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P-V-T equation of state of CaCO_3 aragonite to 29 GPa and 1673 K: *In situ* X-ray diffraction study

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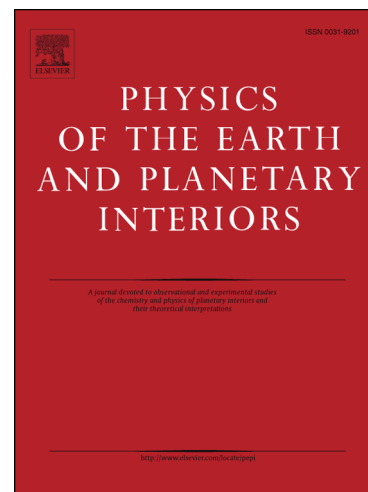
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***P-V-T equation of state of CaCO₃ aragonite to 29 GPa and 1673 K:
In situ X-ray diffraction study***

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Abstract

Pressure–volume–temperature relations have been measured to 29 GPa and 1673 K for CaCO₃ aragonite using synchrotron X-ray diffraction with a multianvil apparatus at the ‘SPring-8’ facility. A least-squares fit of the room-temperature compression data to the Vinet-Rydberg equation of state (EOS) yielded $K_{T0} = 65.7 \pm 0.8$ GPa and $K_T' = 5.1 \pm 0.1$, with fixed $V_0 = 227.11 \text{ \AA}^3$. Further analysis of the high-temperature compression data led to the temperature derivative of the bulk modulus $(\partial K_T / \partial T)_P = -0.016 \pm 0.001$ GPa/K and zero-pressure thermal expansion $\alpha = a_0 + a_1 T$ with $a_0 = 4.98 (22) \times 10^{-5} \text{ K}^{-1}$ and $a_1 = 2.81(38) \times 10^{-8} \text{ K}^{-2}$. The Mie-Gruneisen-Debye approach revealed the Gruneisen parameter $\gamma_0 = 1.39$ at a fixed Debye temperature $\theta_0 = 516$ K and the parameter $q = 1$. Analysis of axial compressibility and thermal expansion indicates that the *c*-axis is two times more compressible than the *b*-axis and four times more compressible than the *a*-axis, whereas zero-pressure thermal expansion of the *a*-axis ($a_{0a} = 2.6 \times 10^{-5} \text{ K}^{-1}$ and $a_{1a} = 2.3 \times 10^{-8} \text{ K}^{-2}$) is weaker than that of the *b*-axis axis ($a_{0b} = 6.3 \times 10^{-5} \text{ K}^{-1}$ and $a_{1b} = 0.1 \times 10^{-8} \text{ K}^{-2}$) and *c*-axis axis ($a_{0c} = 5.2 \times 10^{-5} \text{ K}^{-1}$ and $a_{1c} = 9.5 \times 10^{-8} \text{ K}^{-2}$). A full set of thermodynamic parameters (including heat capacity, enthalpy and free energy) for aragonite and updated equations of state for magnesite and siderite was obtained using the Kunc-Einstein approach. The new EOS parameters were used for

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