baston et al.(1997)	Yes	Yes	Yes (can be used)	class 1	B	A	C/D	A/B	A/B	A/B	C/D	C/D	B	C/D	A/B	C/D	B	B	C	class 3	S. Kunze/M. Ochs, BMG	January 2008	Revision 4b (May 19, 2005)						
46827	Baston et al.(1997)	Yes	Yes	Yes (can be used)	class 1	B	A	C/D	A/B	A/B	A/B	C/D	C/D	unreliable	B	C/D	A/B	C/D	B	C	unreliable	S. Kunze/M. Ochs, BMG	January 2008							

I - Completeness of documentation and title of Kd	II - Technical and scientific quality of reported data	III - Consistency	Operator	Data	Classification Guideline																					
Rating => I-a: Yes/No, I-b: class 1-6	Checkpoints => level: A-D (numerical value: 3-0)/unreliable	Rating => class1-6/unreliable																								
Datapoint	Reference	I-a.1	I-a.2	Rating I-a	Rating I-b	II-a solid phase	II-b pH	II-c redox condition	II-d solution composition	II-e temperature	II-f S/W	II-g sorptive value	II-h initial [RN]	II-i phase separation	II-j reaction time	II-k agitation	II-l RN loading	II-m reaction vessels	II-n error estimates	II-o parameter variation	Rating II	comment/rating				
56677	Nakayama and Sakamoto(1991)	Yes	Yes	Yes (can be used)	class 4	B)	A)	A/B)	C/D)	A/B)	A/B)	A)	A)	A/B)	C/D)	C/D)	A)	D)	C)		class 2	T. Suyama/Y. Tachi(JAEA)	May 2008	Revision 4b (May 19, 2005)		
56678	Nakayama and Sakamoto(1991)	Yes	Yes	Yes (can be used)	class 4	B)	A)	A/B)	C/D)	A/B)	A/B)	C/D)	A)	A)	A/B)	C/D)	C/D)	A)	D)	C)		class 2	T. Suyama/Y. Tachi(JAEA)	May 2008	Revision 4b (May 19, 2005)	
56679	Nakayama and Sakamoto(1991)	Yes	Yes	Yes (can be used)	class 4	B)	A)	A/B)	C/D)	A/B)	A/B)	A)	A)	A)	A/B)	C/D)	C/D)	A)	D)	C)		class 2	T. Suyama/Y. Tachi(JAEA)	May 2008	Revision 4b (May 19, 2005)	
56680	Nakayama and Sakamoto(1991)	Yes	Yes	Yes (can be used)	class 4	B)	A)	A/B)	C/D)	A/B)	A/B)	C/D)	A)	A)	A)	A/B)	C/D)	C/D)	A)	D)	C)		class 2	T. Suyama/Y. Tachi(JAEA)	May 2008	Revision 4b (May 19, 2005)
56703	Nakayama and Sakamoto(1991)	Yes	Yes	Yes (can be used)	class 4	B)	A)	A/B)	C/D)	A/B)	A/B)	A)	A)	A)	A/B)	C/D)	C/D)	A)	D)	C)		class 2	T. Suyama/Y. Tachi(JAEA)	May 2008	Revision 4b (May 19, 2005)	
56704	Nakayama and Sakamoto(1991)	Yes	Yes	Yes (can be used)	class 4	B)	A)	A/B)	C/D)	A/B)	A/B)	A)	A)	A)	A/B)	C/D)	C/D)	A)	D)	C)		class 2	T. Suyama/Y. Tachi(JAEA)	May 2008	Revision 4b (May 19, 2005)	
56705	Nakayama and Sakamoto(1991)	Yes	Yes	Yes (can be used)	class 4	B)	A)	A/B)	C/D)	A/B)	A/B)	A)	A)	A)	A/B)	C/D)	C/D)	A)	D)	C)		class 2	T. Suyama/Y. Tachi(JAEA)	May 2008	Revision 4b (May 19, 2005)	
56706	Nakayama and Sakamoto(1991)	Yes	Yes	Yes (can be used)	class 4	B)	A)	A/B)	C/D)	A/B)	A/B)	A)	A)	A)	A/B)	C/D)	C/D)	A)	D)	C)		class 2	T. Suyama/Y. Tachi(JAEA)	May 2008	Revision 4b (May 19, 2005)	
56707	Nakayama and Sakamoto(1991)	Yes	Yes	Yes (can be used)	class 4	B)	A)	A/B)	C/D)	A/B)	A/B)	A)	A)	A)	A/B)	C/D)	C/D)	A)	D)	C)		class 2	T. Suyama/Y. Tachi(JAEA)	May 2008	Revision 4b (May 19, 2005)	
56708	Nakayama and Sakamoto(1991)	Yes	Yes	Yes (can be used)	class 4	B)	A)	A/B)	C/D)	A/B)	A/B)	A)	A)	A)	A/B)	C/D)	C/D)	A)	D)	C)		class 2	T. Suyama/Y. Tachi(JAEA)	May 2008	Revision 4b (May 19, 2005)	
56709	Nakayama and Sakamoto(1991)	Yes	Yes	Yes (can be used)	class 4	B)	A)	A/B)	C/D)	A/B)	A/B)	A)	A)	A)	A/B)	C/D)	C/D)	A)	D)	C)		class 2	T. Suyama/Y. Tachi(JAEA)	May 2008	Revision 4b (May 19, 2005)	
56710	Nakayama and Sakamoto(1991)	Yes	Yes	Yes (can be used)	class 4	B)	A)	A/B)	C/D)	A/B)	A/B)	A)	A)	A)	A/B)	C/D)	C/D)	A)	D)	C)		class 2	T. Suyama/Y. Tachi(JAEA)	May 2008	Revision 4b (May 19, 2005)	
56711	Nakayama and Sakamoto(1991)	Yes	Yes	Yes (can be used)	class 4	B)	A)	A/B)	C/D)	A/B)	A/B)	A)	A)	A)	A/B)	C/D)	C/D)	A)	D)	C)		class 2	T. Suyama/Y. Tachi(JAEA)	May 2008	Revision 4b (May 19, 2005)	
56712	Nakayama and Sakamoto(1991)	Yes	Yes	Yes (can be used)	class 4	B)	A)	A/B)	C/D)	A/B)	A/B)	A)	A)	A)	A/B)	C/D)	C/D)	A)	D)	C)		class 2	T. Suyama/Y. Tachi(JAEA)	May 2008	Revision 4b (May 19, 2005)	
56713	Nakayama and Sakamoto(1991)	Yes	Yes	Yes (can be used)	class 4	B)	A)	A/B)	C/D)	A/B)	A/B)	A)	A)	A)	A/B)	C/D)	C/D)	A)	D)	C)		class 2	T. Suyama/Y. Tachi(JAEA)	May 2008	Revision 4b (May 19, 2005)	
56714	Nakayama and Sakamoto(1991)	Yes	Yes	Yes (can be used)	class 4	B)	A)	A/B)	C/D)	A/B)	A/B)	A)	A)	A)	A/B)	C/D)	C/D)	A)	D)	C)		class 2	T. Suyama/Y. Tachi(JAEA)	May 2008	Revision 4b (May 19, 2005)	
56715	Nakayama and Sakamoto(1991)	Yes	Yes	Yes (can be used)	class 4	B)	A)	A/B)	C/D)	A/B)	A/B)	A)	A)	A)	A/B)	C/D)	C/D)	A)	D)	C)		class 2	T. Suyama/Y. Tachi(JAEA)	May 2008	Revision 4b (May 19, 2005)	
56716	Nakayama and Sakamoto(1991)	Yes	Yes	Yes (can be used)	class 4	B)	A)	A/B)	C/D)	A/B)	A/B)	A)	A)	A)	A/B)	C/D)	C/D)	A)	D)	C)		class 2	T. Suyama/Y. Tachi(JAEA)	May 2008	Revision 4b (May 19, 2005)	
56717	Nakayama and Sakamoto(1991)	Yes	Yes	Yes (can be used)	class 4	B)	A)	A/B)	C/D)	A/B)	A/B)	A)	A)	A)	A/B)	C/D)	C/D)	A)</								

No		I – Completeness of documentation and type of Kd										II – Technical and scientific quality of reported data															III – Consistency		Operator	Data	Classification Guideline
Rating ⇒ I-a: Yes/No, I-b: class 1–6		Checkpoints ⇒ level: A–D (numerical value: 3–0)/unreliable															Rating ⇒ class1–6/unreliable														
Datapoint	Reference	I-a.1	I-a.2	Rating I-a	Rating I-b	II-a solid phase	II-b pH	II-c redox condition	II-d solution composition	II-e temperature	II-f S/W	II-g sorptive value	II-h initial [RN]	II-i phase separation	II-j reaction time	II-k agitation	II-l RN loading	II-m reaction vessels	II-n error estimates	II-o parameter variation	Rating II	comment/rating									
63971	Morgan et al.(1988)	Yes	Yes	Yes (can be used)	class 1	A)	B)	A/B)	C/D)	C/D)	A/B)	A)	A)	B)	A/B)	A/B)	A)	A)	D)	C)	class 2		T. Suyama/Y. Tachi(JAEA)	May 2008	Revision 4b (May 19, 2005)						
63972	Morgan et al.(1988)	Yes	Yes	Yes (can be used)	class 1	A)	B)	A/B)	C/D)	C/D)	A/B)	A)	A)	B)	A/B)	A/B)	A)	A)	D)	C)	class 2		T. Suyama/Y. Tachi(JAEA)	May 2008	Revision 4b (May 19, 2005)						
63973	Morgan et al.(1988)	Yes	Yes	Yes (can be used)	class 1	A)	B)	A/B)	C/D)	C/D)	A/B)	A)	A)	B)	A/B)	A/B)	A)	A)	D)	C)	class 2		T. Suyama/Y. Tachi(JAEA)	May 2008	Revision 4b (May 19, 2005)						
63974	Morgan et al.(1988)	Yes	Yes	Yes (can be used)	class 1	A)	B)	A/B)	C/D)	C/D)	A/B)	A)	A)	B)	A/B)	A/B)	A)	A)	D)	C)	class 2		T. Suyama/Y. Tachi(JAEA)	May 2008	Revision 4b (May 19, 2005)						
63975	Morgan et al.(1988)	Yes	Yes	Yes (can be used)	class 1	A)	B)	A/B)	C/D)	C/D)	A/B)	A)	A)	B)	A/B)	A/B)	A)	A)	D)	C)	class 2		T. Suyama/Y. Tachi(JAEA)	May 2008	Revision 4b (May 19, 2005)						
63976	Morgan et al.(1988)	Yes	Yes	Yes (can be used)	class 1	A)	B)	A/B)	C/D)	C/D)	A/B)	A)	A)	B)	A/B)	A/B)	A)	A)	D)	C)	class 2		T. Suyama/Y. Tachi(JAEA)	May 2008	Revision 4b (May 19, 2005)						
