Josep Bonet, Montserrat Filella, Peter M May, Ruth F May and Kevin Murray
(under the auspices of Murdoch University and the University of Geneva)

present the

JESS Thermodynamic Database v8.9

Introduction

24-Jan-2023

The 'Joint Expert Speciation System' (JESS) package of software and thermodynamic databases [1-5] is a large body of computer software and data concerned primarily with the modelling of chemical phenomena in water solutions. It is now the world's largest single electronic repository of thermodynamic information relevant to such systems.

At the core of the software package is a thermodynamic database called the 'JESS Parent Database' (JPD). The current work presents the whole contents of this database in a set of associated PDF documents, which have been specifically prepared for free, widespread scientific dissemination.

JPD now comprises over 80,000 chemical reactions for which some 280,000 equilibrium constants and other thermodynamic parameters have been recorded from the chemical literature. Over 70,000 distinct chemical species are involved. While there are a number of key differences due to the specific objectives of JESS, JPD follows the tradition of earlier published compilations of such thermodynamic data such as those of the Chemical Society Special Publications SP17 [6] and SP25 [7]. A significant number of data for common chemical systems from other thermodynamic compilations such as 'Critical Stability Constants' [8] and the 'IUPAC Stability Constants Database' [9] has also been included together with assemblages large and small from numerous more recent sources, *e.g.,* our critical reviews for the 'strategically important elements' tantalum [10], tellurium [11] and niobium [12].

Background

Ongoing progress in computer technology has enabled the assembly of huge sets of thermodynamic information from the chemical literature.

Large-scale critical evaluation of thermodynamic data is generally carried out by institutions like the erstwhile U.S. National Bureau of Standards (NBS), its successor, the U.S. National Institute of Standards and Technology (NIST), the International Union of Pure and Applied Chemistry (IUPAC) or the OECD Nuclear Energy Agency (NEA). Unfortunately, thermodynamic modelling is now overshadowed by a lack of resources to support such internally-consistent compilations of recommended parameters. **As these traditional sources become increasingly outdated, the need grows for alternatives.** In any event, many other thermodynamic systems and quantities beyond those covered by NEA and NIST could and should be available.

doi: 10.5281/zenodo.7700024

The JPD database is already about an order of magnitude larger than any other which can be coupled directly to a computing engine for solving mass balance equations (or minimising Gibbs energies). It differs from other such thermodynamic databases, however, in that it does not purport to hold the best, single set of values for modelling purposes. Neither is it simply an uncritical compilation of relevant literature entries. Rather, it is a hybrid of these two different methods.

Most importantly, JESS does not follow the type of critical evaluation methodology typically carried out by institutions like NBS, NIST, IUPAC or NEA. Instead, JESS simply aims to maximise the information content/knowledge density of the database. This is mainly for reasons of practicality, given the enormous effort required by formal assessments. All possible values are eligible to be recorded; significant inconsistency is the only reason for data to be rejected (still retained but flagged as having no value); other values are subject to various degrees of scrutiny and marked accordingly. The intention is to be as comprehensive as possible for the selected chemical systems. The values from published authoritative critical assessments are, of course, included and given special emphasis. Nevertheless, limitations with this methodology of various kinds are unavoidable and acknowledged. Ultimately, the JESS design aims to leave critical decisions to the modellers (as end users).

The JPD database thus attempts to be as comprehensive as possible, while at the same time clearly indicating the likely reliability of equilibrium constants and, hence, of every reaction. Values in JPD are intended to be used in conjunction with JESS modelling facilities, not as a standalone database. In this context, JESS is designed to ensure thermodynamic modellers are made aware of every chemical species which might be relevant to them, within a framework in which only the worst inconsistencies in the chemical literature have been suppressed. However, the explicit decisions necessary to develop a good set of calculations remain the responsibility of the modeller. Minor / uncertain species often arise; they must be treated and understood appropriately, recognising that thermodynamic modelling rarely (if ever) leads to a singular 'right' answer.

On the other hand, we have now concluded that the JPD compilation may also be useful in its own right. It is a compilation of thermodynamic parameters unmatched in size and scope. A straightforward strategy to ensure the preservation and distribution of the data has accordingly been developed. This document describes the approach we have taken and, simultaneously, seeks feedback from others. Further details can be found in the companion document titled 'Instructions'.

Feedback

The JPD database continues to be developed so feedback is most welcome. Please send us your comments / suggestions. In the first instance, responses concerning the production of the PDF files should be directed to Josep Bonet (josep.bonet@schema.lu) and concerning the content of the database to either or both Peter May (P.May@murdoch.edu.au) and/or Montserrat Filella (montserrat.filella@unige.ch).

doi: 10.5281/zenodo.7700024

Disclaimer

Whilst considerable effort is made to ensure that JESS and JPD are error-free and user-friendly, we give no warranties. All JESS material is made available on an 'as is' basis, under the condition that you use it entirely at your own risk. No person or agency involved in JESS development assumes any responsibility for losses incurred through the use of JESS or of its documentation.

Copyright

References

1 P.M. May and K. Murray, JESS, A Joint Expert Speciation System - I. Raison d'Etre. Talanta, 1991, 38, 1409-1417.

2 P.M. May and K. Murray, JESS, A Joint Expert Speciation System - II. The Thermodynamic Database. Talanta, 1991, 38, 1419-1426.

3 P.M. May and K. Murray, Database of Chemical Reactions Designed to Achieve Thermodynamic Consistency Automatically. J. Chem. Eng. Data, 2001, 46, 1035-1040.

4 P.M. May, D. Rowland, E. Konigsberger and G. Hefter, JESS, a Joint Expert Speciation System - IV: A Large Database of Aqueous Solution Physicochemical Properties with an Automatic Means of Achieving Thermodynamic Consistency. Talanta, 2010, 81, 142-148.

5 P.M. May and D. Rowland, JESS, a Joint Expert Speciation System - VI: Thermodynamically-consistent Standard Gibbs Energies of Reaction for Aqueous Solutions. New J. Chem., 2018, 42, 7617-7629.

6 L.G. Sillen and A.E. Martell, "Stability Constants of Metal-ion Complexes SP17" The Chemical Soc.,London, 1964.

7 L.G. Sillen and A.E. Martell, "Stability Constants of Metal-ion Complexes SP25, Supplement No 1 to Special Publication No 25" Chemical Society, London, 1971.

8 R.M. Smith, A.E. Martell and R.J. Motekaitis, "NIST Critical Stability Constants of Metal Complexes Database, Version 5.0" U.S. Dept. Commerce, Gaithersburg, MD, U.S.A., 1998.

9 L.D. Pettit and H.K.J. Powell, "IUPAC Stability Constants Database, Release 4.71" Academic Software, U.K., 2005.

doi: 10.5281/zenodo.7700024

10 M. Filella and P.M. May, The Aqueous Solution Thermodynamics of Tantalum under Conditions of Environmental and Biological Interest. Appl. Geochem., 2019, 109, 104402-1-104402-7.

11 M. Filella and P.M. May, The Aqueous Chemistry of Tellurium: Critically-selected Equilibrium Constants for the Low-Molecular-Weight Inorganic Species. Environ. Chem., 2019, 16, 289-295.

12 M. Filella and P.M. May, The Aqueous Solution Thermodynamics of Niobium under Conditions of Environmental and Biological Interest. Appl. Geochem., 2020, 122, 104729-1-104729-9.

doi: 10.5281/zenodo.7700024