The future of thermodynamic databases: Community driven data systems fueled by the geoinformatics revolution

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Internally consistent thermodynamic databases are critical community resources that facilitate the calculation of heterogeneous phase equilibria and thereby support geochemical, petrological, and geodynamical modeling. These “databases” are actually derived data/model systems that depend on a diverse suite of physical property measurements, calorimetric data, and experimental phase equilibrium brackets. In addition, such databases are calibrated with the adoption of various models for extrapolation of heat capacities and volumetric equations of state to elevated temperature and pressure conditions. Finally, these databases require specification of models for the mixing properties of solid, liquid, and fluid solutions, which are often rooted in physical theory and, in turn, depend on additional experimental observations. The process of “calibrating” a thermochemical database involves considerable effort and an extensive computational infrastructure. Because of these complexities, the community tends to rely on a limited number of thermochemical databases, generated by a few researchers; these databases are often out-of-date and are universally difficult to maintain. Their longevity is generally linked to that of their creators.

Geoinformatics is poised to alter the manner in which thermodynamic databases are created, maintained, tailored, and applied. By making underlying data resources universally available, and by focusing development on a generalized web-based computing infrastructure that permits a wider community of users to evaluate those data in an internally consistent and thermodynamically rigorous context, the generation of thermodynamic data/model collections can be made more transparent and spontaneous. Through automated generation of web services that standardize the linkage between thermochemical databases and the geochemical, petrological, and geodynamical models they serve, the lag time between generation and evaluation can be shortened and a broader community of users can be empowered to participate in model creation and evaluation. A prototype system that embodies this approach to thermochemical database construction will be demonstrated. Requirements for broad-based application of this geoinformatics architecture will be discussed.

Neoproterozoic granites of Sharm El-Sheikh area, Egypt: Mineralogical and geobarometric variations

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Sharm El- Sheikh District, south Sinai, includes representative granitic outcrops. Mineral of the hosted granites are analyzed to elucidate geobarometric variation, which could prove their evolution. The amphiboles classified as calcic and alkali amphiboles. The calcic amphiboles are Ferro-edenite while the alkali amphiboles are typically riebeckite. Amphiboles varieties are of magmatic nature. Biotites encountered mostly in monzogranites and syenogranites. They classified as meroxene (Mg-rich varieties). They pertain to metamorphic-metasomatic types. Biotites have calc-alkaline affinity for the syenogranites and monzogranites. Feldspars have albite and orthoclase end-members. Coexisting amphiboles and plagioclase are used to estimate the physicochemical parameters of their crystallizing parent magma. It is clarifies that syenogranites underwent temperature and pressure of formation ranges of 520-730 ^{O}C; <3 kbars. The alkali feldspar granites record 450-830 ^{O}C; <4 kbars. The riebeckite-bearing granites record the lowest temperature condition among all varieties since it estimate formation at 350-650 ^{O}C; <4 kbars.

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DOI:10.1180/minmag.2013.077.5.7