

High-pressure structural studies of eskolaite by means of single-crystal X-ray diffraction

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ABSTRACT

The structural behavior of Cr₂O₃ was investigated up to ~70 GPa using single-crystal X-ray diffraction under a quasi-hydrostatic pressure (neon pressure medium) at room temperature. The crystal structure remains rhombohedral with the space group $R\bar{3}c$ (No. 167) and upon compression the oxygen atoms approach an ideal hexagonal close-packing arrangement. An isothermal bulk modulus of Cr₂O₃ and its pressure derivative were found to be 245(4) GPa and 3.6(2), respectively, based on a third-order Birch-Murnaghan equation of state and $V_0 = 288.73 \text{ \AA}^3$. An analysis of the crystal strains suggest that the non-hydrostatic stresses can be considered as negligible even at the highest pressure reached.

Keywords: High pressure, crystal structure, eskolaite