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Growth, Hirshfeld surfaces, Spectral, Quantum Chemical Calculations, Photoconductivity and Chemical Etching analyses of nonlinear optical p- Toluidine p- Toluenesulfonate Single Crystal

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Abstract

A single crystal of p-toluidine p-toluenesulfonate (PTPT) has been grown by slow evaporation solution technique (SEST) at room temperature. Single crystal X-ray analysis confirms that grown crystal belongs to the monoclinic structure with space group $P2_1$. Intermolecular interactions and fingerprint plots of PTPT molecules are executed by Hirshfeld surface analysis. It was found that H···H (44.2 %) contacts have maximum intermolecular interactions contributions in the total Hirshfeld surface area. The characteristic absorption band occurs at below 290 nm. The functional groups were identified using FTIR and FT-Raman analyses and compared with theoretical values. The title molecule contains fourteen C–H bonds and three O–H bonds. The calculated HOMO and LUMO energy values are -6.125 eV and -1.157 eV, respectively. The chemical potential (μ) and electronegativity (χ) values are estimated to be -3.4938 eV and 3.4938 eV, respectively. The strongest negative hyperconjugation occurs due to the charge transfer from the occupied orbital (σ) to the unoccupied orbital (π*) which is calculated for the σ(N20 - C21) → π*(N20 – O18). The green and red lines in the total density of states (TDOS) spectrum indicate the occupied orbital and virtual orbital levels, respectively. Photoconductivity studies have been done for the grown crystal. It is observed that the dark current is greater than photocurrent. It shows