GROWTH, EXPERIMENTAL AND COMPUTATIONAL STUDIES OF L-HISTIDINE BARIUM NITRATE CRYSTALS FOR PHOTONICS, OPTICAL-SENSOR AND RHEOLOGICAL APPLICATIONS

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The L-Histidine Barium Nitrate (LHBN) crystal is properly grown by the customary slow evaporation method using the de-ionized water of lab-quality with the resistivity above 1 *MΩ-cm with high purity. The lattice parameters for LHBN are* $a = 24.0106$ *Å,* $b = 4.7231$ *Å,* $c = 8.3181$ *Å,* $\alpha = 90°$, $\beta = 105.44°$, $\gamma = 90°$ *with* $C2$ *as the space group. The LHBN material is analyzed for the white transparent nature with lower cut-off value of* 320 *nm. By Tauc's plot the optically measured band gap of LHBN is* 3.9 *eV for the macro-photonics utility. The optical sensitivity of the LHBN crystal is analyzed and found to have* 8% *sensitivity with blue and red LED sources. The rheological based work for LHBN is analyzed for enhanced results.*

Keywords: L-Histidine Barium Nitrate (LHBN); optical, sensor, rheology, photonics.

1. Introduction. Single crystals are in high demand across various scientific and industrial fields due to their unique properties and exceptional structural uniformity and optical quality.

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High efficiency non-linear optical (NLO) specimens have attracted significant attention for opto-electronic applications particularly in frequency doublers. Most organic and inorganic crystalline substances offer wide NLO utility in electronics and material engineering [1–3]. In the field of crystal growth, single crystals are primarily developed for the NLO and sensor based applications with the specific focus on Second Harmonic Generation (SHG).

Additional advantages of these materials include multifunctionality via substitution, high laser-damage threshold and device utility [4]. Crystals are typically grown and optimized for NLO efficiency, physical and chemical stability, and the mechanical strength [5]. Materials classified as amino acid frequently exhibit excellent NLO and electro-optic properties [6]. Combining organic and inorganic materials improves the higher order NLO utility by providing lower phase-transforming temperature, faster response and higher transparency and makes them highly sought-after systems [7]. The growth of higher-order NLO crystals is of greater significance for extending the frequency range of standard laser inputs in the UV, IR zones [8–11]. Semi-organic crystals, in particular, offer interesting NLO responses for electronic / opto-electronic usage [12–15]. Previously, vibrational spectra, the optical absorption (200–800 nm), the TG-DTA curves, the permittivity and dielectric loss at various temperatures, conductivity, and hardness of this material have been examined. However, since the crystal under consideration is nonlinear, it is necessary to study the damage threshold and sensor sensitivity. This study investigates LHBN, because of the combination of amino-acid and barium yields higher selectivity, sensitivity, stability and optical activity.

2.Growth of LHBN and computational structural data. Commercially available of L-Histidine (99% purity SRL) and Barium Nitrate (99% purity, Merck) were utilized as starting materials. Single crystals of LHBN were grown via slow evaporation solution growth method using de-ionized water. LHBN was synthesized by mixing L-histidine and barium nitrate in a 2:1 molar ratio; LHBN synthesis is confirmed by the following reaction shown in equation (1) and the grown crystals are shown in Fig. 1; Fig. 2 presents the computationally analyzed structure of LHBN crystal generated via software using the standard crystallographic information file (CIF-data) of LHBN...

Поступила в редакцию 19 ноября 2025 г.
После доработки 9 июня 2026 г.
Принята к публикации 28 июня 2026 г.