AGENCE DE L'OCDE POUR L'ÉNERGIE NUCLÉAIRE
OECD NUCLEAR ENERGY AGENCY

TDB-0

THE NEA THERMOCHEMICAL DATA BASE PROJECT

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Contents

The NEA Thermochemical Data Base Project

This document is intended as a background and brief guide on the chemical thermochemical data base project of the OECD/NEA, often referred to as the TDB project. It aims to explain the general structure of the project, as well as some of the working procedures. This is a revised version for phase II of the project.

Much of the text has been taken directly from the "Agreement on the OECD/NEA Thermochemical Database Project (Phase II)", signed in December 1997 by the participating organisations (see Appendix A).

1 Background

1.1 General

In order to assess the safety of a radioactive waste repository, it is essential to be able to predict the eventual migration of its components into the environment. Numerical simulation and/or modelling of processes affecting the behaviour of radionuclides in natural and man-made systems is an integral part of a radiological assessment methodology. Some of the basic information is provided by speciation calculations using general, non-site-specific, chemical thermodynamic data. The value of the results of geochemical modelling as a predictive tool is strongly dependent on the quality of the thermodynamic data used to calculate the chemical speciation.

1.2 Thermochemical data bases: background

Phase I of the TDB project was initiated in 1984. At the time, it was clear that although a number of thermodynamic data compilations and reviews had already been published [82WAG/EVA, 78ROB/HEM, 82PAN, 78COD], none of them could be used reliably as a complete source data table to study the behaviour of radioelements in the environment. To be useful in performance assessment work, a data base must:

- contain data for all the elements of interest in radioactive waste disposal systems
- document why and how the data were selected
- document the sources of experimental data used
- be internally consistent
- treat all solids and aqueous species of the elements of interest

None of the existing data bases at the time fulfilled all of these criteria. Although several potentially interesting compilations of thermochemical data have been made since then (e. g. [89COX/WAG, 91DIN, 88PHI/HAL, 91MAY/MUR]), still none of these meet all the criteria above. In particular, the documentation

on how and why a particular datum was selected is often omitted, in favour of general guidelines or no information at all. It is also common to find specialised thermochemical databases intended for quite different purposes, such as general geochemical modelling under hydrothermal conditions, metallurgical simulations etc. Consequently, most research groups supporting the performance assessment of radioactive waste disposal still use their own databases for modelling purposes.

However, these individual data bases may lack internal consistency, and they often differ considerably from each other, especially in the data of the actinides. It is thus not surprising that radionuclide speciation and maximum solubilities calculated by different groups, with different geochemical computer codes and data, but for similar conditions, often turn out to differ by orders of magnitude. It has been recognised that these discrepancies are due to shortcomings in different data bases, rather than in the computer codes used.

The OECD/NEA TDB project was started in response to the recognition among the member countries of the NEA of shortcomings in these existing national databases. This work has been described earlier [85MUL, 88WAN, 91WAN]. In the first phase of this project, extensive literature reviews and data evaluations were undertaken to develop a comprehensive, internally consistent and internationally recognised thermodynamic database for the inorganic chemistry of five elements: uranium, americium, technetium, neptunium and plutonium.

1.2.1 CODATA

The ICSU Committee on Data for Science and Technology (CODATA) has had a Task Group on Key Values for Thermodynamics which has published highly reliable critical assessments and recommended values of thermodynamic parameters for selected key substances since 1971. These data have become the *de facto* international standard for chemical thermodynamic data. This group's work, on expanding the set of highly reliable data, continues under the Task Group on Chemical Thermodynamic Tables. To be of general value, any chemical thermodynamic data base developed at the corporate, national or international level, must be consistent with the CODATA data set. This consistency is therefore a primary goal of the NEA TDB project.

1.2.2 IAEA reports

Starting in 1976, the International Atomic Energy Agency published a series of 14 reports on the chemical thermodynamics of the actinides. Since they are as CODATA consistent as possible, these reports are an excellent start for developing a reliable actinide data set. Unfortunately, the IAEA is no longer active in this area. The early reports are out of date. Six of the principal contributors to the

IAEA series were consulted when the NEA review was initiated. All of these contributors agreed that the NEA review would provide a valuable continuation to the IAEA work on the actinides and would supplement it with the work on the selected fission-product elements.

