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Single-crystal X-ray diffraction study of $CaIrO_3$

Masahiko Sugahara,[1,*] Akira Yoshiasa,[1] Akira Yoneda,[2] Takafumi Hashimoto,[1] Syunsuke Sakai,[1] Maki Okube,[3] Akihiko Nakatsuka,[5] and Osamu Ohtaka[4]

[1]Graduate School of Science, Kumamoto University, Kumamoto 860-8555, Japan
[2] Institute for Study of the Earth's Interior, Okayama University, Misasa 682-0193, Japan
[3]Tokyo Institute of Technology, Nagatsuta 4259, Yokohama 226-8502, Japan
[4]Department of Earth and Space Science, Graduate School of Science, Osaka University, 1-1 Machikaneyama, Toyonaka, Osaka 560-0043, Japan
[5]Graduate School Science and Engineering, Yamaguchi University, Ube 755-8611, Japan

Abstract

Single crystals of $CaIrO_3$ were prepared via flux growth method. Crystal structure parameters, including the anisotropic displacement parameters, are determined based on a single-crystal X-ray diffraction experiment. The unit-cell dimensions are a = 3.147(2), b = 9.866(6), and c = 7.302(5) Å. The structure is a three-dimensional dense structure with small vacant spaces. The $CaIrO_3$ structure can be described as a pseudo-one-dimensional oxide and is compared with Ca_4IrO_6 structure. The IrO_6 octahedra are significantly distorted, in contrast to other octahedral Ir^{4+} compounds. The O-O distances for faces and edges shared between polyhedra are shorter than other non-shared edge distances. These effects are explained by Pauling's rules and occur to decrease the repulsion between the cations. Thermal vibrations of Ca and Ir atoms are significantly anisotropic. Thermal vibrations of Ca and Ir atoms are restricted in orientation toward the shared face, shared edges, and shortest cation-cation directions. The single-crystal experiment shows that $CaIrO_3$ crystals grow fastest along the **a** axis and that they assume a prism or needle shape. Strongly preferred orientation of such prism shaped $CaIrO_3$-type post perovskite $MgSiO_3$ crystals may develop under the shear flow in the Earth's mantle.

Keywords: Post-perovskite, $CaIrO_3$, single crystal, X-ray diffraction, lower mantle, D' layer