63977	Morgan et al.(1988)	Yes	Yes	Yes (can be used)	class 1	A)	B)	A/B)	C/D)	C/D)	A/B)	A)	A)	B)	A/B)	A/B)	A)	A)	D)	C)	class 2		T. Suyama/Y. Tachi(JAEA)	May 2008	Revision 4b (May 19, 2005)						
63978	Morgan et al.(1988)	Yes	Yes	Yes (can be used)	class 1	A)	B)	A/B)	C/D)	C/D)	A/B)	A)	A)	B)	A/B)	A/B)	A)	A)	D)	C)	class 2		T. Suyama/Y. Tachi(JAEA)	May 2008	Revision 4b (May 19, 2005)						
63979	Morgan et al.(1988)	Yes	Yes	Yes (can be used)	class 1	A)	B)	A/B)	C/D)	C/D)	A/B)	A)	A)	B)	A/B)	A/B)	A)	A)	D)	C)	class 2		T. Suyama/Y. Tachi(JAEA)	May 2008	Revision 4b (May 19, 2005)						
63980	Morgan et al.(1988)	Yes	Yes	Yes (can be used)	class 1	A)	B)	A/B)	C/D)	C/D)	A/B)	B)	A)	B)	A/B)	A/B)	A)	A)	D)	C)	class 2		T. Suyama/Y. Tachi(JAEA)	May 2008	Revision 4b (May 19, 2005)						
63981	Morgan et al.(1988)	Yes	Yes	Yes (can be used)	class 1	A)	B)	A/B)	C/D)	C/D)	A/B)	A)	A)	B)	A/B)	A/B)	A)	A)	D)	C)	class 2		T. Suyama/Y. Tachi(JAEA)	May 2008	Revision 4b (May 19, 2005)						
63982	Morgan et al.(1988)	Yes	Yes	Yes (can be used)	class 1	A)	B)	A/B)	C/D)	C/D)	A/B)	A)	A)	B)	A/B)	A/B)	A)	A)	D)	C)	class 2		T. Suyama/Y. Tachi(JAEA)	May 2008	Revision 4b (May 19, 2005)						
63983	Morgan et al.(1988)	Yes	Yes	Yes (can be used)	class 1	A)	B)	A/B)	C/D)	C/D)	A/B)	A)	A)	B)	A/B)	A/B)	A)	A)	D)	C)	class 2		T. Suyama/Y. Tachi(JAEA)	May 2008	Revision 4b (May 19, 2005)						
63984	Morgan et al.(1988)	Yes	Yes	Yes (can be used)	class 1	A)	B)	A/B)	C/D)	C/D)	A/B)	A)	A)	B)	A/B)	A/B)	A)	A)	D)	C)	class 2		T. Suyama/Y. Tachi(JAEA)	May 2008	Revision 4b (May 19, 2005)						
63985	Morgan et al.(1988)	Yes	Yes	Yes (can be used)	class 1	A)	B)	A/B)	C/D)	C/D)	A/B)	A)	A)	B)	A/B)	A/B)	A)	A)	D)	C)	class 2		T. Suyama/Y. Tachi(JAEA)	May 2008	Revision 4b (May 19, 2005)						
63986	Morgan et al.(1988)	Yes	Yes	Yes (can be used)	class 1	A)	B)	A/B)	C/D)	C/D)	A/B)	A)	A)	B)	A/B)	A/B)	A)	A)	D)	C)	class 2		T. Suyama/Y. Tachi(JAEA)	May 2008	Revision 4b (May 19, 2005)						
63987	Morgan et al.(1988)	Yes	Yes	Yes (can be used)	class 1	A)	B)	A/B)	C/D)	C/D)	A/B)	A)	A)	B)	A/B)	A/B)	A)	A)	D)	C)	class 2		T. Suyama/Y. Tachi(JAEA)	May 2008	Revision 4b (May 19, 2005)						
63988	Morgan et al.(1988)	Yes	Yes	Yes (can be used)	class 1	A)	B)	A/B)	C/D)	C/D)	A/B)	A)	A)	B)	A/B)	A/B)	A)	A)	D)	C)	class 2		T. Suyama/Y. Tachi(JAEA)	May 2008	Revision 4b (May 19, 2005)						
63989	Morgan et al.(1988)	Yes	Yes	Yes (can be used)	class 1	A)	B)	A/B)	C/D)	C/D)	A/B)	A)	A)	B)	A/B)	A/B)	A)	A)	D)	C)	class 2		T. Suyama/Y. Tachi(JAEA)	May 2008	Revision 4b (May 19, 2005)						
63990	Morgan et al.(1988)	Yes	Yes	Yes (can be used)	class 1	A)	B)	A/B)	C/D)	C/D)	A/B)	A)	A)	B)	A/B)	A/B)	A)	A)	D)	C)	class 2		T. Suyama/Y. Tachi(JAEA)	May 2008	Revision 4b (May 19, 2005)						
63991	Morgan et al.(1988)	Yes	Yes	Yes (can be used)	class 1	A)	B)	A/B)	C/D)	C/D)	A/B)	A)	A)	B)	A/B)	A/B)	A)	A)	D)	C)	class 2		T. Suyama/Y. Tachi(JAEA)	May 2008	Revision 4b (May 19, 2005)						
63992	Morgan et al.(1988)	Yes	Yes	Yes (can be used)	class 1	A)	B)	A/B)	C/D)	C/D)	A/B)	A)	A)	B)	A/B)	A/B)	A)	A)	D)	C)	class 2		T. Suyama/Y. Tachi(JAEA)	May 2008	Revision 4b (May 19, 2005)						
63993	Morgan et al.(1988)	Yes	Yes	Yes (can be used)	class 1	A)	B)	A/B)	C/D)	C/D)	A/B)	B)	A)	B)	A/B)	A/B)	A)	A)	D)	C)	class 2		T. Suyama/Y. Tachi(JAEA)	May 2008	Revision 4b (May 19, 2005)						
63994	Morgan et al.(1988)	Yes	Yes	Yes (can be used)	class 1	A)	B)	A/B)	C/D)	C/D)	A/B)	A)	A)	B)	A/B)	A/B)	A)	A)	D)	C)	class 2		T. Suyama/Y. Tachi(JAEA)	May 2008	Revision 4b (May 19, 2005)						
63995	Morgan et al.(1988)	Yes	Yes	Yes (can be used)	class 1	A)	B)	A/B)	C/D)	C/D)	A/B)	A)	A)	B)	A/B)	A/B)	A)	A)	D)	C)	class 2		T. Suyama/Y. Tachi(JAEA)	May 2008	Revision 4b (May 19, 2005)						
63996	Morgan et al.(1988)	Yes	Yes	Yes (can be used)	class 1	A)	B)	A/B)	C/D)	C/D)	A/B)	A)	A)	B)	A/B)	A/B)	A)	A)	D)	C)	class 2		T. Suyama/Y. Tachi(JAEA)	May 2008	Revision 4b (May 19, 2005)						
63997	Morgan et al.(1988)	Yes	Yes	Yes (can be used)	class 1	A)	B)	A/B)	C/D)	C/D)	A/B)	A)	A)	B)	A/B)	A/B)	A)	A)	D)	C)	class 2		T. Suyama/Y. Tachi(JAEA)	May 2008	Revision 4b (May 19, 2005)						
63998	Morgan et al.(1988)	Yes	Yes	Yes (can be used)	class 1	A)	B)	A/B)	C/D)	C/D)	A/B)	B)	A)	B)	A/B)	A/B)	A)	A)	D)	C)	class 2		T. Suyama/Y. Tachi(JAEA)	May 2008	Revision 4b (May 19, 2005)						
63999	Morgan et al.(1988)	Yes	Yes	Yes (can be used)	class 1	A)	B)	A/B)	C/D)	C/D)	A/B)	A)	A)	B)	A/B)	A/B)	A)	A)	D)	C)	class 2		T. Suyama/Y. Tachi(JAEA)	May 2008	Revision 4b (May 19, 2005)						
64000	Morgan et al.(1988)	Yes	Yes	Yes (can be used)	class 1	A)	B)	A/B)	C/D)	C/D)	A/B)	A)	A)	B)	A/B)	A/B)	A)	A)	D)	C)	class 2		T. Suyama/Y. Tachi(JAEA)	May 2008	Revision 4b (May 19, 2005)						
64001	Morgan et al.(1988)	Yes	Yes	Yes (can be used)	class 1	A)	B)	A/B)	C/D)	C/D)	A/B)	A)	A)	B)	A/B)	A/B)	A)	A)	D)	C)	class 2		T. Suyama/Y. Tachi(JAEA)	May 2008	Revision 4b (May 19, 2005)						
64002	Morgan et al.(1988)	Yes	Yes	Yes (can be used)	class 1	A)	B)	A/B)	C/D)	C/D)	A/B)	A)	A)	B)	A/B)	A/B)	A)	A)	D)	C)	class 2		T. Suyama/Y. Tachi(JAEA)	May 2008	Revision 4b (May 19, 2005)						
64003	Morgan et al.(1988)	Yes	Yes	Yes (can be used)	class 1	A)	B)	A/B)	C/D)	C/D)	A/B)	A)	A)	B)	A/B)	A/B)	A)	A)	D)	C)	class 2		T. Suyama/Y. Tachi(JAEA)	May 2008	Revision 4b (May 19, 2005)						
64004	Morgan et al.(1988)	Yes	Yes	Yes (can be used)	class 1	A)	B)	A/B)	C/D)	C/D)	A/B)	A)	A)	B)	A/B)	A/B)	A)	A)	D)	C)	class 2		T. Suyama/Y. Tachi(JAEA)	May 2008	Revision 4b (May 19, 2005)						

Se	I – Completeness of documentation and type of Kd				II – Technical and scientific quality of reported data																			III – Consistency	Operator	Data	Classification Guideline	
	Rating ⇒ I-a: Yes/No, I-b: class 1-6				Checkpoints ⇒ level: A-D (numerical value: 3=0)/unreliable Rating ⇒ class1-6/unreliable																							
Datapoint	Reference	I-a.1	I-a.2	Rating I-a	Rating I-b	II-a	II-b	II-c	II-d	II-e	II-f	II-g	II-h	II-i	II-j	II-k	II-l	II-m	II-n	II-o	Rating II	comment/rating						
						solid phase	pH	redox condition	solution composition	temperature	S/W	sortive value	initial [RN]	phase separation	reaction time	agitation	RN loading	reaction vessels	error estimates	parameter variation								
51967	Fujikawa and Fukui (1997)	yes	no	no (cannot be used)	unreliable																unreliable	N.E.	S.Kunze/M.Ochs, BMG	November 2007	Revision 4b (May 19, 2005)			
51968	Fujikawa and Fukui (1997)	yes	no	no (cannot be used)	unreliable																unreliable	N.E.	S.Kunze/M.Ochs, BMG	November 2007	Revision 4b (May 19, 2005)			
51969	Fujikawa and Fukui (1997)	yes	no	no (cannot be used)	unreliable																unreliable	N.E.	S.Kunze/M.Ochs, BMG	November 2007	Revision 4b (May 19, 2005)			
51970	Fujikawa and Fukui (1997)	yes	no	no (cannot be used)	unreliable																unreliable	N.E.	S.Kunze/M.Ochs, BMG	November 2007	Revision 4b (May 19, 2005)			
