

Crystal structure of CaRhO₃ polymorph: High-pressure intermediate phase between perovskite and post-perovskite

**Y. SHIRAKO,¹ H. KOJITANI,¹ A.R. OGANOV,^{2,3} K. FUJINO,⁴ H. MIURA,⁵ D. MORI,¹ Y. INAGUMA,¹
K. YAMAURA,⁶ AND M. AKAOGI^{1,*}**

¹Department of Chemistry, Gakushuin University, Toshima-ku, Tokyo 171-8588, Japan

²Department of Geosciences and Department of Physics and Astronomy, Stony Brook University, Stony Brook, New York 11794-2100, U.S.A.

³Geology Department, Moscow State University, 119992 Moscow, Russia

⁴Geodynamics Research Center, Ehime University, Bunkyo-cho, Matsuyama 790-8577, Japan

⁵Division of Earth and Planetary Sciences, Hokkaido University, Kita-ku, Sapporo 060-0810, Japan

⁶National Institute of Materials Science, Namiki, Tsukuba 305-0044, Japan

ABSTRACT

A high-pressure phase of CaRhO₃ stable between perovskite and post-perovskite in *P-T* space was synthesized at 17 GPa and 1650 °C using a multi-anvil apparatus. The crystal structure of CaRhO₃ was solved by the structure prediction evolutionary algorithm and was refined by Rietveld analysis of the synchrotron powder X-ray diffraction pattern, along with transmission electron microscopy observations. The structure is monoclinic with lattice parameters of $a = 12.5114(1) \text{ \AA}$, $b = 3.1241(1) \text{ \AA}$, $c = 8.8579(1) \text{ \AA}$, $\beta = 103.951(1)^\circ$, $V = 336.01(1) \text{ \AA}^3$ with space group $P2_1/m$. The structure contains edge-sharing RhO₆ octahedral chains along the **b**-axis. The six RhO₆ octahedral chains make a unit, which stacks up alternatively with the CaO₈ polyhedral layer along the [101] direction to form the structure of CaRhO₃ intermediate phase.

Keywords: Perovskite, post-perovskite, X-ray diffraction, Rietveld analysis, CaRhO₃, electron microscopy, structure search