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ThermoFun: C++/Python code to fetch standard thermodynamic data from ThermoHub database

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An unavoidable step in any realistic application of geochemical thermodynamic modelling is to collect a consistent set of standard thermodynamic data at temperature and pressure of interest for involved substances or reactions. With a plethora of existing thermodynamic databases, equations of state, modeling codes and file formats, it can be difficult and time-consuming to collect such data and to apply suitable methods of thermodynamic calculations. The open-source ThermoFun code library (thermohub.org/thermofun), supported by the remote ThermoHub property graph database server (thermohub.org/thermohub), solves this extensive problem in a simple, focused, and efficient manner. The library can be linked to any C++ or Python geochemical modelling code; it is currently used as a source of thermodynamic data in GEMS codes (gems.web.psi.ch) and in Reaktoro geochemical modelling framework (reaktoro.org).

ThermoFun can fetch the reference thermodynamic data and parameters from a selected dataset available in ThermoHub. With this, ThermoFun API can be used for obtaining standard thermodynamic properties at temperature T and pressure P of interest and/or their T or P derivatives either for a particular one or for a list of substances or reactions. This is possible because ThermoFun contains a comprehensive collection of models and equations of state (EoS) for solid, aqueous, gaseous, and melt substances. A certain model or EoS is not yet available? No problem - taking advantage of its modular architecture, ThermoFun can be extended easily with new methods and EoS models. The ThermoFun graphical user interface as a desktop or web application are available, e.g., for tabulating thermodynamic properties of substances or reactions at desired ranges of T and P.

ThermoHub represents a centerpiece for storing and maintaining traceable and internally consistent thermodynamic data, built using state-of-the-art data storage, data management, and import-export tools. It contains many internally consistent thermodynamic datasets applicable in various fields such as hydrothermal processes, cementitious materials, nuclear engineering, waste management and disposal, and other (geo)chemical environments.