5th International Conference on

Organic and Inorganic Chemistry

July 12-13, 2018 | Paris, France

Hydrothermal synthesis, crystal structure, and second-harmonic generating (SHG) properties of a new layered bismuth oxyfluoride nitrate

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A new layered noncentrosymmetric (NCS) bismuth oxyfluoride-nitrate was synthesized by a hydrothermal reaction. The crystal structure was determined by powder and single-crystal X-ray diffraction. The material crystallizes in an NCS trigonal space group, R3 (No. 146). The constituting [Bi6O7F3]+ cationic layer contain H2O and nitrate anion makes a charge balance. The powder second harmonic generation (SHG) measurements indicate the title compound is phase-matchable (Type I) and exhibits a strong SHG efficiency of about 90 times that of α -SiO2. Detailed structural examination suggests that the π -conjugate system of nitrate anion directly influence the nonlinear optical (NLO) properties of the material. Infrared and UV-vis diffuse-reflectance spectroscopy, energy dispersive X-ray spectroscopy (EDS), thermogravimetric analysis (TGA), and local dipole moment calculations are also presented.

Biography

Eun Jeong Cho has obtained her Bachelor's degree from Chung-Ang University. She is working on the synthesis and characterization of new bismuth oxyfluoride materials as a graduate student under the guidance of Prof. Kang Min Ok at Chung-Ang University.

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