51971	Fujikawa and Fukui (1997)	yes	no	no (cannot be used)	unreliable																unreliable	N.E.	S.Kunze/M.Ochs, BMG	November 2007	Revision 4b (May 19, 2005)			
51972	Fujikawa and Fukui (1997)	yes	no	no (cannot be used)	unreliable																unreliable	N.E.	S.Kunze/M.Ochs, BMG	November 2007	Revision 4b (May 19, 2005)			
51973	Fujikawa and Fukui (1997)	yes	no	no (cannot be used)	unreliable																unreliable	N.E.	S.Kunze/M.Ochs, BMG	November 2007	Revision 4b (May 19, 2005)			
51974	Fujikawa and Fukui (1997)	yes	no	no (cannot be used)	unreliable																unreliable	N.E.	S.Kunze/M.Ochs, BMG	November 2007	Revision 4b (May 19, 2005)			
51975	Fujikawa and Fukui (1997)	yes	no	no (cannot be used)	unreliable																unreliable	N.E.	S.Kunze/M.Ochs, BMG	November 2007	Revision 4b (May 19, 2005)			
51976	Fujikawa and Fukui (1997)	yes	no	no (cannot be used)	unreliable																unreliable	N.E.	S.Kunze/M.Ochs, BMG	November 2007	Revision 4b (May 19, 2005)			
51977	Fujikawa and Fukui (1997)	yes	no	no (cannot be used)	unreliable																unreliable	N.E.	S.Kunze/M.Ochs, BMG	November 2007	Revision 4b (May 19, 2005)			
51978	Fujikawa and Fukui (1997)	yes	no	no (cannot be used)	unreliable																unreliable	N.E.	S.Kunze/M.Ochs, BMG	November 2007	Revision 4b (May 19, 2005)			
58965	Sato et al. (1997)	yes	yes	yes (can be used)	class 1	A	A	C/D	A/B	A/B	C/D	A	B	B	C/D	C/D	C/D	C/D	C	D	class 3	not inconsistent with other data for Se(IV)	S.Kunze/M.Ochs, BMG	November 2007	Revision 4b (May 19, 2005)			
58966	Sato et al. (1997)	yes	yes	yes (can be used)	class 1	A	A	C/D	A/B	A/B	C/D	C/D	B	B	B	C/D	C/D	C/D	C/D	C	D	class 3	not inconsistent with other data for Se(IV)	S.Kunze/M.Ochs, BMG	November 2007	Revision 4b (May 19, 2005)		
58967	Sato et al. (1997)	yes	yes	yes (can be used)	class 1	A	A	C/D	A/B	A/B	C/D	B	B	B	C/D	C/D	C/D	C/D	C	D	class 3	not inconsistent with other data for Se(IV)	S.Kunze/M.Ochs, BMG	November 2007	Revision 4b (May 19, 2005)			
58968	Sato et al. (1997)	yes	yes	yes (can be used)	class 1	A	A	C/D	A/B	A/B	C/D	A	B	B	C/D	C/D	C/D	C/D	C	D	class 3	not inconsistent with other data for Se(IV)	S.Kunze/M.Ochs, BMG	November 2007	Revision 4b (May 19, 2005)			
58969	Sato et al. (1997)	yes	yes	yes (can be used)	class 1	A	A	C/D	A/B	A/B	C/D	B	B	B	C/D	C/D	C/D	C/D	C	D	class 3	not inconsistent with other data for Se(IV)	S.Kunze/M.Ochs, BMG	November 2007	Revision 4b (May 19, 2005)			
58970	Sato et al. (1997)	yes	yes	yes (can be used)	class 1	A	A	C/D	A/B	A/B	C/D	B	B	B	C/D	C/D	C/D	C/D	C	D	class 3	not inconsistent with other data for Se(IV)	S.Kunze/M.Ochs, BMG	November 2007	Revision 4b (May 19, 2005)			
58971	Sato et al. (1997)	yes	yes	yes (can be used)	class 1	A	A	C/D	A/B	A/B	C/D	C/D	B	B	C/D	C/D	C/D	C/D	C	D	class 3	not inconsistent with other data for Se(IV)	S.Kunze/M.Ochs, BMG	November 2007	Revision 4b (May 19, 2005)			
58972	Sato et al. (1997)	yes	yes	yes (can be used)	class 1	A	A	C/D	A/B	A/B	C/D	B	B	B	C/D	C/D	C/D	C/D	C	D	class 3	not inconsistent with other data for Se(IV)	S.Kunze/M.Ochs, BMG	November 2007	Revision 4b (May 19, 2005)			
58973	Sato et al. (1997)	yes	yes	yes (can be used)	class 1	A	A	C/D	A/B	A/B	C/D	B	B	B	C/D	C/D	C/D	C/D	C	D	class 3	not inconsistent with other data for Se(IV)	S.Kunze/M.Ochs, BMG	November 2007	Revision 4b (May 19, 2005)			
59136	Shibutani et al. (1994)	yes	yes	yes (can be used)	class 2	C/D	A	C/D	A/B	A/B	C/D	C/D	A	B	C/D	C/D	C/D	C/D	D	C	class 3	N.E.	S.Kunze/M.Ochs, BMG	January 2008	Revision 4b (May 19, 2005)			
59137	Shibutani et al. (1994)	yes	yes	yes (can be used)	class 2	C/D	A	C/D	A/B	A/B	C/D	C/D	A	B	C/D	C/D	C/D	C/D	D	C	class 3	N.E.	S.Kunze/M.Ochs, BMG	January 2008	Revision 4b (May 19, 2005)			
59138	Shibutani et al. (1994)	yes	yes	yes (can be used)	class 2	C/D	A	C/D	A/B	A/B	C/D	C/D	A	B	C/D	C/D	C/D	C/D	D	C	class 3	N.E.	S.Kunze/M.Ochs, BMG	January 2008	Revision 4b (May 19, 2005)			
59139	Shibutani et al. (1994)	yes	yes	yes (can be used)	class 2	C/D	A	C/D	A/B	A/B	C/D	C/D	A	B	C/D	C/D	C/D	C/D	D	C	class 3	N.E.	S.Kunze/M.Ochs, BMG	January 2008	Revision 4b (May 19, 2005)			
59140	Shibutani et al. (1994)	yes	yes	yes (can be used)	class 2	C/D	A	C/D	A/B	A/B	C/D	C/D	A	B	C/D	C/D	C/D	C/D	D	C	class 3	N.E.	S.Kunze/M.Ochs, BMG	January 2008	Revision 4b (May 19, 2005)			
59141	Shibutani et al. (1994)	yes	yes	yes (can be used)	class 2	C/D	A	C/D	A/B	A/B	C/D	C/D	A	B	C/D	C/D	C/D	C/D	D	C	class 3	N.E.	S.Kunze/M.Ochs, BMG	January 2008	Revision 4b (May 19, 2005)			
60586	Ticknor and McMurry (1996)	yes	yes	yes (can be used)	class 1	B	A	A/B	A/B	C/D	C/D	C/D	B	C/D	A/B	C/D	B	C/D	D	B	class 3	N.E. (zero sorption)	S.Kunze/M.Ochs, BMG	May 2009	Revision 4b (May 19, 2005)			
60587	Ticknor and McMurry (1996)	yes	yes	yes (can be used)	class 1	B	A	A/B	A/B	C/D	C/D	C/D	B	C/D	A/B	C/D	B	C/D	D	B	class 3	N.E. (zero sorption)	S.Kunze/M.Ochs, BMG	May 2009	Revision 4b (May 19, 2005)			
60588	Ticknor and McMurry (1996)	yes	yes	yes (can be used)	class 1	B	A	A/B	A/B	C/D	C/D	C/D	A	C/D	A/B	C/D	B	C/D	D	B	class 2	N.E. (zero sorption)	S.Kunze/M.Ochs, BMG	May 2009	Revision 4b (May 19, 2005)			
60589	Ticknor and McMurry (1996)	yes	yes	yes (can be used)	class 1	B	A	A/B	A/B	C/D	C/D	C/D	B	C/D	A/B	C/D	B	C/D	D	B	class 3	N.E. (zero sorption)	S.Kunze/M.Ochs, BMG	May 2009	Revision 4b (May 19, 2005)			
60590	Ticknor and McMurry (1996)	yes	yes	yes (can be used)	class 1	B	A	A/B	A/B	C/D	C/D	C/D	B	C/D	A/B	C/D	B	C/D	D	B	class 3	N.E. (zero sorption)	S.Kunze/M.Ochs, BMG	May 2009	Revision 4b (May 19, 2005)			
60591	Ticknor and McMurry (1996)	yes	yes	yes (can be used)	class 1	B	A	A/B	A/B	C/D	C/D	C/D	B	C/D	A/B	C/D	B	C/D	D	B	class 3	N.E. (zero sorption)	S.Kunze/M.Ochs, BMG	May 2009	Revision 4b (May 19, 2005)			
60592	Ticknor and McMurry (1996)	yes	yes	yes (can be used)	class 1	B	A	A/B	A/B	C/D	C/D	C/D	B	C/D	A/B	C/D	B	C/D	D	B	class 3	N.E. (zero sorption)	S.Kunze/M.Ochs, BMG	May 2009	Revision 4b (May 19, 2005)			
60593	Ticknor and McMurry (1996)	yes	yes	yes (can be used)	class 1	B	A	A/B	A/B	C/D	C/D	C/D	B	C/D	A/B	C/D	B	C/D	D	B	class 2	approximately consistent with other data for granitic rocks	S.Kunze/M.Ochs, BMG	May 2009	Revision 4b (May 19, 2005)			
60594	Ticknor and McMurry (1996)	yes	yes	yes (can be used)	class 1	B	A	A/B	A/B	C/D	C/D	B	A	C/D	A/B	C/D	B	C/D	D	B	class 2	approximately consistent with other data for granitic rocks	S.Kunze/M.Ochs, BMG	May 2009	Revision 4b (May 19, 2005)			
60595	Ticknor and McMurry (1996)	yes	yes	yes (can be used)	class 1	B	A	A/B	A/B	C/D	C/D	A	A	C/D	A/B	C/D	B	C/D	D	B	class 2	approximately consistent with other data for granitic rocks	S.Kunze/M.Ochs, BMG	May 2009	Revision 4b (May 19, 2005)			
