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Crystal growth and intramolecular hydrogen bond effects on activity of a novel Schiff base ligand: An experimental and theoretical approach

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ABSTRACT

Reaction of thiosemicarbazide with alkyl halides produce isothiosemicarbazides which in condensation reactions with aldehydes or ketones could yield isothiosemicarbazones. A new tridentate Schiff base compound, salicylaldehyde S-benzylisothiosemicarbazone (H_2L) (Figure), is synthesised and characterized by elemental, IR, ^1H-, ^{13}C-NMR, mass and X-ray diffraction analyses.

The optimized molecular geometry (bond length, bond angle), natural bond orbital (NBO), Mulliken population analysis (MPA), complete vibrational frequencies and the its intensities are calculated by density functional theory (DFT) method (B3LYP) with 6–311++G(d,p) basis set. The optimized geometry and calculated vibrational frequences are performed and compared with the experimental results. NBO analysis explore hyperconjugative interactions and stability of the title compound, especially, reconfirms the existence of O-H⋯N intramolecular hydrogen bond. Calculated HOMO-LUMO band gap energy confirms that charge transfer occurs within the molecule by removing the hydrogen bond in title compound. The hyperconjugative interactions energy $E^{(2)}$ and electron densities of donor (i) and acceptor (j) bonds are calculated using NBO analysis.
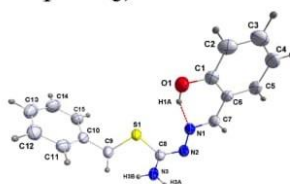
Figure. Salicylaldehyde S-benzylisothiosemicarbazone (H_2L)

Keywords: isothiosemicarbazone, crystal Structure, DFT

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