Single crystal X-ray diffraction analysis and crystal chemistry of CaIrO3

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Single crystals of CaIrO3 were synthesized by a flux method, and its crystal structure was investigated using single-crystal X-ray diffraction analysis. Cell dimensions: a=3.147(1), b=9.865(7), c=7.302(6) (A). The structure is composed of largely distorted IrO6 octahedra. The anisotropic displacement of Ir atom is large toward vacant space. The anisotropic displacement of O(2) atom is large parallel to share edge between IrO6 octahedra. The structure follows the Pauling's law.