60596	Ticknor and McMurry (1996)	yes	yes	yes (can be used)	class 1	B	A	A/B	A/B	C/D	C/D	B	A	C/D	A/B	C/D	B	C/D	D	B	class 2	approximately consistent with other data for granitic rocks	S.Kunze/M.Ochs, BMG	May 2009	Revision 4b (May 19, 2005)			
60597	Ticknor and McMurry (1996)	yes	yes	yes (can be used)	class 1	B	A	A/B	A/B	C/D	C/D	C/D	B	C/D	A/B	C/D	B	C/D	D	B	class 3	approximately consistent with other data for granitic rocks	S.Kunze/M.Ochs, BMG	May 2009	Revision 4b (May 19, 2005)			
60598	Ticknor and McMurry (1996)	yes	yes	yes (can be used)	class 1	B	A	A/B	A/B	C/D	C/D	A	A	C/D	A/B	C/D	B	C/D	D	B	class 2	approximately consistent with other data for granitic rocks	S.Kunze/M.Ochs, BMG	May 2009	Revision 4b (May 19, 2005)			
60599	Ticknor and McMurry (1996)	yes	yes	yes (can be used)	class 1	B	A	A/B	A/B	C/D	C/D	A	A	C/D	A/B	C/D	B	C/D	D	B	class 2	approximately consistent with other data for granitic rocks	S.Kunze/M.Ochs, BMG	May 2009	Revision 4b (May 19, 2005)			
60600	Ticknor and McMurry (1996)	yes	yes	yes (can be used)	class 1	B	A	A/B	A/B	C/D	C/D	A	A	C/D	A/B	C/D	B	C/D	D	B	class 2	approximately consistent with other data for granitic rocks	S.Kunze/M.Ochs, BMG	May 2009	Revision 4b (May 19, 2005)			
60601	Ticknor and McMurry (1996)	yes	yes	yes (can be used)	class 1	B	A	A/B	A/B	C/D	C/D	A	A	C/D	A/B	C/D	B	C/D	D	B	class 2	approximately consistent with other data for granitic rocks	S.Kunze/M.Ochs, BMG	May 2009	Revision 4b (May 19, 2005)			
60602	Ticknor and McMurry (1996)	yes	yes	yes (can be used)	class 1	B	A	A/B	A/B	C/D	C/D	C/D	B	C/D	A/B	C/D	B	C/D	D	B	class 3	approximately consistent with other data for granitic rocks	S.Kunze/M.Ochs, BMG	May 2009	Revision 4b (May 19, 2005)			
60603	Ticknor and McMurry (1996)	yes	yes	yes (can be used)	class 1	B	A	A/B	A/B	C/D	C/D	A	A	C/D	A/B	C/D	B	C/D	D	B	class 2	approximately consistent with other data for granitic rocks	S.Kunze/M.Ochs, BMG	May 2009	Revision 4b (May 19, 2005)			
60604	Ticknor and McMurry (1996)	yes	yes	yes (can be used)	class 1	B	A	A/B	A/B	C/D	C/D	A	A	C/D	A/B	C/D	B	C/D	D	B	class 2	approximately consistent with other data for granitic rocks	S.Kunze/M.Ochs, BMG	May 2009	Revision 4b (May 19, 2005)			
60605	Ticknor and McMurry (1996)	yes	yes	yes (can be used)	class 1	B	A	A/B	A/B	C/D	C/D	A	A	C/D	A/B	C/D	B	C/D	D	B	class 2	approximately consistent with other data for granitic rocks	S.Kunze/M.Ochs, BMG	May 2009	Revision 4b (May 19, 2005)			
60688	Ticknor(1988)	-	yes(tentative)	yes (can be used)	class 1	B	B	C/D	unreliable												unreliable	N.E.	S.Kunze/M.Ochs, BMG	December 2006	Revision 4b (May 19, 2005)			
60689	Ticknor(1988)	-	yes(tentative)	yes (can be used)	class 1	B	B	A/B	C/D(tentative)	A/B	A/B	A	A	B	C/D	A/B	C/D	C/D	D	C	class 3	N.E.	S.Kunze/M.Ochs, BMG	December 2006	Revision 4b (May 19, 2005)			
60690	Ticknor(1988)	-	yes(tentative)	yes (can be used)	class 1	B	B	A/B	C/D(tentative)	A/B	A/B	A	A	B	C/D	A/B	C/D	C/D	D	C	class 3	N.E.	S.Kunze/M.Ochs, BMG	December 2006	Revision 4b (May 19, 2005)			
60691	Ticknor(1988)	-	yes(tentative)	yes (can be used)	class 1	B	B	A/B	C/D(tentative)	A/B	A/B	A	A	B	C/D	A/B	C/D	C/D	D	C	class 3	N.E.	S.Kunze/M.Ochs, BMG	December 2006	Revision 4b (May 19, 2005)			
60692	Ticknor(1988)	-	yes(tentative)	yes (can be used)	class 1	B	B	A/B	unreliable												unreliable	N.E.	S.Kunze/M.Ochs, BMG	December 2006	Revision 4b (May 19, 2005)			
60693	Ticknor(1988)	-	yes(tentative)	yes (can be used)	class 1	B	B	A/B	C/D(tentative)	A/B	A/B	A	A	B	C/D	A/B	C/D	C/D	D	C	class 3	N.E.	S.Kunze/M.Ochs, BMG	December 2006	Revision 4b (May 19, 2005)			
60694	Ticknor(1988)	-	yes(tentative)	yes (can be used)	class 1	B	B	A/B	unreliable												unreliable	N.E.	S.Kunze/M.Ochs, BMG	December 2006	Revision 4b (May 19, 2005)			
60695	Ticknor(1988)	-	yes(tentative)	yes (can be used)	class 1	B	B	C/D	C/D(tentative)	A/B	A/B	A	A	B	C/D	A/B	C/D	C/D	D	C	class 1	N.E.	S.Kunze/M.Ochs, BMG	December 2006	Revision 4b (May 19, 2005)			
60696	Ticknor(1988)	-	yes(tentative)	yes (can be used)	class 1	B	B	C/D	C/D(tentative)	A/B	A/B	A	A	B	C/D	A/B	C/D	C/D	D	C	class 4	N.E.	S.Kunze/M.Ochs, BMG	December 2006	Revision 4b (May 19, 2005)			
50201	Davis and Leckie (1980)	yes	yes	yes (can be used)	class 4	A	A	A/B	A/B	A/B	C/D	A	A	C/D	A/B	A/B	B	C/D	D	B	class 2	consistent with independent data	S.Kunze/M.Ochs, BMG	October 2007	Revision 4b (May 19, 2005)			
50202	Davis and Leckie (1980)	yes	yes	yes (can be used)	class 4	A	A	A/B	A/B	A/B	C/D	A	A	C/D	A/B	A/B	B	C/D	D	B	class 2	consistent with independent data	S.Kunze/M.Ochs, BMG	October 2007	Revision 4b (May 19, 2005)			
50203	Davis and Leckie (1980)	yes	yes	yes (can be used)	class 4	A	A	A/B	A/B	A/B	C/D	A	A	C/D	A/B	A/B	B	C/D	D	B	class 2	consistent with independent data	S.Kunze/M.Ochs, BMG	October 2007	Revision 4b (May 19, 2005)			
50204	Davis and Leckie (1980)	yes	yes	yes (can be used																								

Se	I - Completeness of documentation and title of Kd	II - Technical and scientific quality of reported data	III - Consistency	Operator	Data	Classification Guideline																			
Datapoint	Reference	Rating => I-a: Yes/No, I-b: class 1-6	Rating I-a	Rating I-b	II-a	II-b	II-c	II-d	II-e	II-f	II-g	II-h	II-i	II-j	II-k	II-l	II-m	II-n	II-o	Rating II	comment/rating				
		I-a.1	I-a.2		II-a phase	pH	redox condition	solution composition	temperature	S/W	sortive value	initial [RN]	phase separation	reaction time	aeration	RN loading	reaction vessels	error estimates	parameter variation						
52834	Hayes et al. (1988)	yes	yes (tentative)	yes (can be used)	class 4	A	A	A/B	A/B	C/D	C/D	B	A	C/D	C/D	A/B	C/D	B	D	B	class 2	internally consistent behavior of Se(VI) & Se(IV), consistent with independent data	S.Kunze/M.Ochs, BMG	October 2007	Revision 4b (May 19, 2005)
52835	Hayes et al. (1988)	yes	yes (tentative)	yes (can be used)	class 4	A	A	A/B	A/B	C/D	C/D	B	A	C/D	C/D	A/B	C/D	B	D	B	class 2	internally consistent behavior of Se(VI) & Se(IV), consistent with independent data	S.Kunze/M.Ochs, BMG	October 2007	Revision 4b (May 19, 2005)
52836	Hayes et al. (1988)	yes	yes (tentative)	yes (can be used)	class 4	A	A	A/B	A/B	C/D	C/D	B	A	C/D	C/D	A/B	C/D	B	D	B	class 2	internally consistent behavior of Se(VI) & Se(IV), consistent with independent data	S.Kunze/M.Ochs, BMG	October 2007	Revision 4b (May 19, 2005)
52837	Hayes et al. (1988)	yes	yes (tentative)	yes (can be used)	class 4	A	A	A/B	A/B	C/D	C/D	A	A	C/D	C/D	A/B	C/D	B	D	B	class 2	internally consistent behavior of Se(VI) & Se(IV), consistent with independent data	S.Kunze/M.Ochs, BMG	October 2007	Revision 4b (May 19, 2005)
52838	Hayes et al. (1988)	yes	yes (tentative)	yes (can be used)	class 4	A	A	A/B	A/B	C/D	C/D	A	A	C/D	C/D	A/B	C/D	B	D	B	class 2	internally consistent behavior of Se(VI) & Se(IV), consistent with independent data	S.Kunze/M.Ochs, BMG	October 2007	Revision 4b (May 19, 2005)
