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STRUCTURAL, ELECTRONIC AND NATURAL BONDING ORBITALS (NBOS) ANALYSIS OF CHLOROBENZALDEHYDE SCHIFF BASES: A DFT STUDY

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Abstract

This study investigates the reactivity and stability of Schiff bases (S1–S2), focusing on their geometric and electronic properties. These compounds are of interest due to their potential applications stemming from their conjugated systems and functional groups. The study aims to explore their chemical reactivity descriptors, intramolecular and intermolecular charge transfer behavior, and stability. Additionally, the spectral properties of the Schiff bases were examined through simulated UV-Vis and FTIR spectra, with particular attention to π–π transitions associated with aromatic rings and C=N linkages. Density Functional Theory (DFT) calculations were carried out using the B3LYP functional and the 6-311G(d,p) basis set. Global reactivity parameters including ionization potential (IP), electron affinity (EA), chemical hardness, softness, electronegativity, and electrophilicity were derived from the frontier molecular orbitals (FMO). Hirschfeld surface analysis and Natural Bond Orbital (NBO) analysis were also performed at the same theoretical level to assess molecular interactions and charge transfer. Simulated UV-Vis and FTIR spectra were computed to further support the electronic and vibrational characterization of the Schiff bases.*

INTRODUCTION

Schiff bases have received great attention for last decades due to their versatility and intriguing properties such as thermal stability, catalytic properties, Anti tumors, anti-cancers, anti-fungal, antibacterial, anti-microbial anti-proliferative, anti-diabetic, anti-inflammatory, biocidal activities[1-3].and also act as ligand in the field of coordination chemistry[4]. Schiff base is also known asimine or azomethine. The complexes of Schiff bases showed significant inhibitory activity againstpathogenic bacterial species [5; 6].

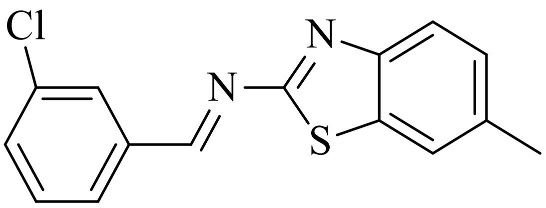
Besides versatile biological applications Schiff base and their derivatives are also employed as fluorescent turn on\ turn off sensors [7; 8] optical sensors [9] corrosion inhibitory [10] fluorescent camphor [11] and chemo sensors [12]. Naked eye sensors are much interested now a days due to their visual detection properties rather employing complex instrumentation. Recent literature studies reveals that Schiff bases containing chlobenzaldehyde and aminothiazole derivatives is of great interest due to its several biological and non-biological applications such as antifungal, antibacterial, Anticancer, antituberculosis, anti-inflammatory, anti-allergic, antihypertensive, Anti-HIV fungicides and herbicides. Fluorescent chemo sensor, bio sorbent, pharmacophore, chromophores, Dyes and pigment [13-16].

The Schiff base with thiazole derivatives were of great interest due to its verities of application, these Schiff base as a ligand have been extensively studied mainly because of their electronic properties responsible for the designing of new electric materials [17; 18]. A lot of theoretical investigation have been made on Schiff bases to calculate different electronic and molecular properties associated with low band gap for designing new conducting materials [19]

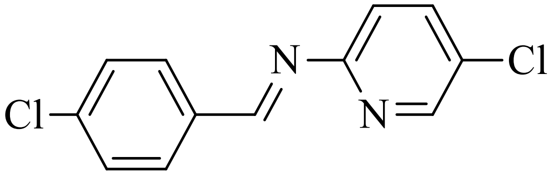
By considering the above mention applications of Schiff bases we are planning to investigate the geometric parameters and molecular properties through density function theory (DFT), Natural bond orbitals (NBOs) and molecular orbitals (MOs) analysis will also carried out to demonstrate electronic properties i.e., EHOMO, ELUMO, band gap (ΔE), ionization potential (IP) electron affinity (EA), global hardness (η) and global electrophilicity (ω) by using computational software gaussian09 with different basis set and some quantum physical calculation.

Computational details

Density functional theory (DFT) was utilized to determine geometry optimization for **S1–S2** given in **figure 1**. This was accomplished by describing all nonmetal atoms using the basis set 6-31++G(d,p) and the hybrid functional B3LYP. Because these approaches performed effectively in our earlier research, they were employed. Vibrational frequency calculations were performed after geometry optimizations to verify that the optimized structures were indeed minima. The NBO program developed in Gaussian was utilized to perform natural bond analysis on the given ground-state geometries. The eager singlet with the lowest position ultraviolet-visible with the TD-DFT, states were examined. Approaches that was employed to carry out the optimizations at the same theoretical level. Every computation was performed using the Gaussian program. The NBO, FMOs, FTIR, UV-vis analysis was also accomplished for electronic properties i.e., E_{HOMO}, $E_{LUMO,}$ Band gap(ΔE), Ionization Potential (IP) Electron Affinity (EA), Global Hardness(η) and Global Electrophilicity (ω) with the help of same theory and basis set The Hirschfield surface analysis was also conducted for molecular interactions sites. By using crystal explorer.



