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Structure and Antiferroelectric Properties of Cesium Niobate, Cs₂Nb₄O₁₁ JIANJUN LIU, WAI-NING MEI, Department of Physics, University of Nebraska at Omaha, Omaha, NE 68182 USA, ROBERT W. SMITH, Department of Chemistry, University of Nebraska at Omaha, Omaha, NE 68182 USA, CHUNHUA HU, Nebraska Center for Materials and Nanoscience, University of NebraskaLincoln, Lincoln, NE 68588 USA, KUAN-JIUH LIN, Department of Chemistry, Center of Nanoscience and Nanotechnology, National Chung-Hsing University, Taichung 402, Taiwan, Republic of China — We determined the crystal structure of Cs₂Nb₄O₁₁ by using single crystal X-ray diffraction. The structural refinements at both 100 and 297 K show it to have a centrosymmetric structure in point group mmm and orthorhombic space group Pnna. The lattice is comprised of niobiumcentered tetrahedra and octahedra connected through shared vertices and edges; cesium atoms occupy channels afforded by the three-dimensional polyhedral network. We also studied the electric-field dependence of the polarization and observed double hysteresis loops which we interpret as the manifestation of antiferroelectricity. We then elucidated the origin of the antiferroelectricity by using symmetry analysis of the structural space groups.

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