

Experimental and theoretical thermal equations of state of MgSiO₃ post-perovskite at multi-megabar pressures

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The MgSiO₃ post-perovskite phase is the most abundant silicate phase in a super-Earth's mantle, although it only exists within the Earth's lowermost mantle. In this study, we established the thermal equation of state (EoS) of the MgSiO₃ post-perovskite phase, which were determined by using both laser-heated diamond anvil cell and density-functional theoretical techniques, within a multi-megabar pressure range, corresponding to the conditions of a super-Earth's mantle. The LHDAC experiments were performed at up to a pressure of 265 GPa at a temperature of 300 K, and 170 GPa at 2560 K. The ab initio calculations were performed at up to 1.2 TPa and 5000 K. The Keane and AP2 EoS models were adopted for the first time to extract meaningful physical properties. The experimentally determined Grüneisen parameter and its volume dependence were found to be consistent with their theoretically obtained values. This reduced the previously reported discrepancy observed between experiment and theory. Both the experimental and theoretical EoS were also found to be in very good agreement for volumes at pressures and temperatures of up to 300 GPa and 5000 K. Our newly developed EoSs are considerably useful to discuss the physical properties of not only the Earth's lowermost mantle, but also a super-Earth's mantle.