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LETTER

Thermochemistry and high-pressure equilibria of the post-perovskite phase transition in $CaIrO_3$

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ABSTRACT

To study the ambient analog of the deep mantle $MgSiO_3$ perovskite to post-perovskite phase transition, high-temperature drop calorimetry experiments of perovskite and post-perovskite phases of $CaIrO_3$ system as well as high-pressure phase equilibrium experiments in the $CaIrO_3$ system were made. The enthalpies for dissociation of $CaIrO_3$ (298 K) to CaO + Ir + O_2 (1573 K) were 486.7 ± 9.2 kJ/mol for post-perovskite and 454.5 ± 12.5 kJ/mol for perovskite. From the difference between them, the phase transition enthalpy from perovskite to post-perovskite at 298 K is –32.2 ± 15.5 kJ/mol. This gives 2.7 ± 15.6 kJ/mol as formation enthalpy of $CaIrO_3$ perovskite from CaO + IrO_2 at 298 K. Using the phase transition enthalpy and volume change of –0.48 ± 0.02 cm^3/mol determined in this study, the phase equilibrium boundary is calculated to be P (GPa) = 0.040 T (K) – 67.1. The strongly positive slope agrees with that obtained in high-pressure experiments. This is consistent with a large positive Clapeyron slope of post-perovskite phase transition in $MgSiO_3$ recently reported from experimental and theoretical studies.

Keywords: $CaIrO_3$, post-perovskite, perovskite, calorimetry, thermodynamics, high pressure