[MS25-P01] Hydrogen bonding interactions in a zwitter-ion derivative: Insights from crystallographic and theoretical studies

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The Schiff-base ligands and their complexes have attracted considerable interest due to their potential applications as analytical reagents [1-4] and their biological activities such as antibacterial and antifungal [5], anticancer [6] etc. Moreover, they are also important in industrial applications of liquid crystals, light-driven switches and image storage devices [7, 8]. Due to the biological importance, the crystal structure of a zwitter-ion derivative- 2-[2hydroxyphenyl) iminomethyl] phenol is determined and hydrogen bonding interactions together with theoretically computed structure are discussed herein. In the title molecule, $C_{13}H_{11}NO_2$, the two independent molecules have orthogonal orientations characterized by dihedral angle of 83.77 (4)° between the mean planes passing through atoms of respective molecule. The quantitative analysis of root mean square fit between non-hydrogen atoms of both the molecules (r.m.s. deviation = 0.017 Å) indicates almost similar conformation for both the molecules. The two intramolecular N-H…O hydrogen bonds with S(6)S(5) graph-set motif [9] and an intermolecular O-H…O hydrogen bond in each of the two molecules form two dimensional hydrogen bonding network in a zigzag fashion along bc-plane. These hydrogen bonded sheets in a crystal are linked through van der Waals force in (1 0 0) direction. The conformational difference between theoretical and experimental structures obtained from semi-empirical quantum chemical and single crystal X-ray diffraction methods respectively [10,11] explain the role of hydrogen bonding interactions in the packing of structure. The small HOMO-LUMO energy gap of 6.959 eV indicates the intermolecular charge transfer between the atoms of two molecule system.

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