2 The TDB project

2.1 TDB phase I

The first phase of the OECD/NEA Thermochemical Database (TDB) Project was initiated in 1984, to fulfil the need as described above for a high-quality database for modelling purposes in safety analyses for radioactive waste repositories. This phase of the project has also described elsewhere [85MUL, 88WAN]. A comprehensive, internally consistent and internationally recognised thermodynamic database has been developed for the inorganic, aqueous and solid chemistry of five elements: uranium, americium, technetium, neptunium and plutonium. Recommended data for uranium and americium have been published and similar publications for technetium, neptunium and plutonium are being finalised. The result is a set of reliable thermodynamic parameters that can be used to describe the behaviour of these elements under conditions relevant for radioactive waste disposal systems and the geochemical environments.

2.2 TDB phase II

Due to the *ad hoc* structure of the first phase of the TDB Project, important delays were encountered, and the project did not meet the schedule of certain national radioactive waste management programmes. In order to avoid further delays, a second phase of the TDB Project, based on a more rigorous organisation, was agreed upon by the following organisations:

ANSTO, Australia
NIRAS/ONDRAF, Belgium,
RAWRA, Czech Republic,
POSIVA, Finland,
ANDRA, France,
IPSN, France,
FZK, Germany,
PNC, Japan,
ENRESA, Spain
SKB, Sweden,
SKI, Sweden,

HSK, Switzerland,
NAGRA, Switzerland,
PSI, Switzerland,
BNFL, UK,
NIREX, UK,
DoE, USA,

This project is referred to as the TDB phase II project, or simply TDB II.

2.3 How the TDB II project is organised

The second phase of the TDB Project is organised as a semi-autonomous project under the guidance of a Management Board, representing the participating organisations or countries. The OECD/NEA acts as the Project Co-ordinator, assisted and advised in technical matters by an Executive Group of the Management Board. Review Teams are set up (one per element or group of elements/ligands) to review available information, evaluate existing data and to prepare interim and final reports. A schematic layout of the organisation structure is shown in Figure 1.

The Management Board is ultimately responsible for the project and defines and approves the annual Programme of Work and Budget of the TDB Project. The Management Board will decide the details of the work programme as the need arises.

The Executive Group, which consists of three to five persons with a strong technical background, acts as a technical adviser to the Management Board. It also gives advice and assists the Project Co-ordinator in the conduct of its work.

The OECD/NEA acts as the Project Co-ordinator. The main part of this work is performed by the NEA Data Bank and covers predominantly two areas of responsibility: the co-ordination of the Review Teams and the update and maintenance of the TDB database. The NEA Data Bank will also continue to service other scientists in OECD/NEA Member countries with information from the TDB database.

The Review Teams, one for each element or group of elements/ligands, consist of approximately three to five experts per team, approved by the Management Board. Their main tasks are to critically review the chemical thermodynamic data available for the element/ligand in question, recommend a set of data, and present these data, together with a justification for the selection, in a report. The report is peer-reviewed before final publication. The members of the review team have to be highly qualified in the area of science covered by the review, together covering a wide range of direct experimental experience. This experimental experience is

crucial for the experts to be able to judge the quality and completeness of the scientific publications to be reviewed.

Each review team has an "initiator" and a chairman, which may or may not be the same person. The role of the initiator is to propose suitable members of the review team. The initiators are chosen by the Executive Group and the NEA Project Coordinator jointly, on grounds of availability as well as sufficient expertise in the field.

The initiators proposal for review team is subject to approval by the Executive Group and ultimately the Management Board. The formal nomination of the review team to the Management Board is made by the project coordinator (cf. Appendix A). Once the review team has been approved by the management board, the work of the initiator is over.

The role of the chairman of the review team, is to coordinate the work within the review team once the work has started. The chairman of the review team is also ultimately responsible for the quality of the report. It is the task of the chairman to ensure that the contributions from all authors arrive in a timely fashion. In addition to authoring parts of the review, the chairman of the review team has the overview of the review, and makes sure that consistency is maintained within the report, and that the review is complete in terms of covering the chemical systems of interest.

The chairman of the review team is elected by the members of the review team. As the task of being chairman can be quite time-consuming, availability and organizational skills should be emphasized when electing a chairman, alongside with expert knowledge.

