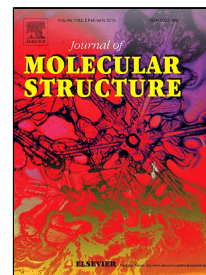


# Accepted Manuscript



On the molecular structure, vibrational spectra, HOMO-LUMO, molecular electrostatic potential, UV-Vis, first order hyperpolarizability, and thermodynamic investigations of 3-(4-chlorophenyl)-1-(pyridine-3-yl) prop-2-en-1-one by quantum chemistry calculations

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**HIGHLIGHTS**

- The optimized geometry is computed using HF and DFT methods
- Spectroscopic properties were calculated and compared with the experimental ones
- The complete vibration assignments are performed on the basis of PED
- The nonlinear optical properties have been evaluated at different levels of theory
- MEP of the title compound was calculated

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