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present the

JESS Thermodynamic Database v8.9

Instructions

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It is assumed herein that you have already read the **Introduction** document associated with this one. If not, it is advisable to do so.

This work presents a large set of documents in PDF format which contain, as the entire contents of the JESS Thermodynamic Database v8.9, equilibrium constants and other thermodynamic parameters for more than 80,000 chemical reactions. These reactions are all pertinent to aqueous solutions but they are not confined to aqueous species (*i.e.*, relevant solids and gases are included).

Due to the magnitude of the dataset, it has been subdivided into separate PDF files, each of which deals with entries for a particular chemical element. This is intended to divide the whole body of information from the database into segments which are kept to a reasonable file size.

The elements O and H are omitted from the above subdivision process because they are involved in too many reactions. Instead, just one file (H2OR.PDF) holds the equilibrium constant data for the specific reactions of water. Similarly, all redox reactions (i.e., those having the electron, 'e-') appear in their own file (E.PDF). The elements C, N, F, P, S and Cl are also treated exceptionally. With C, the data are further subdivided into segments based on ranges of carbon by molecular formulae. Regarding the rest (elements N, F, P, S and Cl), reactions involving C (in addition to the element) are omitted – they appear only in the respective files of carbon-containing reactions. In essence, only inorganic ligands thus appear in the files for N, F, P, S and Cl.

Each chemical element (or segment) gives rise to two PDF files. The first PDF contains all the appropriate chemical reactions and their thermodynamic parameters. The second contains information defining every chemical species which appears in those chemical reactions, including molecular formula and electronic charge and, where available, chemical names and CAS registry numbers. The PDF file names in general have the format EER.PDF and EES.PDF where EE represents the letters (or letter) of the chemical element symbol, R identifies the file with reaction (equilibrium constant) data and S identifies the file with species information. The order of entries of chemical species ('S files') is alphabetical but the order of the chemical reactions ('R files) is merely as they were entered into the database.

Look at the files H2OR.PDF and H2OS.PDF as examples of how the contents of JPD are presented.

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JESS identifies chemical species and chemical reactions using an exact but general and flexible symbolic notation suitable for computer processing with a human-user interface. Details are as follows.

Every species in the JPD database is represented by an alphanumeric string without spaces. For example, the ion of Zinc(II) has the symbol **Zn+2** (in which, conventionally, the element's chemical abbreviation is followed by the ion's signed electronic charge). Symbols like **Zn+2** are called 'primitive' to indicate that they are a basic building-block of the database. For convenience, it is also possible to describe species in terms of combinations of primitive symbols. In such cases, the symbol is referred to as a 'composite'. In constructing a composite symbol, simply append appropriate primitive symbols together, separating them from one another with underscore characters, **_**. For instance, the first-stepwise complex of Zn(II) with glycinate is represented as **Zn+2_Gly-1** and the second-stepwise complex is represented as **Zn+2_Gly-1(2)**.

Chemical reactions are described using these species symbols in much the same way as they are in ordinary chemical writing, *i.e*. the symbols of the reactant species appear on the left hand side of an equals sign, =, and the symbols of the products appear on the right hand side. Species on the same side of the equation are usually separated from one another by plus signs, +, but minus is also acceptable, if that happens to be appropriate. Note that in the representation of a chemical equation as just described, the signs =, +, - are always surrounded by blank spaces.

Consider the JESS format for reactions used in the following examples.

```
H+1 + OH-1 = H2O
Cu+2 + 2<OH-1> = Cu+2_OH-1(2)
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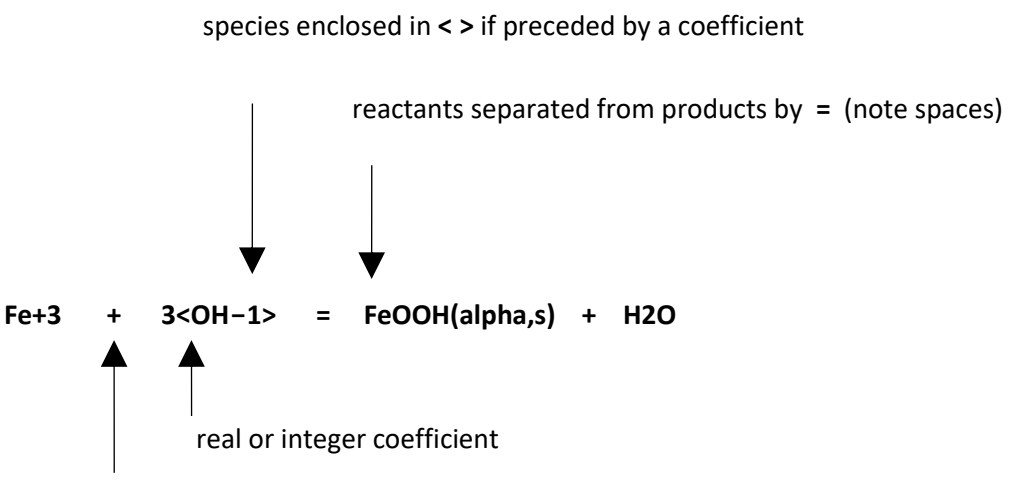
Here, **H+1**, **OH−1**, **H2O** and **Cu+2** are primitive symbols and **Cu+2_OH−1(2)** is a composite symbol. Note how the non-unit stoichiometry is dealt with, using angle brackets and parentheses.

Some other rules for representing reactions are indicated in the following diagram.



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Concerning the tables of reaction data, the temperature (t) is always given in Celsius and the pressure (P) is 1 bar / 1 atm unless indicated explicitly. **Unless otherwise specified**, ionic strengths (I-Str) are given on the molar (mol dm^{-3}) scale, Gibbs energies (dG) and enthalpies (dH) of reaction are given in kilocalories (per mole), heat capacities of reaction are given in calories (per K per mol). The alternatives are indicated explicitly by '/m' (for mol kg^{-1}), 'kJ', and 'J/K' respectively. The solvent is water unless otherwise specified. All reaction standard potentials (E) are given in volts. The precision of values (Dev) reflects what was reported in the literature source, expressed in terms of significant figures (SF), standard deviations (SD) or maximum deviations (MD). The weight (W) gives the JESS assessment of data reliability, the method by which the datum was determined is given by the technique (Tech) and its literature source by a reference acquisition number (Ref. #). Lists with details for the weights, techniques and literature references appear at the end of the 'R' documents, after the main data tables. Where no literature reference appears, the datum was determined during the process of database compilation, usually estimated by linear combination (ELC) of other reactions deemed to be more reliable.

Modellers who require estimates of equilibrium constants and other reaction parameters at any particular temperature and ionic strength should consult the relevant JESS publications, especially references [1,2].

To find less obvious JESS species symbols, you can search the files listing chemical species for molecular formulae or chemical names. These filenames end in 'S.PDF'. Molecular formula have the form 'C(2)H(4)O(2)' (this being for acetic acid), where the elements are arranged according to the Hill system [3] with C first followed by H for C-containing substances or, otherwise, alphabetically by element symbol.

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 (pep.bonet@proton.me) 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).

Disclaimer

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