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Letter

A simple method for obtaining heat capacity coefficients of minerals

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Abstract

Heat capacity data are unavailable or incomplete for many minerals at geologically relevant temperatures. Despite the availability of entropy and enthalpy values in numerous thermodynamic tables (even sometimes at elevated temperatures), there remains need for extrapolation beyond, or interpolation between, temperatures. This approach inevitably results in estimates for entropy and enthalpy values because the heat capacity coefficients required for optimal thermodynamic treatment are less frequently available. Here we propose a simple method for obtaining heat capacity coefficients of minerals. This method requires only the empirically measured temperature-specific heat capacity for calculation via a matrix algorithm. The system of equations solver is written in the Python computing language and has been made accessible in an online repository. Thermodynamically, the solution to a system of equations represents the heat capacity coefficients that satisfy the mineral-specific polynomial. Direct coefficient calculation will result in more robust thermodynamic data, which are not subject to fitting uncertainties. Using hematite as an example, this method provides results that are comparable to conventional means and is applicable to any solid material. Coefficients vary within the traditional large 950 K temperature interval, indicating that best results should instead utilize a smaller 400 K temperature interval. Examples of large-scale implications include the refinement of geothermal gradient estimation in rapidly subsiding sedimentary basins or metamorphic and hydrothermal evolution.

Keywords: Gaussian elimination, heat capacity, hematite, system of equations