

Equations of state of CaCO_3 phases based on the Helmholtz free energy

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The carbonates in the CaCO_3 system are important carbon carrier in the Earth's interior, transporting of carbon in the Earth's crust and mantle. Moreover, CaCO_3 phases are often found as inclusions in natural diamonds, being a source of information about their genesis. The CaCO_3 system was widely considered many authors, but the reliable thermodynamic description of CaCO_3 phases based on modern x-ray diffraction measurements is relevant. The thermodynamic properties of CaCO_3 phases can be calculated from their equations of state (EOS). The proposed equations of state of calcite, aragonite and postaragonite are based on the Helmholtz free energy by analogy with our previous studies for the Mg_2SiO_4 and CaSiO_3 systems [1–3]. The calculated equations of CaCO_3 phases contain group of fixed parameters and group of fitting parameters derived by least squares method in Excel worksheets. It is easy to calculate a full set of thermodynamic functions (entropy, enthalpy, Gibbs energy, etc.) at given P-T parameters by the proposed approach.

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