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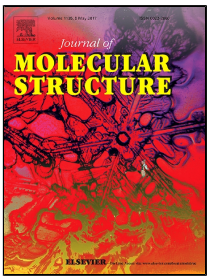

Comparative studies on Molecular structure, Vibrational Spectra and Hyperpolarizabilities of NLO Chromophore Ethyl 4-Dimethylaminobenzoate

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- DFT calculations have been performed on the NLO crystal Ethyl 4-Dimethylaminobenzoate (EDAB)
- Theoretical Optimized geometry, NBO, charge and Hyperpolarizabilities were calculated
- Comparative studies of geometry, Hyperpolarizability and charge were made
- The IR and Raman spectra of the compound were analyzed.
- The NLO activity of the crystal was confirmed by SHG analysis.
- UV-Visible analysis was recorded and analysed