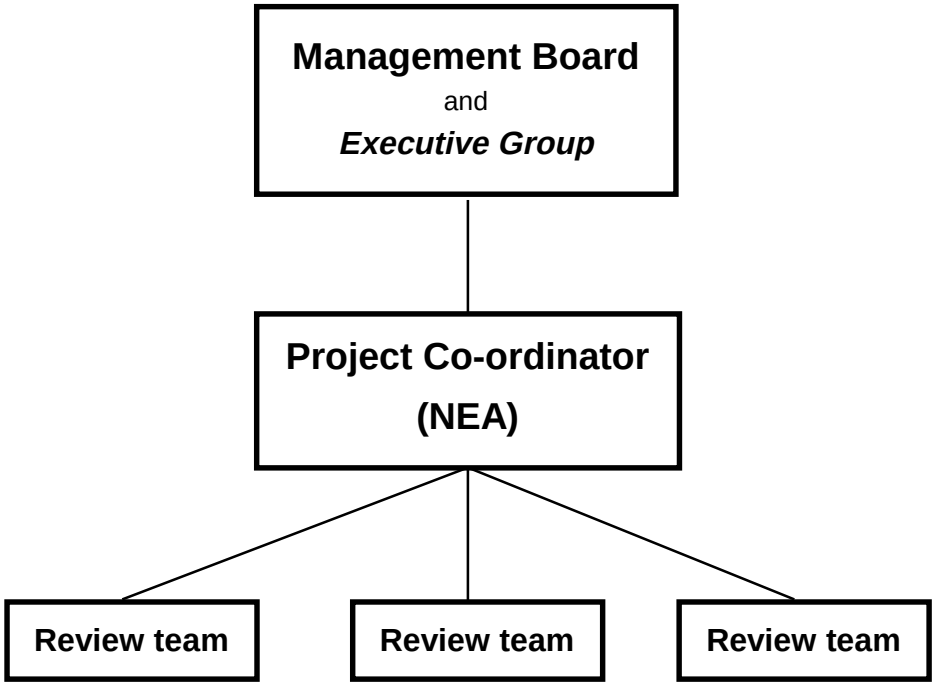
2.4 The new reviews of TDB phase II

The following new reviews are planned within the TDB phase II project.

- An update of the U/Am/Tc/Np/Pu reviews (one review team for all elements).
- Inorganic complexes and compounds of Ni.
- Inorganic complexes and compounds of Se.
- Simple organic ligands (isosaccharinic acid (ISA), EDTA, citrate and oxalate) of U, Am, Tc, Np, Pu, Ni, Se, Zr and some selected competing cations.
- Inorganic complexes and compounds of Zr.

These review areas were decided on taking into account the mobility, radioactivity and half-lives of the commonly occurring nuclides in radioactive waste, as well as the particular areas of interest of the funding organisations.

Figure 1: The organization of the NEA-TDB Project



3 Rationale for the selection of parameters

A variety of parameters could be included in a chemical thermodynamic data base. The selection of which parameters to include in the NEA data base was based on the needs of existing chemical models, the generality of applications and the availability of data.

Most geochemical modelling codes work with equilibrium constants. Although solubility and equilibrium constant data would thus appear appropriate for inclusion in the data base, different models may, and often do, use different sets of thermodynamic components, in the Gibbs' phase rule sense of the word, for the chemical reactions associated with the equilibrium constants. To avoid having to recalculate the selected equilibrium constants for different sets of components, the data set collected in the TDB project includes standard molar Gibbs energy ($\Delta_f G^\circ_m$) and enthalpy ($\Delta_f H^\circ_m$) of formation, standard molar entropy (S°_m) and heat capacity at constant pressure ($C^\circ_{p,m}$). The equilibrium constants needed can then be derived from these parameters for the aqueous species and solid phases of interest. This approach also makes it easier to check the internal consistency of the selected thermodynamic parameters.

As the parameters in this set vary as a function of temperature, provision has been made to include the compilation of the coefficients of empirical temperature functions for these thermodynamic data, as well as the temperature ranges over which they are valid. In these cases, the data are fitted to obtain the most significant coefficients of the following empirical function:

$$\begin{aligned} F(T) &= a + bT + cT^2 + dT^{-1} + eT^{-2} + f\ln T + gT\ln T + h\sqrt{T} \\ &\quad + i\frac{1}{\sqrt{T}} + jT^3 + kT^{-3} \end{aligned} \tag{1}$$

Most temperature variations can be described with two to four parameters, a, b, c (or d) and e being the ones most frequently used.

Although in principle the temperature dependence can be recorded for any of the selected parameters, only temperature dependencies for $C_{p,m}$ have been selected in the TDB data base so far.

