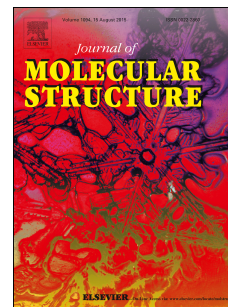


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N–H···O hydrogen bonded novel nonlinear optical semiorganic crystal (4-methoxyanilinium trifluoroacetate) studied through theoretical and experimental methods

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Abstract

The new semi-organic crystal of 4-methoxyanilinium trifluoroacetate (4MATFA) was designed through strong N–H···O hydrogen bonds in the perspective of its nonlinear optical (NLO) properties. The crystalline state of 4MATFA was successfully attained by slow evaporation solution growth method at room temperature. The molecular structure of the grown crystal was determined by single crystal X-ray diffraction technique which confirms the importance of N–H···O hydrogen bonds in the molecular assembly. The amino group of the cation and carboxylate group of the anion are hydrogen bonded through two primary chains $C_1^2(4)$ and $C_2^2(6)$ motifs and a secondary ring $R_4^4(12)$ motif leading to alternate hydrophobic and hydrophilic layers at $z = 0$ or 1 and at $z = 1/2$, respectively. The molecular geometry was optimized theoretically by Hartree-Fock (HF) and Density Functional Theory (DFT) methods with 6-311++G(d,p) basis set. The optimized molecular geometrical parameters and computed vibrational spectra demonstrated the presence of N–H···O hydrogen bonds and the absence of expected N–H···F hydrogen bonds. The strong N–H···O tendency between the ions are observed as strong intensity isolated peak in computed IR spectra and strong intensity broad peak in experimental IR spectrum. Further, the calculated first (β) and second order hyperpolarizability (γ) values showed that the compound is good candidate for NLO applications. The chemical hardness, electro-negativity and chemical potential of the molecule were computed by HOMO - LUMO plot. The frontier orbital has lower band gap value, which indicate the possible optical activity of the molecule. The thermal stability of the grown crystals were confirmed by TG/DTA which showed the thermal stability of the compound upto 150°C.

Keywords: Single Crystal XRD, hydrogen bonds, vibrational spectra, quantum chemical methods and nonlinear optical (NLO)

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