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Structural investigations, theoretical analysis, chemosensing characteristics and molecular docking studies of t-butyl carbazate based novel aldimine

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ABSTRACT

The reaction of tert-butyl carbazate and 2-hydroxybenzaldehyde in a methanol solvent with a catalytic amount of glacial acetic acid produced tert-butyl (E)-2-(2-hydroxybenzylidene)hydrazine-1-carboxylate (TBCS) and was characterised by experimental NMR (^{1}H, ^{13}C), FT-IR spectrum (4000-400 cm^{-1}). In the P bca space group, X-ray crystallography established the orthorhombic crystal structure of the target molecule, $C_{12}H_{16}N_2O_3$. One molecule makes up the asymmetric unit, which has unit cell dimensions of a = 10.8241(4) Å, b = 10.4072(4) Å, c = 21.9875(8) Å, and angles α=β=γ= 90°. There are several hydrogen bonding connections and π stacking interactions between the molecules in the crystal packing. The study of the Hirshfeld surface employed various energy frameworks, enabling a thorough examination of the solid-state structure. The results demonstrate that electrostatic energy plays a vital role in maintaining the stability of molecular sheets, while hydrogen bonds primarily contribute to their expansion. Fingerprint plots were created to evaluate the relative importance of noncovalent interactions in the target compound, TBCS. Energy framework calculations have also been performed to delve deeper into understanding the intermolecular interactions. The enrichment ratios show that the favorable contacts accountable for the crystal packing are O···H-C, N···H-C, O···H, and N···H. The intermolecular interactions are further characterized using Bader's theory of "atoms in molecules" (QTAIM) and the "noncovalent" (NCI) interaction plot index. The nature and strength of noncovalent interactions are analyzed from the topological parameters at (3, −1) bond critical points(BCPs). The application of density functional theory (DFT) calculations utilising the B3LYP hybrid functional alongside a TZVP basis set improved the accuracy of structural coordinates, Infrared intensities, harmonic vibrational fundamentals, potential energy distribution (PED) and various electronic parameters in both gas phase and a range of solvents, such as methanol, water, DMSO, and chloroform. TBCS functions as an effective fluorescent chemosensor specifically designed for the detection of Zn^{2+} ions. The probe exhibits increased fluorescence upon immersion in methanol solutions that contain Zn^{2+} ions. This study utilised UV-Vis and fluorescence titration methods to examine the binding mechanism of TBCS

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