52839	Hayes et al. (1988)	yes	yes (tentative)	yes (can be used)	class 4	A	A	A/B	A/B	C/D	C/D	A	A	C/D	C/D	A/B	C/D	B	D	B	class 2	internally consistent behavior of Se(VI) & Se(IV), consistent with independent data	S.Kunze/M.Ochs, BMG	October 2007	Revision 4b (May 19, 2005)
52840	Hayes et al. (1988)	yes	yes (tentative)	yes (can be used)	class 4	A	A	A/B	A/B	C/D	C/D	A	A	C/D	C/D	A/B	C/D	B	D	B	class 2	internally consistent behavior of Se(VI) & Se(IV), consistent with independent data	S.Kunze/M.Ochs, BMG	October 2007	Revision 4b (May 19, 2005)
52841	Hayes et al. (1988)	yes	yes (tentative)	yes (can be used)	class 4	A	A	A/B	A/B	C/D	C/D	A	A	C/D	C/D	A/B	C/D	B	D	B	class 2	internally consistent behavior of Se(VI) & Se(IV), consistent with independent data	S.Kunze/M.Ochs, BMG	October 2007	Revision 4b (May 19, 2005)
52842	Hayes et al. (1988)	yes	yes (tentative)	yes (can be used)	class 4	A	A	A/B	A/B	C/D	C/D	A	A	C/D	C/D	A/B	C/D	B	D	B	class 2	internally consistent behavior of Se(VI) & Se(IV), consistent with independent data	S.Kunze/M.Ochs, BMG	October 2007	Revision 4b (May 19, 2005)
52843	Hayes et al. (1988)	yes	yes (tentative)	yes (can be used)	class 4	A	A	A/B	A/B	C/D	C/D	B	A	C/D	C/D	A/B	C/D	B	D	B	class 2	internally consistent behavior of Se(VI) & Se(IV), consistent with independent data	S.Kunze/M.Ochs, BMG	October 2007	Revision 4b (May 19, 2005)
52844	Hayes et al. (1988)	yes	yes (tentative)	yes (can be used)	class 4	A	A	A/B	A/B	C/D	C/D	A	A	C/D	C/D	A/B	C/D	B	D	B	class 2	internally consistent behavior of Se(VI) & Se(IV), consistent with independent data	S.Kunze/M.Ochs, BMG	October 2007	Revision 4b (May 19, 2005)
52845	Hayes et al. (1988)	yes	yes (tentative)	yes (can be used)	class 4	A	A	A/B	A/B	C/D	C/D	A	A	C/D	C/D	A/B	C/D	B	D	B	class 2	internally consistent behavior of Se(VI) & Se(IV), consistent with independent data	S.Kunze/M.Ochs, BMG	October 2007	Revision 4b (May 19, 2005)
52846	Hayes et al. (1988)	yes	yes (tentative)	yes (can be used)	class 4	A	A	A/B	A/B	C/D	C/D	B	A	C/D	C/D	A/B	C/D	B	D	B	class 2	internally consistent behavior of Se(VI) & Se(IV), consistent with independent data	S.Kunze/M.Ochs, BMG	October 2007	Revision 4b (May 19, 2005)
52847	Hayes et al. (1988)	yes	yes (tentative)	yes (can be used)	class 4	A	A	A/B	A/B	C/D	C/D	A	A	C/D	C/D	A/B	C/D	B	D	B	class 2	internally consistent behavior of Se(VI) & Se(IV), consistent with independent data	S.Kunze/M.Ochs, BMG	October 2007	Revision 4b (May 19, 2005)
52848	Hayes et al. (1988)	yes	yes (tentative)	yes (can be used)	class 4	A	A	A/B	A/B	C/D	C/D	A	A	C/D	C/D	A/B	C/D	B	D	B	class 2	internally consistent behavior of Se(VI) & Se(IV), consistent with independent data	S.Kunze/M.Ochs, BMG	October 2007	Revision 4b (May 19, 2005)
52849	Hayes et al. (1988)	yes	yes (tentative)	yes (can be used)	class 4	A	A	A/B	A/B	C/D	C/D	A	A	C/D	C/D	A/B	C/D	B	D	B	class 2	internally consistent behavior of Se(VI) & Se(IV), consistent with independent data	S.Kunze/M.Ochs, BMG	October 2007	Revision 4b (May 19, 2005)
52850	Hayes et al. (1988)	yes	yes (tentative)	yes (can be used)	class 4	A	A	A/B	A/B	C/D	C/D	A	A	C/D	C/D	A/B	C/D	B	D	B	class 2	internally consistent behavior of Se(VI) & Se(IV), consistent with independent data	S.Kunze/M.Ochs, BMG	October 2007	Revision 4b (May 19, 2005)
52851	Hayes et al. (1988)	yes	yes (tentative)	yes (can be used)	class 4	A	A	A/B	A/B	C/D	C/D	A	A	C/D	C/D	A/B	C/D	B	D	B	class 2	internally consistent behavior of Se(VI) & Se(IV), consistent with independent data	S.Kunze/M.Ochs, BMG	October 2007	Revision 4b (May 19, 2005)
52852	Hayes et al. (1988)	yes	yes (tentative)	yes (can be used)	class 4	A	A	A/B	A/B	C/D	C/D	A	A	C/D	C/D	A/B	C/D	B	D	B	class 2	internally consistent behavior of Se(VI) & Se(IV), consistent with independent data	S.Kunze/M.Ochs, BMG	October 2007	Revision 4b (May 19, 2005)
52853	Hayes et al. (1988)	yes	yes (tentative)	yes (can be used)	class 4	A	A	A/B	A/B	C/D	C/D	A	A	C/D	C/D	A/B	C/D	B	D	B	class 2	internally consistent behavior of Se(VI) & Se(IV), consistent with independent data	S.Kunze/M.Ochs, BMG	October 2007	Revision 4b (May 19, 2005)
52854	Hayes et al. (1988)	yes	yes (tentative)	yes (can be used)	class 4	A	A	A/B	A/B	C/D	C/D	A	A	C/D	C/D	A/B	C/D	B	D	B	class 2	internally consistent behavior of Se(VI) & Se(IV), consistent with independent data	S.Kunze/M.Ochs, BMG	October 2007	Revision 4b (May 19, 2005)
52855	Hayes et al. (1988)	yes	yes (tentative)	yes (can be used)	class 4	A	A	A/B	A/B	C/D	C/D	A	A	C/D	C/D	A/B	C/D	B	D	B	class 2	internally consistent behavior of Se(VI) & Se(IV), consistent with independent data	S.Kunze/M.Ochs, BMG	October 2007	Revision 4b (May 19, 2005)
52856	Hayes et al. (1988)	yes	yes (tentative)	yes (can be used)	class 4	A	A	A/B	A/B	C/D	C/D	A	A	C/D	C/D	A/B	C/D	B	D	B	class 2	internally consistent behavior of Se(VI) & Se(IV), consistent with independent data	S.Kunze/M.Ochs, BMG	October 2007	Revision 4b (May 19, 2005)
52857	Hayes et al. (1988)	yes	yes (tentative)	yes (can be used)	class 4	A	A	A/B	A/B	C/D	C/D	A	A	C/D	C/D	A/B	C/D	B	D	B	class 2	internally consistent behavior of Se(VI) & Se(IV), consistent with independent data	S.Kunze/M.Ochs, BMG	October 2007	Revision 4b (May 19, 2005)
52858	Hayes et al. (1988)	yes	yes (tentative)	yes (can be used)	class 4	A	A	A/B	A/B	C/D	C/D	A	A	C/D	C/D	A/B	C/D	B	D	B	class 2	internally consistent behavior of Se(VI) & Se(IV), consistent with independent data	S.Kunze/M.Ochs, BMG	October 2007	Revision 4b (May 19, 2005)
52859	Hayes et al. (1988)	yes	yes (tentative)	yes (can be used)	class 4	A	A	A/B	A/B	C/D	C/D	A	A	C/D	C/D	A/B	C/D	B	D	B	class 2	internally consistent behavior of Se(VI) & Se(IV), consistent with independent data	S.Kunze/M.Ochs, BMG	October 2007	Revision 4b (May 19, 2005)
52860	Hayes et al. (1988)	yes	yes (tentative)	yes (can be used)	class 4	A	A	A/B	A/B	C/D	C/D	A	A	C/D	C/D	A/B	C/D	B	D	B	class 2	internally consistent behavior of Se(VI) & Se(IV), consistent with independent data	S.Kunze/M.Ochs, BMG	October 2007	Revision 4b (May 19, 2005)
52861	Hayes et al. (1988)	yes	yes (tentative)	yes (can be used)	class 4	A	A	A/B	A/B	C/D	C/D	A	A	C/D	C/D	A/B	C/D	B	D	B	class 2	internally consistent behavior of Se(VI) & Se(IV), consistent with independent data	S.Kunze/M.Ochs, BMG	October 2007	Revision 4b (May 19, 2005)
52862	Hayes et al. (1988)	yes	yes (tentative)	yes (can be used)	class 4	A	A	A/B	A/B	C/D	C/D	A	A	C/D	C/D	A/B	C/D	B	D	B	class 2	internally consistent behavior of Se(VI) & Se(IV), consistent with independent data	S.Kunze/M.Ochs, BMG	October 2007	Revision 4b (May 19, 2005)
52863	Hayes et al. (1988)	yes	yes (tentative)	yes (can be used)	class 4	A	A	A/B	A/B	C/D	C/D	A	A	C/D	C/D	A/B	C/D	B	D	B	class 2	internally consistent behavior of Se(VI) & Se(IV), consistent with independent data	S.Kunze/M.Ochs, BMG	October 2007	Revision 4b (May 19, 2005)
