Organic-inorganic compounds with strong nonlinear optical properties based on 2,4,6-trimethylpyridinium and tetrahedral BF_4^- networks.

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Streszczenie

A different organic-inorganic crystal—[2,4,6-trimethylpyridinium][BF4]—of nonlinear optical propertiesat room temperature was synthesized and characterized. The compound is built up of the organic [2,4,6-trimethylpyridinium] cations incorporated into inorganic, tetrahedral BF4anions. It crystallizes at roomtemperature in the polar space groupPmn21, and undergoes three first-order phase transitions at [cooling(heating)] 241 (245) K, 297 (328) K, and 389 (406) K. The lowest temperature ferroic phase transition (ferroelastic;mm2→mtype) is related to the significant pyroelectric effect. The compound was studied by single-crystalx-ray diffraction at several temperatures, using thermal (differential scanning calorimetry and thermogravimetricanalysis) methods and dielectric spectroscopy. The piezoelectric, pyroelectric, and second-harmonic generation(SHG) properties were determined. Density-functional theory calculations in two stable phases are given. The[2,4,6-trimethylpyridinium][BF4] crystal exhibits a SHG efficiency of 1.7 times that of KDP. The mechanism ofstructural phase transitions in the title compound is discussed.

Adres publiczny

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