Since various publications in the scientific literature contain equilibrium constants or thermodynamic data of reaction rather than the thermodynamic data of formation of single species, the database can also store chemical reactions, as well as the corresponding reaction data (including temperature dependencies) with uncertainties in SI units. This also allows selected data to be stored for reactions where no formation data can be extracted, as well as giving users of the data base the possibility to use the selected reaction data directly without having to recalculate these data from formation data. Such recalculations usually lead to

uncertainties that are much larger than those assigned to the original experimental data.

The following reaction data are stored:

$\log_{10} K$	the equilibrium constant of the reaction, logarithmic	
$\Delta_r G_m$	the molar Gibbs energy of reaction	(kJ·mol^{-1})
$\Delta_r H_m$	the molar enthalpy of reaction	(kJ·mol^{-1})
$\Delta_r S_m$	the molar entropy of reaction	(J·K^{-1}·mol^{-1})
$\Delta_r C_{p,m}$	the molar heat capacity of reaction	(J·K^{-1}·mol^{-1})

The temperature functions of these data, if available, are also stored, according to Eq. (1).

As a rule, selected data are presented for a temperature of 298.15 K and a pressure of 1 bar (1×10^5 Pa). The pressure dependence of thermodynamic data is not considered in the NEA/TDB reviews. The specific reference conditions used in the NEA TDB project reviews are described in the TDB guideline report TDB-5 [99NEA].

For many modelling purposes, equilibrium constants are required for temperatures different from 25°C. Ideally, the temperature function of the reaction heat capacity, $\Delta_r C^\circ_{p,m}(T)$, is used to calculate the temperature dependence of the corresponding equilibrium constant. When the required heat capacity functions are not available, various methods to estimate heat capacities and entropies must be used (see [97ALL/BAN, Chapter X], which is also available as the TDB-4 Guideline [99NEA]).

4 Compilation of literature data

The first step of the review procedure is the compilation of data published in the scientific literature for each key element. In principle, the literature search should cover everything relevant that has ever been published on the subject (for update reviews, the literature search will obviously start at the date where the previous review report stopped). For most reviews, however, some restrictions have to be made since the resources available are not sufficient to cover everything that could possibly be included. These restrictions are subject to the endorsement of the Executive Group and ultimately the approval of the Management Board. The restrictions are made taking into account primarily the needs of the radioactive waste disposal performance assessment community. The restrictions made are documented in the respective review reports. Some common restrictions are described in section 5.1.

5 Critical review procedure and data selection

5.1 Restrictions in the literature reviewed

As mentioned above, the TDB project covers only selected thermodynamic quantities, not non-thermodynamic data such as diffusion and kinetic data.

Normally, the collection of literature data is done keeping in mind the target audience for the review reports, i. e. the nuclear waste storage performance assessment (PA) community. Hence, data which are of no or little interest for PA calculations are normally not considered in the reviews. Examples of areas that are normally excluded are:

- Complexation in non-aqueous solvents
- Sorption
- Diffusion and kinetic data
- Low-temperature data (below 200 K)
- Alloys and other non-stoichiometric compounds
- Polyelectrolytes and organic ligands other than those treated by the review group for simple organic ligands.
- Melts

Minerals are normally excluded because of the lack of well-defined stoichiometries; reliable thermodynamic data for minerals are rather scarce (see e. g. [95SIL/BID, Appendix D]).

The authors of the review reports may, however, decided to include one or more of the areas above, if the available resources allow. Such inclusions must be cleared with the TDB project coordinator before any work in these areas is started.

5.2 Estimates

In general, the OECD/NEA TDB reviews only take into account primary experimental data, not estimates, values from compilations or calculated parameters. However, if scientifically well established procedures for making estimates of otherwise unavailable data (i. e. by analogies with similar elements) exist, such procedures may be employed. If no reliable experimental data exist and no data are available for similar elements that would allow estimates to be made, the TBD reviews do not attempt to fill the resulting gaps in the thermodynamic data base. Areas that merit further experimental investigation are pointed out in the review

reports. The selection procedure is described in detail in the TDB-1 guideline [99NEA].

5.3 Data sources used

As stated above, in general the OECD/NEA TDB reviews only take into account primary experimental data. It is essential to, to the largest extent possible, obtain the original publication containing the experimental details when performing the review work.

When possible, experimental source data are re-evaluated by using chemical models which are found to be more accurate than those used by the original authors. The final result is a selected set of data of formation and reaction for each key element considered by the review, as well as for the auxiliary data that were used for recalculations in the critical review. It is essential that the consistent auxiliary data set is used in conjunction with the data set of the key element. The selected data and their uncertainties are stored in the TDB data base.