S1



S2

Figure 1. Structure formulae of Schiff bases (S1-S2)

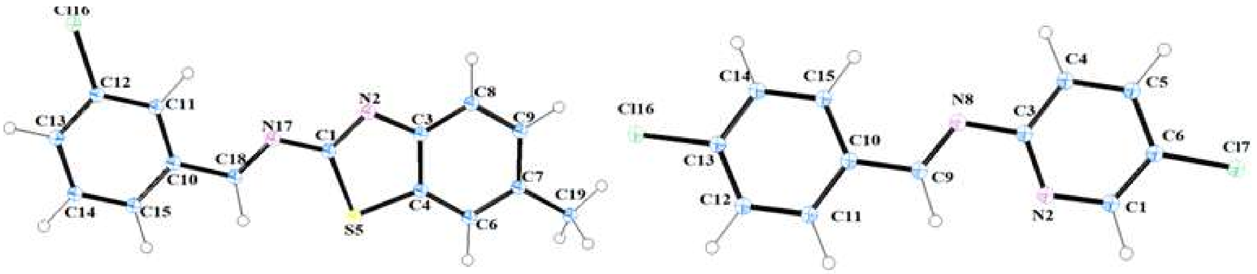
Results and Discussion

Geometric parameters

It is a well-known fact that DFT can accurately and quickly predict the molecular geometries[20] of the compounds. The Schiff bases **(S1-S2)** were selected for the title study. The quantum chemical investigation of the said compound **(S1-S2)** was carried out with gaussian09 software by using the same theory and basis set as mention above. Ball and stick diagram was drawn via Ortep molecular graphics software from optimized file to calculate and compare the geometric parameters of schiff base as shown below in **figure 2.** The geometric bond distances for **S1** (C1-S5), (N17-C18), (C12-C11), and (C8-C9) are 1.668, 1.289, 1.399, and 1.407 Å and that for **S2** (C3-C4), (Cl7-C6), (C1-N2), and (N8-C9) are 1.390, 1.715, 1.357, and 1.291 Å respectively. The calculated bonds angles of **S1** (S5-C4-C6), (C13-C14-C15), (N17-C1-N2), and (Cl16-C12-C11) are 130.68°, 120.14°, 122.99°, and 119.98° and that for **S2** (C1-N2-C3), (Cl16-C13-C14), (C10-C9-N8), and (C4-C5-C6) are 116.91°, 119.73°, 121.18°, and 118.18° respectively are given in **table 1**. The least deviated values were found to be 0.001 Å for **S1,** and **S2**. However, the most deviated values were recorded 0.002 Å.

Table 1. Parameters of Schiff base S1-S2 bond length (Å) and bond angles (°)

Compounds	Atoms	Bond Length (Å)		Atoms	Bond Angle (°)	
		Experimental	Calculated		Experimental	Calculated
S1	C1-S5	1.669	1.668	S5-C4-C6	130.68	130.68
	N17-C18	1.290	1.289	C13-C14-C15	120.45	120.14
	C12-C11	1.400	1.399	N17-C1-N2	122.99	122.99
	C8-C9	1.408	1.407	Cl16-C12-C11	119.99	119.98
S2	C3-C4	1.390	1.390	C1-N2-C3	116.91	116.91
	Cl7-C6	1.715	1.715	Cl16-C13-C14	118.72	119.73
	C1-N2	1.357	1.357	C10-C9-N8	121.98	121.18
	N8-C9	1.293	1.291	C4-C5-C6	118.81	118.18



S1

S2

Figure 2. Optimized geometry of Schiff base (S1-S2).

Theoretical investigation of Ultra-violet/visible (UV/Vis) spectrum:

The simulated absorption spectra are given in Figure 3. Both Schiff bases produced a distinct peak for the excitation of π electrons in the π-π* transition, allocated to the overall absorption band peaks at 295 and 265 nm. Corresponding to 50000, and 42000 cm^{-1} for **S1-S2** respectively It is important to note that the transition π-π* is due to the aromatic rings and C=N linking in both of the Schiff bases **(S1-S2)**

