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Polar noncentrosymmetric $\text{ZnMoSb}_2\text{O}_7$ and nonpolar centrosymmetric $\text{CdMoSb}_4\text{O}_{10}$: d^{10} transition metal size effect influencing the stoichiometry and the centricity

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Functional oxides have attracted attention owing to their various applications in electronics, catalyst and optical devices with superior thermal stability. One of them, noncentrosymmetric (NCS) oxides have been studied by plenty of research group because they have diverse properties such as pyroelectricity, ferroelectricity, piezoelectricity and nonlinear optical properties at the same time. Thus, several strategies for synthesizing novel NCS materials have been continuously proposed. In this research, we successfully synthesized two novel NCS materials by combining Second-Order Jahn-Teller (SOJT) distortive d^0 cations, lone pair cations, and polar displacive d^{10} cations, i.e. Mo^{6+} , Sb^{3+} , and Zn^{2+} (or Cd^{2+}). Two new molybdenum antimonites have been synthesized by hydrothermal and standard solid state reactions. The $\text{ZnMoSb}_2\text{O}_7$ crystallizes polar space group $P2_1$ along with three-dimensional framework composed of MoO_4 , SbO_4 , and ZnO_4 polyhedra. While $\text{CdMoSb}_4\text{O}_{10}$ crystallizes nonpolar centrosymmetric space group $P21/m$ along with one-dimensional framework consisting of MoO_4 , SbO_3 , and CdO_6 polyhedra. For $\text{ZnMoSb}_2\text{O}_7$, structural analysis suggests that it has a net polarization in the $[0-10]$ direction due to parallel alignment of MoO_4 distorted tetrahedra. Local dipole moment calculation is consistent with structural analysis. The result of synthetic experiments for $\text{ZnMoSb}_4\text{O}_{10}$ and $\text{CdMoSb}_2\text{O}_7$ show that the size of d^{10} cation affect stoichiometry as well as symmetry. The two molybdenum antimonites were also fully characterized by powder X-ray diffraction, IR spectroscopy, UV-vis spectroscopy, and powder second-harmonic generation measurements.

Biography

Jo Hongil has completed his bachelor degree at the age of 26 years from Chung-Ang University and pursues his combined master's and doctorate program at Chung-Ang University. He is studying solid chemistry and advised by Prof. Ok Kang Min. He has published 3 papers in reputed journals.

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