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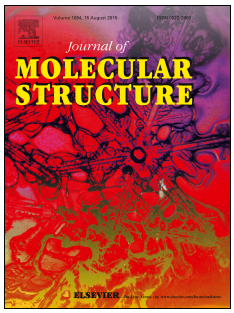

Hydrogen bonding interactions and supramolecular assemblies in 2-amino guanidinium 4-methyl benzene sulphonate crystal structure: Hirshfeld surfaces and computational calculations

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Hydrogen bonding interactions and supramolecular assemblies in 2-amino guanidinium 4-methyl benzene sulphonate crystal structure: Hirshfeld surfaces and computational calculations

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Abstract

2-aminoguanidinium 4-methyl benzene sulphonate (AGMS), an organic compound with big assembly of hydrogen bonding interactions was crystallized at room temperature. The structure of the compound was confirmed by FT-IR, NMR and single crystal X-ray diffraction analysis. Numerous hydrogen bonded interactions were found to form supramolecular assemblies in the molecular structure. Fingerprint plots of Hirshfeld surface analysis spells out the interactions in various directions. The molecular structure of AGMS was optimised by HF, MP2 and DFT (B3LYP and CAM-B3LYP) methods at 6-311G (d,p) basis set and the geometrical parameters were compared. Electrostatic potential calculations of the reactants and product confirm the transfer of proton. Optical properties of AGMS were ascertained by UV absorbance and reflectance spectra. The band gap of AGMS is found to be 2.689 eV. Due to numerous hydrogen bonds, the crystal is thermally stable up to 200 ºC. Hyperconjugative interactions which are responsible for the second hyperpolarizabilities were accounted by NBO analysis. Static and frequency dependent optical properties were calculated at HF and DFT methods. The hyperpolarizabilities of AGMS increase rapidly at frequencies 0.0428 and 0.08 a.u. compared to static one. The compound exhibits violet and blue emission.

Keywords: Single crystal XRD, Hirshfeld Surfaces, Hyperpolarizability, NBO analysis