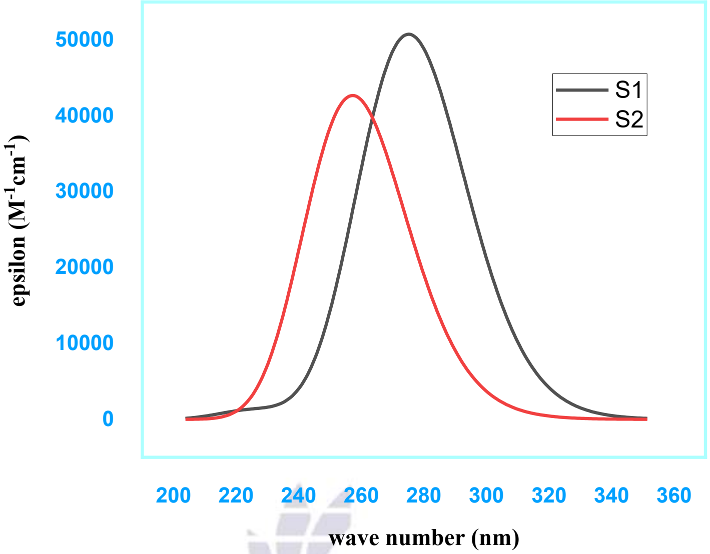


Figure 3. Simulated absorption spectra of Schiff bases (S1-S2).

Theoretical investigation of FT-IR spectrum:

The FT-IR spectra of the Schiff bases under theoretical investigation exposed a variety of fascinating binding characteristics of the functional group with regard to the formation of the Schiff base complexes.[21-23] The strong sharp band was associated with the stretching vibration of the azo methine (C=N) functional group at 1658.6 cm^{-1} **(S1)** and 1702 cm^{-1} **(S2).** The peaks seen in the Schiff base between 600 cm^{-1} **(S1)** is attributable to the presence of C-S, which demonstrated the existence of the thiazole group. Both Schiff bases **(S1-S2)** exhibit the stretching vibration band between 1300 and 1495 cm^{-1}, which is caused, respectively, by C-O and C=C. The broad absorption band developing at about 600 to 1400 cm^{-1} is likewise related to the aromatic ring vibration. The weak absorption band was present at 3258.2 cm^{-1} **(S1)** and 3047 cm^{-1} **(S2)** which showed the aromatic C-H vibrational frequency. DFT/B3LYP and 6-311G (d, p) calculated FT-IR spectra are shown in the **figure 4.**

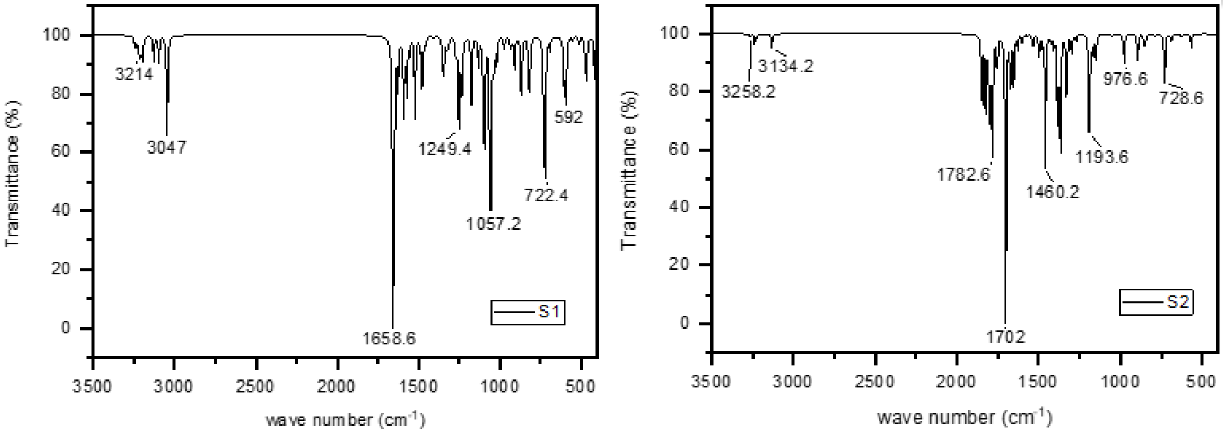


Figure 4. Simulated FT-IR spectra of Schiff bases (S1-S2).

Natural Bond Orbital (NBO) Analysis:

NBO [24-26] research of Schiff bases **(S1-S2)** sheds light on inter- and intramolecular interactions in filled and simulated orbitals. And detailed of charge transfer or conjugative interactions in molecular systems the second-order perturbation energies were used to evaluate the donor(i)-acceptor(j) interactions inside the NBO analysis, and the stabilization energy $E^{(2)}$ associated with the delocalization of each donor and acceptor of Schiff bases **(S1-S2)** was determined following available protocol. B3LYP functional with 6-31+G (d, p) basis was used for NBO calculation.by using Gaussian 09 software. And by using following equation as given below

