**Quantum Chemical Computations with Structural, Topological and Electronic Investigations on Cu Cl Para Nitro Flavonol**

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ABSTRACT

The electronic studies, topological interpretations, and optimal molecular geometry were computed using the density functional theory (DFT/B3PW91) method LANL2DZ as the basis set. To investigate the chemical reactivity, frontier molecular orbitals and molecular electrostatic potential were examined. The HOMO-LUMO energies are used to compute the bandgap energy of the title molecule, which comes out to be 1.3532 eV. The charge transfer interactions verified the intermolecular charge transport inside the molecule. The Localized Orbital Locator (LOL) and Electron Localization Function (ELF) were used to describe the chemical consequences of the molecule.

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