52864	Hayes et al. (1988)	yes	yes (tentative)	yes (can be used)	class 4	A	A	A/B	A/B	C/D	C/D	A	A	C/D	C/D	A/B	C/D	B	D	B	class 2	internally consistent behavior of Se(VI) & Se(IV), consistent with independent data	S.Kunze/M.Ochs, BMG	October 2007	Revision 4b (May 19, 2005)
52865	Hayes et al. (1988)	yes	yes (tentative)	yes (can be used)	class 4	A	A	A/B	A/B	C/D	C/D	A	A	C/D	C/D	A/B	C/D	B	D	B	class 2	internally consistent behavior of Se(VI) & Se(IV), consistent with independent data	S.Kunze/M.Ochs, BMG	October 2007	Revision 4b (May 19, 2005)
52866	Hayes et al. (1988)	yes	yes (tentative)	yes (can be used)	class 4	A	A	A/B	A/B	C/D	C/D	A	A	C/D	C/D	A/B	C/D	B	D	B	class 2	internally consistent behavior of Se(VI) & Se(IV), consistent with independent data	S.Kunze/M.Ochs, BMG	October 2007	Revision 4b (May 19, 2005)
52867	Hayes et al. (1988)	yes	yes (tentative)	yes (can be used)	class 4	A	A	A/B	A/B	C/D	C/D	C/D	A	C/D	C/D	A/B	C/D	B	D	B	class 2	internally consistent behavior of Se(VI) & Se(IV), consistent with independent data	S.Kunze/M.Ochs, BMG	October 2007	Revision 4b (May 19, 2005)
52868	Hayes et al. (1988)	yes	yes (tentative)	yes (can be used)	class 4	A	A	A/B	A/B	C/D	C/D	C/D	A	C/D	C/D	A/B	C/D	B	D	B	class 2	internally consistent behavior of Se(VI) & Se(IV), consistent with independent data	S.Kunze/M.Ochs, BMG	October 2007	Revision 4b (May 19, 2005)
52869	Hayes et al. (1988)	yes	yes (tentative)	yes (can be used)	class 4	A	A	A/B	A/B	C/D	C/D	C/D	A	C/D	C/D	A/B	C/D	B	D	B	class 2	internally consistent behavior of Se(VI) & Se(IV), consistent with independent data	S.Kunze/M.Ochs, BMG	October 2007	Revision 4b (May 19, 2005)
52870	Hayes et al. (1988)	yes	yes (tentative)	yes (can be used)	class 4	A	A	A/B	A/B	C/D	C/D	C/D	A	C/D	C/D	A/B	C/D	B	D	B	class 2	internally consistent behavior of Se(VI) & Se(IV), consistent with independent data	S.Kunze/M.Ochs, BMG	October 2007	Revision 4b (May 19, 2005)
52871	Hayes et al. (1988)	yes	yes (tentative)	yes (can be used)	class 4	A	A	A/B	A/B	C/D	C/D	C/D	A	C/D	C/D	A/B	C/D	B	D	B	class 2	internally consistent behavior of Se(VI) & Se(IV), consistent with independent data	S.Kunze/M.Ochs, BMG	October 2007	Revision 4b (May 19, 2005)
52872	Hayes et al. (1988)	yes	yes (tentative)	yes (can be used)	class 4	A	A	A/B	A/B	C/D	C/D	C/D	A	C/D	C/D	A/B	C/D	B	D	B	class 2	internally consistent behavior of Se(VI) & Se(IV), consistent with independent data	S.Kunze/M.Ochs, BMG	October 2007	Revision 4b (May 19, 2005)
52873	Hayes et al. (1988)	yes	yes (tentative)	yes (can be used)	class 4	A	A	A/B	A/B	C/D	C/D	C/D	A	C/D	C/D	A/B	C/D	B	D	B	class 2	internally consistent behavior of Se(VI) & Se(IV), consistent with independent data	S.Kunze/M.Ochs, BMG	October 2007	Revision 4b (May 19, 2005)
52874	Hayes et al. (1988)	yes	yes (tentative)	yes (can be used)	class 4	A	A	A/B	A/B	C/D	C/D	A	A	C/D	C/D	A/B	C/D	B	D	B	class 2	internally consistent behavior of Se(VI) & Se(IV), consistent with independent data	S.Kunze/M.Ochs, BMG	October 2007	Revision 4b (May 19, 2005)
52875	Hayes et al. (1988)	yes	yes (tentative)	yes (can be used)	class 4	A	A	A/B	A/B	C/D	C/D	A	A	C/D	C/D	A/B	C/D	B	D	B	class 2	internally consistent behavior of Se(VI) & Se(IV), consistent with independent data	S.Kunze/M.Ochs, BMG	October 2007	Revision 4b (May 19, 2005)
52876	Hayes et al. (1988)	yes	yes (tentative)	yes (can be used)	class 4	A	A	A/B	A/B	C/D	C/D	A	A	C/D	C/D	A/B	C/D	B	D	B	class 2	internally consistent behavior of Se(VI) & Se(IV), consistent with independent data	S.Kunze/M.Ochs, BMG	October 2007	Revision 4b (May 19, 2005)
52877	Hayes et al. (1988)	yes	yes (tentative)	yes (can be used)	class 4	A	A	A/B	A/B	C/D	C/D	A	A	C/D	C/D	A/B	C/D	B	D	B	class 2	internally consistent behavior of Se(VI) & Se(IV), consistent with independent data	S.Kunze/M.Ochs, BMG	October 2007	Revision 4b (May 19, 2005)
52878	Hayes et al. (1988)	yes	yes (tentative)	yes (can be used)	class 4	A	A	A/B	A/B	C/D	C/D	A	A	C/D	C/D	A/B	C/D	B	D	B	class 2	internally consistent behavior of Se(VI) & Se(IV), consistent with independent data	S.Kunze/M.Ochs, BMG	October 2007	Revision 4b (May 19, 2005)
52879	Hayes et al. (1988)	yes	yes (tentative)	yes (can be used)	class 4	A	A	A/B	A/B	C/D	C/D	A	A	C/D	C/D	A/B	C/D	B	D	B	class 2	internally consistent behavior of Se(VI) & Se(IV), consistent with independent data	S.Kunze/M.Ochs, BMG	October 2007	Revision 4b (May 19, 2005)
52880	Hayes et al. (1988)	yes	yes (tentative)	yes (can be used)	class 4	A	A	A/B	A/B	C/D	C/D	A	A	C/D	C/D	A/B	C/D	B	D	B	class 2	internally consistent behavior of Se(VI) & Se(IV), consistent with independent data	S.Kunze/M.Ochs, BMG	October 2007	Revision 4b (May 19, 2005)
52881	Hayes et al. (1988)	yes	yes (tentative)	yes (can be used)	class 4	A	A	A/B	A/B	C/D	C/D	A	A	C/D	C/D	A/B	C/D	B	D	B	class 2	internally consistent behavior of Se(VI) & Se(IV), consistent with independent data	S.Kunze/M.Ochs, BMG	October 2007	Revision 4b (May 19, 2005)
52882	Hayes et al. (1988)	yes	yes (tentative)	yes (can be used)	class 4	A	A	A/B	A/B	C/D	C/D	A	A	C/D	C/D	A/B	C/D	B	D	B	class 2	internally consistent behavior of Se(VI) & Se(IV), consistent with independent data	S.Kunze/M.Ochs, BMG	October 2007	Revision 4b (May 19, 2005)
52883	Hayes et al. (1988)	yes	yes (tentative)	yes (can be used)	class 4	A	A	A/B	A/B	C/D	C/D	A	A	C/D	C/D	A/B	C/D	B	D	B	class 2	internally consistent behavior of Se(VI) & Se(IV), consistent with independent data	S.Kunze/M.Ochs, BMG	October 2007	Revision 4b (May 19, 2005)
52884	Hayes et al. (1988)	yes	yes (tentative)	yes (can be used)	class 4	A	A	A/B	A/B	C/D	C/D	A	A	C/D	C/D	A/B	C/D	B	D	B	class 2	internally consistent behavior of Se(VI) & Se(IV), consistent with independent data	S.Kunze/M.Ochs, BMG	October 2007	Revision 4b (May 19, 2005)
52885	Hayes et al. (1988)	yes	yes (tentative)	yes (can be used)	class 4	A	A	A/B	A/B	C/D	C/D	A	A	C/D	C/D	A/B	C/D	B	D	B	class 2	internally consistent behavior of Se(VI) & Se(IV), consistent with independent data	S.Kunze/M.Ochs, BMG	October 2007	Revision 4b (May 19, 2005)
52886	Hayes et al. (1988)	yes	yes (tentative)	yes (can be used)	class 4	A	A	A/B	A/B	C/D	C/D	A	A	C/D	C/D	A/B	C/D	B	D	B	class 2	internally consistent behavior of Se(VI) & Se(IV), consistent with independent data	S.Kunze/M.Ochs, BMG		

Se	I – Completeness of documentation and type of Kd	II – Technical and scientific quality of reported data	III – Consistency	Operator	Data	Classification Guideline																
	Rating ⇒ I-a: Yes/No, I-b: class 1-6	Checkpoints ⇒ level: A-D (numerical value: 3-0)/unreliable	Rating ⇒ class1-6/unreliable																			
Datapoint	Reference	I-a.1	I-a.2	Rating I-a	Rating I-b	II-a	II-b	II-c	II-d	II-e	II-f	II-g	II-h	II-i	II-j	II-k	II-l	II-m	II-n	II-o	Rating II	comment/rating
