



**(ICAPMS - 2025)**

Proceedings of the International Conference on  
Advanced Perspectives in Materials Science

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**07<sup>th</sup> January, 2025**

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*Organised by*

**PG & Research Department of Physics  
Jamal Mohammed College (Autonomous)**

Accredited with A++ Grade by NAAC (4<sup>th</sup> Cycle) with CGPA 3.69 out of 4.0  
(Affiliated to Bharathidasan University)

**Tiruchirappalli**



*In association with*

**Indian SpectroPhysics Association  
(ISPA), Chennai, India**

**Editors- In - Chief**

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**Founder President, ISPA**

**Dr. A. Ishaq Ahamed, Ph.D.**

**Associate Professor, Department of Physics**

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

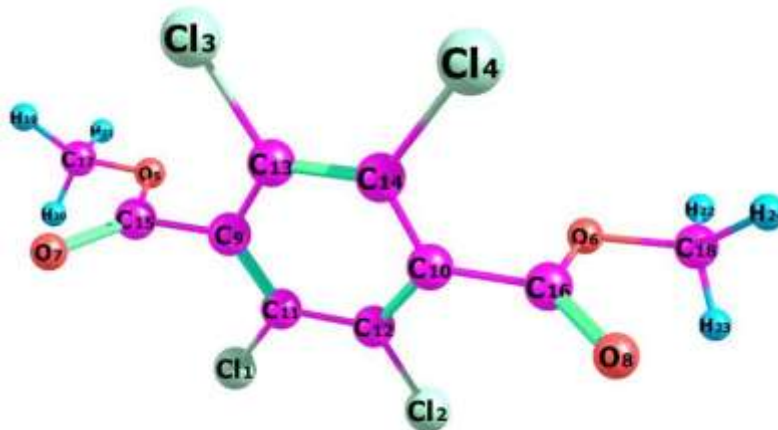
*B. Shantha Lakshmi<sup>a</sup>, V. Sabari<sup>b\*</sup>, C.P. Devipriya<sup>a</sup>, B. Sumathi<sup>a</sup> and J. Udayaseelan<sup>a</sup>*

<sup>a</sup>Department of Physics, Govt. Thirumagal Mills College, Gudiyatham-632602, Vellore, Tamil Nadu, India

<sup>b</sup>Department of Physics, Marudhar Kesari Jain College for Women, Vaniyambadi-635751, (Thiruvalluvar University Serkadu, Vellore -632115)

\*Corresponding author: V. Sabari (vrsabari86@gmail.com)

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