Detailed guidelines for the review procedure can be found in the following documents:

TDB-1 Guidelines for the review procedure and data selection [99NEA]

TDB-2 Guidelines on the extrapolation to zero ionic strength [99NEA]

TDB-3 Guidelines on the assignment of uncertainties [99NEA]

TDB-4 Guidelines for temperature corrections [99NEA]

TDB-5 Standards and conventions in TDB publications [99NEA]

TDB-6 Guidelines for the independent peer review of TDB reports [99NEA]

5.4 Extrapolation to zero ionic strength

Thermodynamic data always refer to a selected standard state. The standard state in the NEA critical review for dissolved species is the hypothetical ideal solution at unit activity (molality scale), as it is for the CODATA Key Values [89COX/WAG], see also the TDB-5 guideline [99NEA]. Hence, the data which are evaluated from experimental measurements need to be corrected for activity coefficients. The method used by the NEA for this purpose is the specific ion interaction method (SIT), which was first outlined by Brønsted [22BRØ, 23BRØ] and elaborated by Scatchard [36SCA] and Guggenheim [66GUG]. The SIT method was established as the method of choice for the TDB project during Phase I of the project, and it will be used also in Phase II. The TDB-2 guideline [99NEA]

gives detailed information about the procedures used for extrapolation to zero ionic strength.

There are other virial expansion methods, *e.g.*, the one proposed by Pitzer [79PIT], which are sometimes more precise than the SIT theory, and are also useable over wider ranges of ionic strengths. Two or three interaction coefficients are needed in the Pitzer method, and these are available in the literature for many simple ionic species. However, equilibrium constants from different sources are rarely consistent enought to allow a determination of these parameters.

The SIT method has several advantages that make it more suitable for the TDB project:

- it is simpler (fewer parameters are needed)
- missing parameters can easily be estimated from values for ions of similar charge and size,
- the extraction of relevant parameters requires fewer experimental data,
- changing from the SIT would require a large amount of recalculation work for already selected data, and
- although there are cases (e. g. brines) where the SIT method is clearly not applicable, its accuracy and range of usefulness is adequate for geochemical modelling of a majority of the environments encountered in radioactive waste disposal sites.

For an extensive discussion on different methods for the estimation and calculation of activity coefficients in electrolyte solutions, see Chapter IX of Ref. [97ALL/BAN].

5.5 Uncertainty estimates of equilibrium data

One of the principal objectives of the OECD/NEA TDB effort is to provide an idea of the uncertainties associated with the data selected in this review. This makes the calculation of confidence limits for the derived quantities possible, although it should be noted that few geochemical modelling codes exist today that make use of this information. In general, the uncertainties should define the range within which the corresponding data can be reproduced with a probability of 95% at any place and by any appropriate method. In many cases, statistical treatment is limited or impossible due to insufficient availability of data. A particular problem has to be solved when significant discrepancies occur between different source data. The TDB-3 guideline [99NEA] contains a description of the statistical procedures that are used for the problems encountered, of the limits of these procedures, as well as guidelines for what to do when statistics are inapplicable.

6 Independent peer review

The reports resulting from the critical reviews of chemical thermodynamics within the NEA-TDB project are reviewed independently by qualified experts nominated by the review team members and the NEA, and approved by the TDB Management Board. The independent peer review is performed according to the procedures described in the TDB-6 [99NEA] document. The reports to be reviewed contain detailed discussions of the data selection resulting from the critical review of the chemical thermodynamics of a particular element. The purpose of the additional peer review is to receive an independent view of the judgements and assessments made by the primary reviewers, to verify assumptions, results and conclusions, and to check whether the relevant literature has been exhaustively considered. The independent peer review is performed by personnel having technical expertise in the subject matter to be reviewed, to a degree at least equivalent to that needed for the original review.

7 Publication of recommended data

For each element, the selected data set and the selection procedure are published under the authorship of the corresponding reviewers. The publication includes a detailed discussion of key data sources, a presentation of the re-evaluations done by the NEA reviewers, as well as a complete set of auxiliary data used in the evaluation. Usually, one volume is published for each review.

8 Data retrieval

As soon as the selected data for a certain review have passed peer review, they are made available for downloading at the NEA web site `http://www.nea.fr/html/dbtdb`.

