



Crystal structure and characterization of a novel acentric imidazolium analog $[C_3N_2H_5^+][Br^-]$.

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A novel nonlinear optical crystal has been synthesized and characterized by a single-crystal X-ray diffraction, calorimetric, dilatometric and dielectric measurements. Above 200 K the crystal structure is polar, with symmetry $R3$. It consists of a highly disordered imidazolium cations and discrete anions. The compound reveals a first order phase transition at 199/201 K (cooling/heating cycle) which leads to the monoclinic centrosymmetric space group . The exceptionally large increment of dielectric permittivity accompanying the structure transformation is related to the freezing of cation motions and a significant rebuilding of the anionic substructure.

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