Radiation from Relativistic Electrons in Periodic Structures "RREPS-23" & Electron, Positron, Neutron and X-ray Scattering under External Influences "Meghri-23"



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Li2·3IO3·H3O: Crystal Structure and IR Spectrum

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In recent years studies have shown that doping a crystal with amino acids improves the non-linear optical properties of α -LiIO3crystal [1, 2]. The authors[3] have studied the interaction of lithium with iodic acid and have shown that, at compositions close to $0.2 \le x \le 0.34$, 2LiIO3•HIO3crystals are formed in a mixture of Li1-xHxIO3.

The present work deals with the synthesis, IR spectrum, thermal, and crystal structure study of the new lithium iodate crystal Li2•3IO3•H3O.The crystal was obtained by doping the α -LiIO3 crystal with amino acids of more than 5mol.%.Crystal structure of 2(Li)+(H3O)+3(IO3)–was determined by single-crystal X-Ray diffraction analysis at 100(2) K. It crystallizes in the monoclinic system (P21/n) with the parameters: a=8.3266(12) Å, b = 10.9893(17) Å, c = 11.2472(17) Å, $\alpha = \gamma = 90^\circ$, $\beta = 111.360(4)^\circ$ and Z(Z') = 4(1). The structure was refined to R = 0.0215 and ω R = 0.0580 for 2276 reflections. The structure contains a hydronium cation(H3O)+, three crystallographic independent trigonal pyramidal IO3 anions, two independent cations(Li+) coordinated each by four oxygen atoms (3IO3) at apices of strongly deformed tetrahedrons, see Fig. 1. The Li-O bond lengths are similar to the bond lengths in the Li2HPO3•H2O crystal [4]. The research results have revealed the mechanisms of crystal formation and the characteristic absorption bands of functional groups, which is of scientific importance.

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