References

[22BRØ] Brønsted, J. N., "Studies of solubility: IV. The principle of specific interaction of ions", *J. Am. Chem. Soc.*, **44** (1922) 877–898. Cited pages 11

[23BRØ] Brønsted, J. N., "The individual thermodynamic properties of ions", *J. Am. Chem. Soc.*, **45** (1923) 2898–2910. Cited pages 11

[36SCA] Scatchard, G., "Concentrated solutions of strong electrolytes", *Chem. Rev.*, **19** (1936) 309–327. Cited pages 11

[66GUG] Guggenheim, E. A., *Applications of Statistical Mechanics*, Oxford: Clarendon Press, 1966. Cited pages 11

[78COD] "CODATA recommended key values for thermodynamics 1977", Committee on Data for Science and Technology (CODATA) Bulletin 28, International council for Scientific Unions, Paris, 1978, 6 p. Cited pages 2

[78ROB/HEM] Robie, R. A., Hemingway, B. S., Fisher, J. R., "Thermodynamic properties of minerals and related substances at 298.15 K and 1 bar (10^5 Pascals) pressure and at higher temperatures", *US Geol. Surv. Bull.*, **1452**. Cited pages 2

[79PIT] Pitzer, K. S., *Activity coefficients in electrolyte solutions*, vol. 1, chap. "Theory: Ion Interaction Approach", Boca Raton: CRC Press, 1979, pp. 157–208. Cited pages 12

[82PAN] Pankratz, L. B., "Thermodynamic properties of elements and oxides", Bulletin, US Bureau of Mines, 1982, 509 p. Cited pages 2

[82WAG/EVA] Wagman, D. D., Evans, W. H., Parker, V. B., Schumm, R. H., Halow, I., Bailey, S. M., Churney, K. L., Nuttall, R. C., "The NBS tables of chemical thermodynamic properties: Selected values for inorganic and C_1 and C_2 organic substances in SI units", *J. Phys. Chem. Ref. Data*, **11, supp. 2** (1982) 1–392. Cited pages 2

[85MUL] Muller, A. B., "International Chemical Thermodynamic Data Base for Nuclear Applications", *Radioact. Waste Manage. Nucl. Fuel Cycle*, **6** (1985) 131–141. Cited pages 3, 4

[88PHI/HAL] Philips, S. L., Hale, F. V., Silvester, L. F., Siegel, M. D., "Thermodynamic tables for nuclear waste isolation: Vol.1, Aqueous solutions database", Report LBL-22860, NUREG/CR-4864, SAND87–0323, Lawrence Berkeley Lab., Berkeley, CA, USA, 1988. Cited pages 2

[88WAN] Wanner, H., "The NEA Thermochemical Data Base Project", *Radiochim. Acta*, **44/45** (1988) 325–329. Cited pages 3, 4

[89COX/WAG] Cox, J. D., Wagman, D. D., Medvedev, V. A., *CODATA Key Values for Thermodynamics*, New York: Hemisphere Publ. Corp., 1989, 271 p. Cited pages 2, 11

[91DIN] Dinsdale, A. T., "SGTE data for pure elements", *CALPHAD*, **15(4)** (1991) 317–425. Cited pages 2

[91MAY/MUR] May, P. M., Murray, K., "JESS, a joint expert speciation system: II. The thermodynamic database", *Talanta*, **38(12)** (1991) 1419–1426. Cited pages 2

[91WAN] Wanner, H., "On the problem of consistency of chemical thermodynamic data bases", in: "Scientific basis for nuclear waste management XIV", vol. 212 of *Mat. Res. Soc. Symp. Proc.*, Materials Research Society, 1991, pp. 815–822. Cited pages 3

[95SIL/BID] Silva, R. J., Bidoglio, G., Rand, M. H., Robouch, P. B., Wanner, H., Puigdomenech, I., *Chemical thermodynamics of americium*, Amsterdam: Elsevier Science Publishers B.V., 1995, 374 p. Cited pages 10

[97ALL/BAN] Allard, B., Banwart, S. A., Bruno, J., Ephraim, J. H., Grauer, R., Grenthe, I., Hadermann, J., Hummel, W., Jakob, A., Karapiperis, T., Plyasunov, A. V., Puigdomènech, I., Rard, J. A., Saxena, S., Spahiu, K., *Modelling in Aquatic Chemistry*, Paris: OECD Nuclear Energy Agency, 1997, 724 p. Cited pages 9, 12

[99NEA] "TDB-0–TDB-6, TDB project guidelines", NEA Web site PDF documents, 1999, URL `http://www.nea.fr/html/dbtdb/guidelines/guidelines.html`. Cited pages 9, 11, 12, 13