52956	Hayes et al. (1988)	yes	yes (tentative)	yes (can be used)	class 4	A	A	A/B	A/B	C/D	C/D	C/D	A	C/D	C/D	A/B	C/D	B	D	B	class 2	internally consistent behavior of Se(VI) & Se(IV), consistent with independent data
52957	Hayes et al. (1988)	yes	yes (tentative)	yes (can be used)	class 4	A	A	A/B	A/B	C/D	C/D	C/D	A	C/D	C/D	A/B	C/D	B	D	B	class 2	internally consistent behavior of Se(VI) & Se(IV), consistent with independent data
52958	Hayes et al. (1988)	yes	yes (tentative)	yes (can be used)	class 4	A	A	A/B	A/B	C/D	C/D	A	A	C/D	C/D	A/B	C/D	B	D	B	class 2	internally consistent behavior of Se(VI) & Se(IV), consistent with independent data
52959	Hayes et al. (1988)	yes	yes (tentative)	yes (can be used)	class 4	A	A	A/B	A/B	C/D	C/D	B	A	C/D	C/D	A/B	C/D	B	D	B	class 2	internally consistent behavior of Se(VI) & Se(IV), consistent with independent data
52960	Hayes et al. (1988)	yes	yes (tentative)	yes (can be used)	class 4	A	A	A/B	A/B	C/D	C/D	B	A	C/D	C/D	A/B	C/D	B	D	B	class 2	internally consistent behavior of Se(VI) & Se(IV), consistent with independent data
52961	Hayes et al. (1988)	yes	yes (tentative)	yes (can be used)	class 4	A	A	A/B	A/B	C/D	C/D	B	A	C/D	C/D	A/B	C/D	B	D	B	class 2	internally consistent behavior of Se(VI) & Se(IV), consistent with independent data
52962	Hayes et al. (1988)	yes	yes (tentative)	yes (can be used)	class 4	A	A	A/B	A/B	C/D	C/D	B	A	C/D	C/D	A/B	C/D	B	D	B	class 2	internally consistent behavior of Se(VI) & Se(IV), consistent with independent data
52963	Hayes et al. (1988)	yes	yes (tentative)	yes (can be used)	class 4	A	A	A/B	A/B	C/D	C/D	B	A	C/D	C/D	A/B	C/D	B	D	B	class 2	internally consistent behavior of Se(VI) & Se(IV), consistent with independent data
52964	Hayes et al. (1988)	yes	yes (tentative)	yes (can be used)	class 4	A	A	A/B	A/B	C/D	C/D	A	A	C/D	C/D	A/B	C/D	B	D	B	class 2	internally consistent behavior of Se(VI) & Se(IV), consistent with independent data
52965	Hayes et al. (1988)	yes	yes (tentative)	yes (can be used)	class 4	A	A	A/B	A/B	C/D	C/D	A	A	C/D	C/D	A/B	C/D	B	D	B	class 2	internally consistent behavior of Se(VI) & Se(IV), consistent with independent data
52966	Hayes et al. (1988)	yes	yes (tentative)	yes (can be used)	class 4	A	A	A/B	A/B	C/D	C/D	A	A	C/D	C/D	A/B	C/D	B	D	B	class 2	internally consistent behavior of Se(VI) & Se(IV), consistent with independent data
52967	Hayes et al. (1988)	yes	yes (tentative)	yes (can be used)	class 4	A	A	A/B	A/B	C/D	C/D	A	A	C/D	C/D	A/B	C/D	B	D	B	class 2	internally consistent behavior of Se(VI) & Se(IV), consistent with independent data
52968	Hayes et al. (1988)	yes	yes (tentative)	yes (can be used)	class 4	A	A	A/B	A/B	C/D	C/D	A	A	C/D	C/D	A/B	C/D	B	D	B	class 2	internally consistent behavior of Se(VI) & Se(IV), consistent with independent data
52969	Hayes et al. (1988)	yes	yes (tentative)	yes (can be used)	class 4	A	A	A/B	A/B	C/D	C/D	A	A	C/D	C/D	A/B	C/D	B	D	B	class 2	internally consistent behavior of Se(VI) & Se(IV), consistent with independent data
52970	Hayes et al. (1988)	yes	yes (tentative)	yes (can be used)	class 4	A	A	A/B	A/B	C/D	C/D	A	A	C/D	C/D	A/B	C/D	B	D	B	class 2	internally consistent behavior of Se(VI) & Se(IV), consistent with independent data
52971	Hayes et al. (1988)	yes	yes (tentative)	yes (can be used)	class 4	A	A	A/B	A/B	C/D	C/D	A	A	C/D	C/D	A/B	C/D	B	D	B	class 2	internally consistent behavior of Se(VI) & Se(IV), consistent with independent data
52972	Hayes et al. (1988)	yes	yes (tentative)	yes (can be used)	class 4	A	A	A/B	A/B	C/D	C/D	A	A	C/D	C/D	A/B	C/D	B	D	B	class 2	internally consistent behavior of Se(VI) & Se(IV), consistent with independent data
52973	Hayes et al. (1988)	yes	yes (tentative)	yes (can be used)	class 4	A	A	A/B	A/B	C/D	C/D	A	A	C/D	C/D	A/B	C/D	B	D	B	class 2	internally consistent behavior of Se(VI) & Se(IV), consistent with independent data
52974	Hayes et al. (1988)	yes	yes (tentative)	yes (can be used)	class 4	A	A	A/B	A/B	C/D	C/D	A	A	C/D	C/D	A/B	C/D	B	D	B	class 2	internally consistent behavior of Se(VI) & Se(IV), consistent with independent data
59142	Shibutani et al. (1994)	yes	yes	yes (can be used)	class 2	B	A	C/D	A/B	A/B	A/B	A	A	B	C/D	C/D	C/D	C/D	D	C	class 3	appears to represent detection limit (tentative)
59143	Shibutani et al. (1994)	yes	yes	yes (can be used)	class 2	B	A	C/D	A/B	A/B	A/B	A	A	B	C/D	C/D	C/D	C/D	D	C	class 3	appears to represent detection limit (tentative)
59144	Shib																					

I – Completeness of documentation and type of Kd										II – Technical and scientific quality of reported data												III – Consistency			Operator	Data	Classification Guideline
Rating ⇒ I-a: Yes/No, I-b: class 1–6										Checkpoints ⇒ level: A–D (numerical value: 3–0)/unreliable Rating ⇒ class1–6/unreliable																	
Datapoint	Reference	I-a.1	I-a.2	Rating I-a	Rating I-b	II-a solid phase	II-b pH	II-c redox condition	II-d solution composition	II-e temperature	II-f S/W	II-g sorptive value	II-h initial [RN]	II-i phase separation	II-j reaction time	II-k agitation	II-l RN loading	II-m reaction vessels	II-n error estimates	II-o parameter variation	Rating II	comment/rating					
42459	Allard et al. (1979b)	yes	yes	yes (can be used)	class 1	C/D	C	A/B	A/B	A/B	C/D		unreliable								unreliable	fairly consistent with independent data	S.Kunze/M.Ochs, BMG	November 2008	Revision 4b (May 19, 2005)		
42460	Allard et al. (1979b)	yes	yes	yes (can be used)	class 1	C/D	C	A/B	A/B	A/B	C/D		A	A	unreliable							fairly consistent with independent data	S.Kunze/M.Ochs, BMG	November 2008	Revision 4b (May 19, 2005)		
42461	Allard et al. (1979b)	yes	yes	yes (can be used)	class 1	C/D	C	A/B	A/B	A/B	C/D	C/D	A		C/D	A/B	C/D	C/D	D	C	class 6	fairly consistent with independent data	S.Kunze/M.Ochs, BMG	November 2008	Revision 4b (May 19, 2005)		
42462	Allard et al. (1979b)	yes	yes	unreliable	class 1	C/D	C	A/B	A/B	A/B	C/D		unreliable								unreliable	fairly consistent with independent data	S.Kunze/M.Ochs, BMG	November 2008	Revision 4b (May 19, 2005)		
42463	Allard et al. (1979b)	yes	yes	yes (can be used)	class 1	C/D	C	A/B	A/B	A/B	C/D		unreliable								unreliable	fairly consistent with independent data	S.Kunze/M.Ochs, BMG	November 2008	Revision 4b (May 19, 2005)		
42464	Allard et al. (1979b)	yes	yes	yes (can be used)	class 1	C/D	C	A/B	A/B	A/B	C/D	C/D	A	A	unreliable						class 6	fairly consistent with independent data	S.Kunze/M.Ochs, BMG	November 2008	Revision 4b (May 19, 2005)		
42465	Allard et al. (1979b)	yes	yes	yes (can be used)	class 1	C/D	C	A/B	A/B	A/B	C/D		unreliable								unreliable	fairly consistent with independent data	S.Kunze/M.Ochs, BMG	November 2008	Revision 4b (May 19, 2005)		
