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Quantum Computational Calculations, DFT, Vibrational Spectroscopy and Molecular Docking Investigations of Dimethyl Tetrachloroterephthalate

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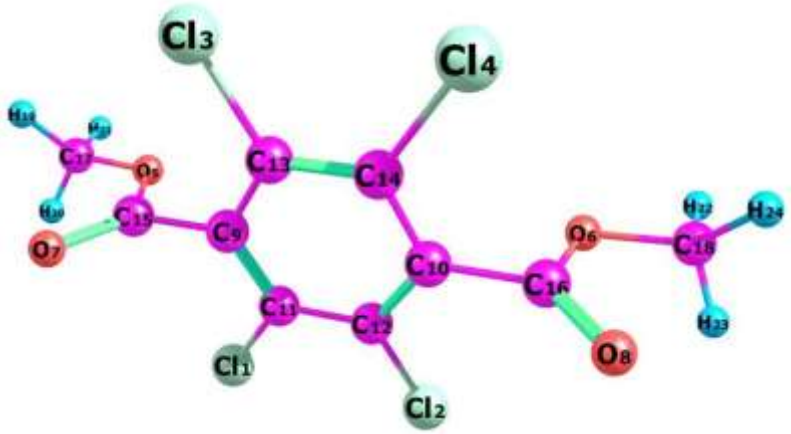
The title compound Dimethyl Tetrachloroterephthalate was characterized through the interpretation by FT-IR, FT-Raman, UV spectral analyses. The stable molecular conformations, optimized molecular geometry, vibrational wave numbers, infrared intensities, and the Raman scattering activities were carefully analyzed by using Density Functional Theory (DFT). The computed HOMO and LUMO energies depict that the charge transfer takes place in the molecule. Intermolecular reliability of the molecule emanating from hyper conjugative interactions of charge delocalization by NBO have been examined with the accomplishment of Molecular Electrostatic Potential (MEP) for the molecule. The molecular docking studies put forward the idea that the amino acid .



Keywords: DFT, FTIR, FT-Raman, Chemical reactivity, Molecular docking