American Mineralogist, Volume 92, pages 1760–1763, 2007

LETTER

Equations of state of $CaIrO_3$ perovskite and post-perovskite phases

TIZIANA BOFFA BALLARAN,[1,*] REIDAR G. TRØNNES,[2] AND DANIEL J. FROST[1]

[1]Bayerisches Geoinstitut, Universität Bayreuth, D-95440 Bayreuth, Germany
[2]Natural History Museum, Geology, University of Oslo, Box 1172, Blindern, N-0318 Oslo, Norway

ABSTRACT

Unit-cell lattice parameters have been measured to ~8 GPa in a diamond anvil cell for two single crystals of $CaIrO_3$: one with the perovskite (*Pbnm*) and the other with the post-perovskite (*Cmcm*) structure. The $CaIrO_3$ post-perovskite structure is more compressible than the perovskite. A third-order Birch Murnaghan equation of state has been used to fit the measured *P-V* data with the following refined parameters: V_0 = 229.463(8) Å^3, K_0 = 198(3) GPa, K' = 1.2(8); and V_0 = 226.38(1) Å^3, K_0 = 181(3) GPa, K' = 2.3(8) for $CaIrO_3$ perovskite and post-perovskite, respectively. The compressibility of the unit-cell axes of the perovskite structure is highly anisotropic with $\beta_a >> \beta_c >> \beta_b$. In contrast, the **b** axis is the most compressible in the post-perovskite structure, whereas the **a** and **c** axes have similar compressibilities (with **c** slightly less compressible than **a**) and are much stiffer. A comparison between the compressibility of $CaIrO_3$ perovskite and post-perovskite with the isostructural $MgSiO_3$ phases, reveals a similar general behavior, although in detail $CaIrO_3$ perovskite is more and the post-perovskite less anisotropic than the corresponding $MgSiO_3$ compounds.

Keywords: $CaIrO_3$ phases, high-pressure X-ray single-crystal diffraction, equation of state, perovskite and post-perovskite analogues