42466	Allard et al. (1979b)	yes	yes	yes (can be used)	class 1	C/D	C	A/B	A/B	A/B	C/D		unreliable								unreliable	fairly consistent with independent data	S.Kunze/M.Ochs, BMG	November 2008	Revision 4b (May 19, 2005)		
42467	Allard et al. (1979b)	yes	yes	yes (can be used)	class 1	C/D	C	A/B	A/B	A/B	C/D	B	A	A	C/D	A/B	C/D	C/D	D	C	class 6	fairly consistent with independent data	S.Kunze/M.Ochs, BMG	November 2008	Revision 4b (May 19, 2005)		
42468	Allard et al. (1979b)	yes	yes	yes (can be used)	class 1	C/D	C	A/B	A/B	A/B	C/D	B	A	A	C/D	A/B	C/D	C/D	D	C	class 6	fairly consistent with independent data	S.Kunze/M.Ochs, BMG	November 2008	Revision 4b (May 19, 2005)		
42469	Allard et al. (1979b)	yes	yes	yes (can be used)	class 1	C/D	C	A/B	A/B	A/B	C/D	B	A	A	C/D	A/B	C/D	C/D	D	C	class 6	fairly consistent with independent data	S.Kunze/M.Ochs, BMG	November 2008	Revision 4b (May 19, 2005)		
42470	Allard et al. (1979b)	yes	yes	yes (can be used)	class 1	C/D	C	A/B	A/B	A/B	C/D		unreliable								unreliable	fairly consistent with independent data	S.Kunze/M.Ochs, BMG	November 2008	Revision 4b (May 19, 2005)		
42230	Allard et al. (1978)	yes	yes	yes (can be used)	class 1	C/D	D (tent.)	A/B	A/B	A/B	C/D	N.E.	A	C/D	C/D	C/D	C/D	C/D	D	D	N.E.	fairly consistent with independent data	S.Kunze/M.Ochs, BMG	November 2008	Revision 4b (May 19, 2005)		
42231	Allard et al. (1978)	yes	yes	yes (can be used)	class 1	C/D	D (tent.)	A/B	unreliable												unreliable	fairly consistent with independent data	S.Kunze/M.Ochs, BMG	November 2008	Revision 4b (May 19, 2005)		
54053	Koskinen et al. (1985)	yes	yes	yes (can be used)	class 1	C/D	A	A/B	A/B	A/B	C/D	C/D	A	B	C/D	A/B	C/D	B	D	D	class 3	N.E. (limiting values only)	S.Kunze/M.Ochs, BMG	November 2008	Revision 4b (May 19, 2005)		
54054	Koskinen et al. (1985)	yes	yes	yes (can be used)	class 1	C/D	A	A/B	A/B	A/B	C/D	C/D	A	B	C/D	A/B	C/D	B	D	D	class 3	N.E. (limiting values only)	S.Kunze/M.Ochs, BMG	November 2008	Revision 4b (May 19, 2005)		
54055	Koskinen et al. (1985)	yes	yes	yes (can be used)	class 1	C/D	A	A/B	A/B	A/B	C/D	C/D	A	B	C/D	A/B	C/D	B	D	D	class 3	N.E. (limiting values only)	S.Kunze/M.Ochs, BMG	November 2008	Revision 4b (May 19, 2005)		
54056	Koskinen et al. (1985)	yes	yes	yes (can be used)	class 1	C/D	A	A/B	A/B	A/B	C/D	C/D	A	B	C/D	A/B	C/D	B	D	D	class 3	N.E. (limiting values only)	S.Kunze/M.Ochs, BMG	November 2008	Revision 4b (May 19, 2005)		
61613	Ueta (1998)	yes	yes	yes (can be used)	class 1	C/D	A	A/B	unreliable												unreliable	N.E.	S.Kunze/M.Ochs, BMG	January 2008	Revision 4b (May 19, 2005)		
61614	Ueta (1998)	yes	yes	yes (can be used)	class 1	C/D	A	A/B	unreliable												unreliable	N.E.	S.Kunze/M.Ochs, BMG	January 2008	Revision 4b (May 19, 2005)		
61615	Ueta (1998)	yes	yes	yes (can be used)	class 1	C/D	A	A/B	unreliable												unreliable	N.E.	S.Kunze/M.Ochs, BMG	January 2008	Revision 4b (May 19, 2005)		
61616	Ueta (1998)	yes	yes	yes (can be used)	class 1	C/D	A	A/B	unreliable												unreliable	N.E.	S.Kunze/M.Ochs, BMG	January 2008	Revision 4b (May 19, 2005)		
61617	Ueta (1998)	yes	yes	yes (can be used)	class 1	C/D	A	A/B	A/B	A/B	C/D	A	C/D	A	C/D	A/B	C/D	C/D	D	D	class 3	approximately consistent with independent data	S.Kunze/M.Ochs, BMG	January 2008	Revision 4b (May 19, 2005)		
61618	Ueta (1998)	yes	yes	yes (can be used)	class 1	C/D	A	A/B	A/B	A/B	C/D	A	C/D	A	C/D	A/B	C/D	C/D	D	D	class 3	approximately consistent with independent data	S.Kunze/M.Ochs, BMG	January 2008	Revision 4b (May 19, 2005)		
61619	Ueta (1998)	yes	yes	yes (can be used)	class 1	C/D	A	A/B	A/B	A/B	C/D	A	C/D	A	C/D	A/B	C/D	C/D	D	D	class 3	approximately consistent with independent data	S.Kunze/M.Ochs, BMG	January 2008	Revision 4b (May 19, 2005)		
61620	Ueta (1998)	yes	yes	yes (can be used)	class 1	C/D	A	A/B	A/B	A/B	C/D	A	C/D	A	C/D	A/B	C/D	C/D	D	D	class 3	approximately consistent with independent data	S.Kunze/M.Ochs, BMG	January 2008	Revision 4b (May 19, 2005)		
53524	Hunter et al. (1988)	yes	yes	yes (can be used)	class 4	A	A	A/B	A/B	A/B	A/B	A	A	C/D	C/D	A/B	C/D	C/D	D	C	class 2	consistent with independent data	S.Kunze/M.Ochs, BMG	February 2008	Revision 4b (May 19, 2005)		
53525	Hunter et al. (1988)	yes	yes	yes (can be used)	class 4	A	A	A/B	A/B	A/B	A/B	A	A	C/D	C/D	A/B	C/D	C/D	D	C	class 2	consistent with independent data	S.Kunze/M.Ochs, BMG	February 2008	Revision 4b (May 19, 2005)		
53526	Hunter et al. (1988)	yes	yes	yes (can be used)	class 4	A	A	A/B	A/B	A/B	A/B	A	A	C/D	C/D	A/B	C/D	C/D	D	C	class 2	consistent with independent data	S.Kunze/M.Ochs, BMG	February 2008	Revision 4b (May 19, 2005)		
58545	Righetto et al. (1988)	yes	yes	yes (can be used)	class 4	A	A	A/B	A/B	C/D	C/D	A	A	B	A/B	A/B	C/D	B	D	C	class 2	consistent with independent data	S.Kunze/M.Ochs, BMG	January 2008	Revision 4b (May 19, 2005)		
58546	Righetto et al. (1988)	yes	yes	yes (can be used)	class 4	A	A	A/B	A/B	C/D	C/D	A	A	B	A/B	A/B	C/D	B	D	C	class 2	consistent with independent data	S.Kunze/M.Ochs, BMG	January 2008	Revision 4b (May 19, 2005)		
58547	Righetto et al. (1988)	yes	yes	yes (can be used)	class 4	A	A	A/B	A/B	C/D	C/D	A	A	B	A/B	A/B	C/D	B	D	C	class 2	consistent with independent data	S.Kunze/M.Ochs, BMG	January 2008	Revision 4b (May 19, 2005)		

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	立方メートル	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
比透磁率 ^(b)	(数字の)	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、工事率、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	ウェーバ	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
光束流	ルーメン	lm		cd sr ^(c)
照射度	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 sA
表面電荷	クーロン毎平方メートル	C/m ²	m ⁻² sA
電束密度、電気変位	クーロン毎平方メートル	C/m ²	m ⁻² sA
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 sA
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=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	1ha=1hm ² =10 ⁴ m ²
リットル	L, l	1L=1l=1dm ³ =10 ³ cm ³ =10 ⁻³ m ³
トン	t	1t=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	1eV=1.602 176 53(14)×10 ⁻¹⁹ J
ダルトン	Da	1Da=1.660 538 86(28)×10 ⁻²⁷ kg
統一原子質量単位	u	1u=1 Da
天文単位	ua	1ua=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=100kPa=10 ⁵ Pa
水銀柱ミリメートル	mmHg	1mmHg=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
バイン	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 =0.1Pa s
ストークス	St	1 St=1cm ² s ⁻¹ =10 ⁻⁴ m ² s ⁻¹
スチルブ	sb	1 sb=1cd cm ⁻² =10 ⁴ cd m ⁻²
フオト	ph	1 ph=1cd sr cm ⁻² 10 ⁴ lx
ガリ	Gal	1 Gal=1cm 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=1Mx 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=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	f	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=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
カロリー	cal	1cal=4.1858J（「15℃」カロリー）、4.1868J（「IT」カロリー）4.184J（「熱化学」カロリー）
マイクロン	μ	1 μ =1μm=10 ⁻⁶ m

