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Open Access to the JESS Chemical Reaction Database

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Abstract
The JESS (Joint Expert Speciation System) Thermodynamic Database (v8.9) is now available as a set of freely available PDF files. This reaction database contains about 280,000 thermodynamic parameters (equilibrium constants, enthalpies, etc.) as published in the literature for over 80,000 chemical reactions. It is grounded in the tradition of the Stability Constants Special Publications (by the Chemical Society) but it has become much more extensive and it includes some quantitative indication of parameter reliability based mainly on intra- and extra-reaction consistency.

Keywords Chemical reactions · Chemical speciation · Thermodynamic modelling equilibrium constants · Gibbs energy · Enthalpy · Water solutions · Aqueous systems · Complex formation · Metal-ligand interactions · Formation constants · Acidity constants · pKa · pH buffers · Water dissociation

1 Introduction

The purpose of this paper is to announce the recent release on the internet of the JESS (Joint Expert Speciation System) Thermodynamic Database (v8.9). Now specifically prepared as a set of freely available PDF documents, it contains the whole contents of the JESS reaction database called JPD—about 280,000 thermodynamic parameters as published in the literature for over 80,000 chemical reactions. Anyone can access this resource without cost. The PDF documents are available individually at https://doi.org/10.5281/zenodo.7700023 or in one (289 MB) bundle at the Murdoch University research repository (specific web address given at the end of the Zenodo opening statement).

This compendium of thermodynamic data will be useful to those seeking values and literature sources for the equilibrium constants, their thermodynamic equivalents, and the enthalpies of chemical reactions relevant to aqueous systems. These thermodynamic parameters are

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at the foundation of every thermodynamic modelling calculation dealing with chemical species in solution. The collection attempts to provide good coverage of published parameters for chemical reactions having broad interest. An assessment of every datum is given (as a numerical weight in the range 0:9) through a concerted, up-to-date effort to identify those equilibrium constant values at 1 bar, 25 °C and infinite dilution which are most reliable and most thermodynamically consistent.

2 Implementation of the JESS Chemical Reaction Database in Zenodo

The key motivation behind this latest JESS initiative has been to preserve the enormous effort which has been put into compiling the JPD database. The fate of other electronic databases of stability constants has been stark and regrettable. The NIST [1] and IUPAC [2, 3] products are two particular cases in point, being no longer maintained or even generally available [4, https://equilibriumdata.github.io/guide/index.html). The general-purpose open repository Zenodo [https://zenodo.org] offers an enduring remedy for the preservation of otherwise frail datasets. It also ensures the free universal access to the files, following FAIR principles. The choice of the PDF format is a robust preservation option while offering a general search facility within individual PDF documents. However, these advantages come with their own disadvantages, particularly concerning searching. Searching for a required reaction or portion of the data is unavoidably primitive, as described in the following paragraphs. Obviously, searches using the native JESS database facilities are much more sophisticated and powerful, although even these do have a learning curve which is sometimes criticised.

For inspection/download convenience, the JPD dataset on Zenodo has been subdivided into manageable portions. The main mechanism for this purpose has been to classify the subdivisions by chemical element and, in the case of carbon, into 28 separate files divided by molecular formula. Elements are indicated by the initial letter(s) of the PDF file names. Moreover, to help locate required data, the information for each element has been further separated into two subsets. The first subset contains the main body of chemical reaction data and is indicated by an R as the last letter of the PDF file name. The second subset for each element contains the chemical names, molecular formulae, and (where available) CAS registry numbers for every chemical species involved in the reactions of the corresponding element. These latter files, indicated by an S as the last letter of the file name, give the JESS symbol for every chemical species relevant to that element. Thus, to find a chemical reaction of interest, you will generally search first for a chemical species, identifying the JESS symbol for it (using the S file corresponding to the most relevant element), and then locate all chemical reactions with that JESS symbol in them, by searching through the element's corresponding R file.

A full description of the data in the PDF files is given in the accompanying Zenodo file named 'Instructions'. This includes explanations of the many abbreviations which are used. It is advisable to read the preamble documents to avoid various all-too-easy confusions.

3 A Few Useful Hints/Complementary Information

Users of the Zenodo compilation should realise that values in the database are intended to be used in conjunction with JESS modelling facilities, not as a standalone database. The interested reader will find more information about JESS in references [5-9]. The following information is pertinent to a standalone use of the database.

- A proprietary syntax is used for chemical reactions. It allows chemical reactions to be expressed in any form, based on a set of alphanumeric symbols to represent the panoply of chemical species. The resulting expression of chemical reactions is sufficiently recognisable to human users but, at the same time, chemically definitive, such that it could be processed unambiguously by computers. It is easily familiarised by reading the Instructions file.
- JESS includes strategies to evaluate and improve the reliability of the database as well as mechanisms for determining reaction parameters by least squares fitting [10] and estimating values when there are too few data to fit. This implies that multiple reactions are recorded in JPD even though they are thermodynamically redundant. This is desirable because decisions regarding the best sets of data to use then can be readily modified, as well as being amenable to automatic processing mechanisms which can exploit them [7]—redundant data are by no means useless [11].
- A rating is given for every datum (as a numerical weight in the range 0:9). It is important for the user to understand that this weighting takes into account not only the quality of the data as usually evaluated (e.g. adequate control and description of the experimental method, purity of the ligand, calibration, adequate definition of the equilibrium quotients, and reliability of the investigator, as in NIST [12]) but also the overall thermodynamic consistency of the values. For this reason, the user may encounter some reactions in which all published data are weighted zero and an ELC (Estimated from Linear Combination of Reactions) value is added.
- Chemical reactions appear in the format decided at the time they were entered (including choice of reactants vs. products). This makes any search through the PDF more difficult, especially when the chemical species of interest occurs in many reactions but it reduces the possibility of errors or omissions. Capabilities exist within JESS to make such searching much easier, particularly through mechanisms for including and excluding multiple species. Similarly, the equilibrium constants (or Gibbs energies of reaction) can be calculated within JESS for any arbitrary reaction whenever sufficient information appears in JPD and whether or not the reaction has been entered into JPD as such.
- This snapshot of the reaction parameters from the literature is, despite its size, far from exhaustive. It is a major difference between this database and the much more comprehensive IUPAC SC-Database developed by Kip Powell and Leslie & Gwyneth Pettit [2, 3]. With JESS, a conscious decision was made early on to omit hundreds of less common compounds (usually ligands) and to concentrate on those which are of most value in general aqueous chemistry applications. This is not due to any software restriction. Modellers interested in chemical systems which have not so far been incorporated can easily enter the data themselves and thereafter take steps to get them permanently integrated into JPD.

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Declarations

Competing Interests There is no conflict of interest to declare.

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