A Extract from the "Agreement on the OECD/NEA Thermochemical Database Project (Phase II)"

Article I
OBJECTIVES

1. The objectives of the TDB Project shall be:

   (a) to make available a comprehensive, internally consistent, internationally recognised and quality-assured chemical thermodynamic database of selected chemical elements;

   (b) to meet the specialised modelling requirements for safety assessments of radioactive waste disposal systems centred around performance assessment (PA) technical needs;

   (c) to maintain and update the existing database as well as the on-line services;

   (d) to provide the obtained data to the OECD/NEA Member countries;

   (e) to promote an exchange of information on activities in Member countries of relevance to the TDB project.

Article II
MANAGEMENT BOARD

1. Control of the TDB Project shall be vested in the Management Board constituted under this Article and decisions reached by the Management Board shall be binding on each Participant.

2. The Management Board shall consist of one member designated by each Participant. Participants shall also designate alternate members to represent them in the event of members being unable to do so. Participants shall notify the OECD/NEA of the members designated to represent them on the Management Board.

3. A representative of the Project Co-ordinator (as provided for under Article IV of this Agreement) shall attend the meetings of the Management Board in an advisory capacity. If the Chairperson of the Executive Group (as provided for under Article III of this Agreement) is not a member of the Management Board, this person shall also attend the meetings of the Management Board in an advisory capacity.

4. The Management Board may invite one or more members of the Executive Group or any other person to attend meetings of the Management Board as observers, if they are not already members of the Management Board.

5. The Management Board shall:

   (a) take overall responsibility for the TDB Project;

   (b) review the progress of the TDB Project annually with reference to the milestones or the revised milestones, as the case may be;

   (c) following the annual review referred to in 5b above, vote formally on any significant change to the Programme of Work;

   (d) approve each year the annual Programme of Work to meet the milestones, or the revised milestones, as the case may be;

   (e) approve each year the financial report covering the previous year;

   (f) approve annually the budget and the schedule and arrangements for the payment of contributions by Participants;

   (g) nominate the members of the Executive Group;

   (h) approve the composition of the Review Teams as proposed by the Project Co-ordinator;

   (i) make such rules of procedure, directives and regulations, consistent with the objectives and provisions of this Agreement, as may be required for the sound management of the TDB Project;

   (j) assess the results of the work carried out within the TDB Project;

   (k) consider other items submitted to it by the Project Co-ordinator, the Executive Group or any Participant;

   (l) carry out other functions conferred upon it by this Agreement.

6. The Management Board shall keep the Steering Committee for Nuclear Energy regularly informed of the general progress of work, through the OECD/NEAŠs Radioactive Waste Management Committee (RWMC) and its Advisory Group on Performance Assessment (PAAG).

7. The Management Board shall elect each year a Chairperson and a Vice-Chairperson from amongst its members. The role of the Vice-Chairperson is to replace the Chairperson in case of his/her absence.

8. The Management Board shall meet once a year or more frequently in special meetings, which shall be convened by the Chairperson upon request of a Participant, provided the latter can demonstrate the need for such a special meeting.

9. To the extent possible, the Management Board shall operate and reach its decisions by consensus. However, when formal voting is requested, decisions of the Management Board shall be taken by a two-thirds majority of the votes cast, unless unanimity is required. Members of the Management Board shall have one vote each.

10. If necessary, decisions of the Management Board may also be reached by mail, telefax, E-mail or other types of cable communication as agreed by the Management Board. The Chairperson shall be responsible for ensuring that all members are informed of each decision made pursuant to this paragraph.

11. At least 30 days before each regular meeting, notice of the time, place and agenda of the meeting shall be given by the Chairperson to each member and to other persons invited to attend the meeting.

12. The Management Board Chairperson shall, after each meeting, send to all the Participants, the members of the Management Board, the Project Co-ordinator, the Chairperson of the Executive Group and to all other persons invited to attend the meeting, a letter that contains the minutes of the meeting, including any decisions taken by the Management Board.

13. The Management Board shall conduct its business in English. Reports and other documents to be submitted to the Management Board under this Agreement shall also be in English.

Article III
EXECUTIVE GROUP

1. An Executive Group shall act as a technical adviser to the Management Board.

2. The Executive Group shall consist of a limited number of experts (ideally three to five) with a strong technical background, nominated by the Management Board from amongst its members. If it is not possible to find appropriate experts among the members of the Management Board, the Board may nominate external experts from participating countries as members of the Executive Group, taking into account their technical expertise in the field and their availability.

