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Theoretical and Experimental Electrostatic Potential around the M-Nitrophenol Compound

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Abstract : Our work is about a comparison of experimental and theoretical results of the electron charge density distribution and the electrostatic potential around the M-Nitrophenol Molecule (m-NPH) kwon for its interesting physical characteristics. The molecular experimental results have been obtained from a high-resolution X-ray diffraction study. Theoretical investigations were performed under the Gaussian program using the Density Functional Theory at B3LYP level of theory at 6-31G*. The multipolar model of Hansen and Coppens was used for the experimental electron charge density distribution around the molecule, while we used the DFT methods for the theoretical calculations. The electron charge density obtained in both methods allowed us to find out the different molecular properties such us the electrostatic potential and the dipole moment which were finally subject to a comparison leading to an outcome of a good matching results obtained in both methods.

Keywords : electron charge density, m-nitrophenol, nonlinear optical compound, electrostatic potential, optimized geometric
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