FreeGs: A web-enabled thermodynamic database for geochemical modelling

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Using multiple computer packages for modelling geochemical processes requires standardisation of the thermodynamic data. This is critical in a "virtual" collaborative environment, where remote researchers, with different skill sets and levels of thermodynamic literacy, work on the same or similar problems.

Standardisation is hindered by multiple sources of recommended thermodynamic data, disparities in speciation models, different models for extrapolation of thermodynamic properties, and program-specific database formats. This situation often precludes the choice of the best (or the favourite) package for the problem at hand, or benchmarking different packages on the basis of common data. The problem is exacerbated by the tendency to collect and modify data on personal computers, resulting in multiple mutated data sets of variable quality and consistency.

The Predictive Mineral Discovery Cooperative Research Centre (*pmd**CRC), has established FreeGs: a web-enabled database of thermodynamic properties hosted at Geoscience Australia. FreeGs contains mineral, gas, and aqueous species parameters that permit calculation of thermodynamic properties within a wide range of geological temperatures and pressures. The database provides a choice of the depth of the database interrogation ("casual" or "novice" user vs an expert); a choice of the data versions ("recommended" values for the species of interest vs all the available data); a choice of the available extrapolation models (equations of state); and a choice of formats of the output data.

Storage and access to primary FreeGs data are available via Web forms and reports. An integrated software enables users to calculate thermodynamic properties of species and chemical reactions at high T&P (e.g., $\Delta g(T,P)$ or $\log K_r(T,P)$). In future, users' applications will be able to acces the system as a web-service using XML.

The project is run in collaboration with the Cooperative Research Centre for Landscape Environments and Mineral Exploration (CRCLEME).

The URL is www.ga.gov.au/rural/projects/geofluids.jsp

A modified hydrogen electrode concentration cell (HECC): Study of scheelite solubility

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We have constructed a hydrogen electrode concentration cell modified from the design being used at Oak Ridge National Laboratory[1-5]. This experimental setup incorporates nested PTFE cups which communicate through a porous PTFE liquid junction. The inner cup contains a solution of known hydrogen ion concentration; the outer cup contains a suspension of the solid of interest within a test solution. Teflon-sheathed platinum electrodes inserted in the two cells allow measurement of the potential difference between them. The test cell is plumbed for sampling of the test cell fluid and titration of fluids into the test cell.

Our design differs in several respects from that in use at ORNL. The ORNL liquid junction is friction-fitted by tamping a porous PTFE plug into a hole in the reference cell cup, whereas our LJ is placed in the bottom of a fitting detail in the reference cup and held in place with a PFA Teflon nut. Samples in the ORNL system are filtered through a Pt frit that is gold-welded to the end of the dip tube. Our samples are withdrawn through an in-line filter attached to the dip tube with conventional PFA Teflon 1/16" fittings.

We are using this experimental setup to examine the solubility of scheelite at saturated water vapor pressure from 50° - 290°C as a function of pH and ionic strength in non-complexing sodium trifluoromethanesulfonate (triflate) media. Solid scheelite is reacted in the test cell with a solution of sodium triflate and either sodium hydroxide or triflic acid. We will use the experimental results to derive equilibrium constants for the dissolution of scheelite, for the first dissociation of tungstic acid, and ultimately for the dissolution of ferberite at the experimental conditions.

References

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