3. The Executive Group shall be considered as a sub-group of the Management Board.

4. The Executive Group shall accomplish and be responsible for specific tasks on behalf of the Management Board. In particular it shall:

(a) oversee the technical content of the TDB Project;

(b) monitor the completion of the milestones of the TDB Project as defined in the Programme of Work;

(c) advise and assist the Project Co-ordinator in the conduct of its work;

(d) submit progress reports to the Management Board twice a year, prepared jointly with the Project Co-ordinator.

5. The Executive Group shall elect each year a Chairperson from amongst its members.

6. The Executive Group shall meet as it deems necessary, and shall be convened by its Chairperson. A representative of the Project Co-ordinator shall attend the meetings in an advisory capacity. The Executive Group may invite the Team Leader of one or more Review Teams to attend one or more specific meetings of the Group.

7. At least 30 days before each meeting, notice of the time, place and agenda of the meeting shall be given by the Chairperson to each member and to other persons entitled to attend the meeting.

8. The Executive Group Chairperson shall, after each meeting, send to all Participants, the members of the Executive Group, the Management Board, the Project Co-ordinator and to all other persons invited to attend the meetings, a letter containing the minutes of the meeting, including any advice and recommendations of the Management Board to the Review Teams.

9. The Executive Group shall conduct its business in English. Reports and other documents to be submitted to the Executive Group under this Agreement shall also be in English.

Article IV
PROJECT CO-ORDINATOR

1. The OECD Nuclear Energy Agency is invited to act as Project Co-ordinator for the TDB Project.

2. The Project Co-ordinator shall be responsible for the co-ordination of the TDB Project activities, exercise operational control over the TDB Project and take all steps required to implement the TDB Project in accordance with the terms and conditions of this Agreement and the decisions of the Management Board. The Project Co-ordinator reports directly to the Management Board.

3. The Project Co-ordinator shall be responsible for:

   (a) ensuring that the TDB Project is administered in accordance with the Programme of Work and within the limits of funds;

   (b) preparing, in accordance with a format agreed by the Management Board, the draft annual Programme of Work and Budget not later than three months before the beginning of the financial year as defined in Article VI;

   (c) proposing to the Management Board the schedule and arrangements for payment of contributions by Participants;

   (d) submitting progress reports to the Management Board twice a year, prepared jointly with the Executive Group;

   (e) submitting a financial report covering the previous year to the Management Board, not later than two months after the end of each financial year;

   (f) nominating the members of the Review Teams and submit the nominations to the Management Board for approval.

4. Furthermore, the Project Co-ordinator shall carry out specific technical tasks. These are the following:

   (a) maintain and update the thermochemical database;

   (b) provide on-line services;

   (c) organise the meetings of the Review Teams and co-ordinate their work;

   (d) organise a peer-review process of the final recommendations of the Review Teams;

   (e) organise the publication of the reports;

   (f) provide secretariat services to the Management Board and to the Executive Group.

Article V
REVIEW TEAMS

1. Review Teams shall be set up according to the needs of the TDB Project.

2. Each Review Team shall comprise a limited number of experts (ideally three to five). The members of each Review Team shall be nominated by the Project Co-ordinator and their names shall be submitted to the Management Board for approval. The Executive Group should be consulted by the

Project Co-ordinator prior to submission of the names to the Management Board. The members of a Review Team shall be selected taking into account their strong technical expertise in the field and their availability. A member of the Review Team may not at the same time be a member of the Management Board or of the Executive Group.

3. A framework for each Review Team shall be established by the Project Co-ordinator and agreed by the Management Board. In general, the tasks of the Review Teams shall be to examine available information in accordance with the TDB Project, evaluate existing data and prepare interim and final reports. The reports are to be submitted first to the Project Co-ordinator and the Executive Group and then transmitted to the Management Board for information.

Article VII
INFORMATION

1. Documents strictly related to the carrying out of the TDB Project (annual Programme of Work and Budget, Annual Financial Report, Progress Reports, etc.) shall be made available to the Participants of the TDB Project only.

2. The Project Co-ordinator will collect and preserve all information and data of direct relevance to the TDB project.

3. The recommended sets of thermodynamic data and associated documents provided under this Project which are considered to be in a final stage and are not considered to be confidential by the Management Board shall be made available to all OECD/NEA Member countries.

4. The final technical reports will be published in the open literature.