ASRP 2025 - Alpic School for Radiation Physics



Contribution ID: 108

Type: not specified

Theoretical and Experimental Study of L-Arginine Sulfates and L-Nitroarginine Sulfosalicylate Crystals

Tuesday 17 June 2025 17:10 (1 minute)

The subjects of the present study are L-arginine sulfates (LAS·2H2O & LAS) and L-nitroarginine sulfosalicylate (L-NNA·SSA). The thermal properties, vibrational spectra, UV-Vis transmittance spectrum and second harmonic generation activity were experimental studied. The crystal and molecular structure of crystals were determined by the single-crystal X-ray diffraction method. The optimized lattice parameters of the crystal structures of L-NNA·2SSA and L-arginine sulfate (LAS) are presented in Table, together with their experimental values. Thus the optimized unit cell volume was reduced by 6.24% for L-NNA·SSA, 9.9% for LAS·2H2O and 5.02% for LAS crystal. As well as, theoretically obtained optical properties are consistent with the experimental ones. In particular, the absorption spectrum of LAS·2H2O decreases rapidly at low energy regions, which agrees well with the transmittance spectrum of LAS, suggesting a dielectric nature of both materials. Moreover, the bands originating from the orbital electrons of oxygen (O), nitrogen (N) and carbon (C) are responsible for the formation of energy gaps of about 2.9 eV for L-NNA·SSA, 4.2 eV for LAS·2H2O and 4.6 eV for LAS crystals.

Author: GHARIBYAN, Nelli (Institute of Applied Problems of Physics)

Co-authors: Dr ATANESYAN, Armen (Institute of Applied Problems of Physics); Mrs DANGHYAN, Astghik (Institute of Applied Problems of Physics); Dr SAHAKYAN, Mane (Institute of Low Temperature and Structure Research, Polish Academy of Sciences, ul. Okólna 2, 50-422 Wrocław, Poland); Dr SUKIASYAN, Ruzan (Institute of Applied Problems of Physics); Mr TER-BALYANTS, Sargis (Institute of Applied Problems of Physics); Dr BED-NARCHUK, Tamara (Institute of Low Temperature and Structure Research, Polish Academy of Sciences, ul. Okólna 2, 50-422 Wrocław, Poland) (Institute of Competitional Structure Research, Polish Academy of Sciences, ul. Okólna 2, 50-422 Wrocław, Polish Academy of Sciences, ul. Okólna 2, 50-422 Wrocław, Poland)

Presenter: GHARIBYAN, Nelli (Institute of Applied Problems of Physics)

Session Classification: Poster Session P17