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Pressure-induced volume collapse in PbCrO_3 — a combined experimental and theoretical investigation P. GANESH, R.E. COHEN, Geophysical Lab., Carnegie Institution of Washington, Washington DC, USA, WENSHENG XIAO, Guangzhou Institute of Geochemistry, Chinese Academy of Sciences, Guangzhou, China, HO-KWANG MAO, Geophysical Lab., Carnegie Institution of Washington, Washington DC, USA — PbCrO_3 in perovskite structure surprisingly has a larger volume ($a \sim 4.0 \text{ \AA}$) [1, 2] compared to PbTiO_3 ($a \sim 3.95 \text{ \AA}$). We synthesized a powder sample of PbCrO_3 and performed x-ray diffraction studies in a diamond anvil cell up to $\sim 30 \text{ GPa}$. Our experiments show a pressure induced volume collapse at 1.6 GPa by $\sim 9.8\%$. To investigate its origin we performed DFT computations with LDA+U and GGA+U using ABINIT, relaxing the strain and the internal coordinates, for different distorted perovskite phases and spin configurations. We identified the volume collapse with the high pressure phase being cubic and the low-pressure phase being tetragonal and non-centrosymmetric. The spin-configuration is G-AFM with a local moment of $\sim 2.2\mu_B$, comparable to experiments [1]. No spin or metal-insulator transition is observed in our computations. Rather, orbital ordering stabilizes the low pressure phase. Computations show the bulk moduli of the two phases to be very different, consistent with our experiments. Both phases are metallic. [1] W. L. Roth *et.al.*, J. Appl. Phys. **38**, 951 (1967), [2] Angel M. Arivalo-Lopez *et.al.*, J. Solid State Chemistry **180**, 3271 (2007)

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