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Thermal equation of state of ice-VII revisited by single-crystal X-ray diffraction

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Abstract

Ice-VII is a high-pressure polymorph of H_2O ice and an important mineral widely present in many planetary environments, such as in the interiors of large icy planetary bodies, within some cold subducted slabs, and in diamonds of deep origin as mineral inclusions. However, its stability at high pressures and high temperatures and thermoelastic properties are still under debate. In this study, we synthesized ice-VII single crystals in externally heated diamond-anvil cells and conducted single-crystal X-ray diffraction experiments up to 78 GPa and 1000 K to revisit the high-pressure and high-temperature phase stability and thermoelastic properties of ice-VII. No obvious unit-cell volume discontinuity or strain anomaly of the high-pressure ice was observed up to the highest achieved pressures and temperatures. The volume-pressure-temperature data were fitted to a high-temperature Birch-Murnaghan equation of state formalism, yielding bulk modulus $K_{T0} = 21.0(4)$ GPa, its first pressure derivative $K'_{T0} = 4.45(6)$, $dK/dT = -0.009(4)$ GPa/K, and thermal expansion relation $\alpha_T = 15(5) \times 10^{-5} + 15(8) \times 10^{-8} \times (T - 300)$ K^{-1}. The determined phase stability and thermoelastic properties of ice-VII can be used to model the inner structure of icy cosmic bodies. Combined with the thermoelastic properties of diamonds, we can reconstruct the isomeke *P*-*T* paths of ice-VII inclusions in diamond from depth, offering clues on the water-rich regions in Earth's deep mantle and the formation environments of those diamonds.

Keywords: High-pressure ice, diamond-anvil cell, thermal equation of state, icy planetary bodies, ice-VII diamond inclusions