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Original Article

Studies on Molecular Structure and Vibrational Spectra of NLO Crystal L-Glutamine Oxalate by DFT Method

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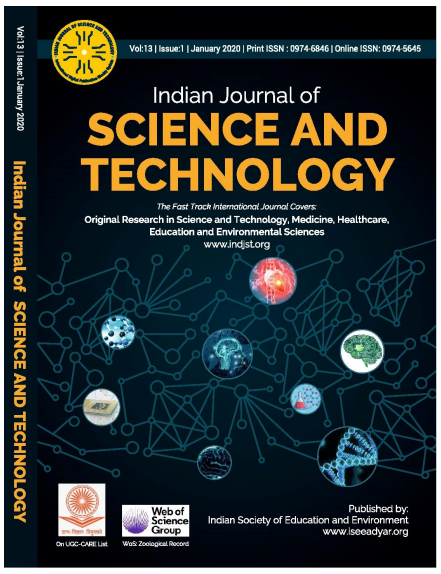

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ABSTRACT

Objectives: To explicate structural features of L-GLUTAMINE OXALATE (LGO) using vibrational spectroscopic methods and DFT computations. To identify the functional groups and hydrogen bonding interactions of the molecule by recording FTIR and FT-Raman spectra. To confirm NLO activity by performing SHG test. **Methods/Statistical Analysis:** Crystals were grown by slow evaporation method and characterized by powder X-Ray diffraction method. FTIR, FT-Raman,

UV-Vis analysis and second harmonic generation test were predicted. DFT analysis using Gaussian'09 program package were performed to confirm the NLO properties theoretically. **Findings:** Lowering of HOMO-LUMO energy gap value explains the intramolecular charge-transfer interaction which indicates NLO property. Second Harmonic Generation of the sample shows good nonlinearity of the sample. **Application/Improvements:** LGO sample shows good NLO Properties and can be used in optical field.

Keywords: HOMO-LUMO, MEP, NLO, NCA

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