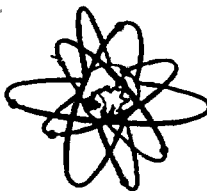


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NDB/5681/ef

8 April 1987

Dear Dr. Kelly

Thank you for your letter of 12th March 1987 in which you express your interest in receiving detailed information on the development of the NEA Thermochemical Data Base (TDB).

Let me try to give you some information on the points in which you are especially interested :

1) Evaluation Procedure : I enclose two recent publications which describe the TDB Project in more detail. As you see, we established for each element considered a special team of internationally acknowledged experts who are performing a critical review on the thermodynamic data available for all known chemical species of this element. The review and the final selection of recommended data is based on experimental evidence, and sometimes reevaluations have to be done of measurements which are reported in the scientific literature. The evaluation procedure is thus based on very fundamental information and is for this reason extremely time-consuming. It should be mentioned that each expert team includes one member who is involved in CODATA evaluations, and who has the responsibility for assuring compatibility of the reviews with the CODATA recommendations.

2) Schedules : Since the TDB Project is still at an early stage, it is difficult to set up a schedule for the publication of the selected data sets and the detailed reviews. The Uranium Review is in full momentum now, but the uranium experts decided recently that the experiments on a couple of very fundamental reactions (the redox reaction  $UO_2^{2+}/U^{4+}$ , and the hydrolysis of  $U^{4+}$ ) need to be repeated in the course of this year. Under these circumstances, the Uranium Review is not likely to be completed before the end of the year. Nevertheless, we hope to be able to submit the final report for publication in early 1988. The Technetium volume will follow in late 1988, and the ones on Americium, Palladium, and Iodine in 1989.

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224

The Neptunium Review will start immediately after the Uranium Review has been finished because some experts are members of both teams. The Neptunium Report is thus not to be expected before 1990.

3) Results to Date : These are no "results" in terms of selected thermodynamic data sets available at NEA at the moment. However, sets of compiled data on specific elements are available at any time on request. They represent the current state of our compilation of thermodynamic data at NEA, prior to the selection procedure.

4) Compatibility with geochemical codes : Since the thermodynamic data sets, which will be selected by the NEA review teams, consist of very fundamental "data of formation" rather than the "data of reaction" used in most geochemical codes, we have developed an interface program which recalculates "data of reaction" out of "data of formation", and factors them to the format in which they can directly be used as input data to geochemical codes like PHREEQE, MINEQL, and EQ 3/6. This service can, of course, be used as soon as selected data sets are available from NEA.

We are aware of the work by Dr. S. Phillips at LBL. His chemical thermodynamic data base will certainly be of value in Radioactive Waste Management studies, because it can offer internally consistent data which is available now, or in the near future. However in my opinion the validity of the procedures used is weakened by the underlying experimental data compilation, where as far as I could see the data sets were not themselves always critically selected, so that the averaging process may include poor data as well as good. I do believe that the combined experience of a group of specialised reviewers for each element studied is essential in selecting a high quality and up to date data base which in turn will guarantee the validity of the final recommended data sets.

I hope that this information will satisfy your request. Please do not hesitate to contact me if you have further questions.

Yours sincerely,

  
Hans Wanner