Crystal structure studies, computational analysis, and hydrogen bonding attributes of halogen bonded sulfonyl Schiff bases

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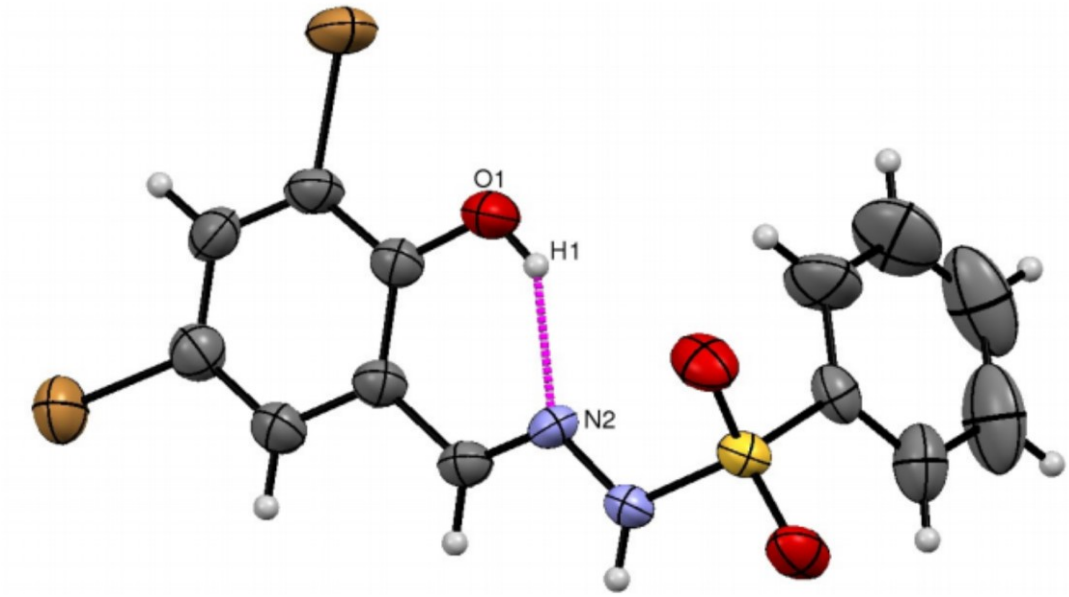
Halogen bond has been the focus of crystallography and chemical engineering for many decades. The effect of intramolecular halogen bonds on adjacent intramolecular hydrogen bonding has hardly been investigated. O-hydroxy sulfonyl Schiff bases are a suitable class of compounds to shed light on these bonding aspects. Series of halogen bonded sulfonyl Schiff bases were synthesized and characterized spectroscopically using mass, FTIR, and NMR methods. The three-dimensional molecular structures of all the sulfonyl Schiff base compounds were confirmed through single-crystal X-ray diffraction studies. The crystal structures of Schiff bases exhibit both inter and intramolecular hydrogen bond interactions. Packing of the structures shows hydrogen bonded 1D chain and π---π interaction generates 2D supramolecular structure. O–H···N intramolecular interactions form the five-membered pseudo chelate rings. The Schiff base structures are also stabilized by C–O···π, N–O···π, π···π interactions and leads to the 3D network through supramolecular synthons. The intermolecular interactions were then quantified using Hirshfeld surface analysis. Further, the density functional theory calculations were employed using B3LYP hybrid functional with a 6-311+G (d, p) level basis set to optimize the structural coordinates. The chemically active regions of the Schiff base molecules were identified from the plot of the molecular electrostatic potential surface. Furthermore, the atoms in molecules (AIM) and their applications to chemical bonding based on Bader's theory have been studied to understand the molecular interactions.



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