$$E^{(2)} = qi\,\frac{(Fi.j)2}{\mathrm{Ei-Ej}}$$

The probable transition consisting of enormous stabilization energies such as π (C8-C9) π*(C6-C7) and π(C1-N2) π*(N17-C18) contain 22.41 kcal/mol each for **S1**. π (N8-C9) π*(C10-C11) and π(C10-C11) π*(N21-C32) has an energy value of 1.21 kcal/mol each for **S2**. The calculation of energy links to π-π* interactions is important to know about the existence of conjugation as well as charge transfer phenomenon in Schiff bases electronic transitions containing of 1.21 kcal/mol are related with least energy in **S2**. The collaboration between the electron donor-acceptor moieties leads to minimum energies. The σ (C14-C15) σ*(C14-H26), σ (N2-C3) σ*(C1-N2) transitions contained 1.31 kcal/mol each in **S1**. The σ (C1-N2) σ*(C1-C6), σ (C12-C13) σ*(C11-C12) transitions contained 21.94 kcal/mol each in **S2**. Higher stabilization energies among all σ-σ* interactions were 21.49 kcal/mol. transition associated with 1.3, 4.4, 4.50, 6.25.and 2.751 kcal/mol energy were with least stabilization energy values. Interactions correspond to resonance were also observed in Schiff bases **S1-S2**, for example, LP1(S5) π*(C3-C4), LP1(C17) π*(C5-C6), LP1(S13) π*(C13-C14), LP1(O11) π*(C3-C4), LP1(O11) π*(C5-C10) and LP1(O11) π*(C3-C4) produced 20.22, 147.31, 20.04, 35.89, 40.72 and 37.23 kcal/mol in **S1-S2** and were the highest values. Given in **Table 2**

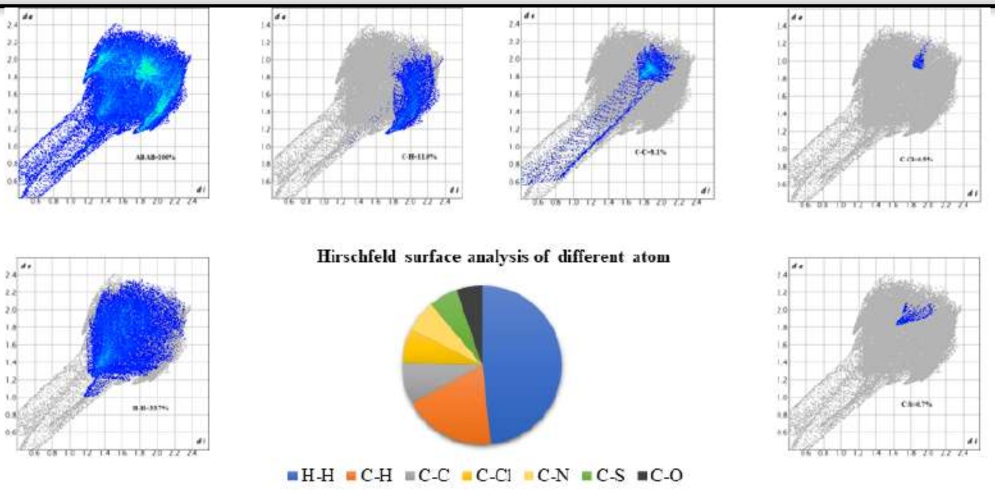
Table.2. The second-order perturbation energies representative values of NBOs investigated for Schiff bases (S1-S6). ^{a}E $^{(2)}$ represents "energy of hyper conjugative interaction (stabilization energy in kcal/mol)" ^{b}Energy difference between i and j NBOs. ^{c}F(i, j) is the Fock matrix element between i and j.

Comp	Donor(i)	Type	Acceptor(j)	Type	E (2)^{a} k j /mole	E(j)-E (i)^{b} (a. u)	F (i, j)^{c} (a. u)
S1	C8-C9	π	C6-C7	π*	22.41	0.27	0.071
	C1-N2	π	N17-C18	π*	13.3	0.32	0.058
	C6-C7	π	C19-H30	σ*	0.95	0.68	0.025
	C14-C15	σ	C15-H26	σ*	1.31	1.17	0.035
	N2-C3	σ	C1-N2	σ*	0.51	1.31	0.023
	S5	LP (2)	C3-C4	π*	20.22	0.26	0.068
	Cl16	LP (1)	C11-C12	σ*	0.83	1,49	0.032
S2	N8-C9	π	C10-C11	π*	1.22	1.09	0.033
	C10-C11	π	C12-C13	π*	0.76	1.14	0.026
	C1-N2	σ	C1-C6	σ*	21.94	0.25	0.067
	C12-C13	σ	C11-C12	σ*	7.03	0.32	0.044
	Cl7	LP (1)	C5-C6	σ*	147.31	0.02	0.082
	Cl16	LP (3)	C12-C13	π*	1.21	1.36	0.036

Hirschfeld Surface Analysis:

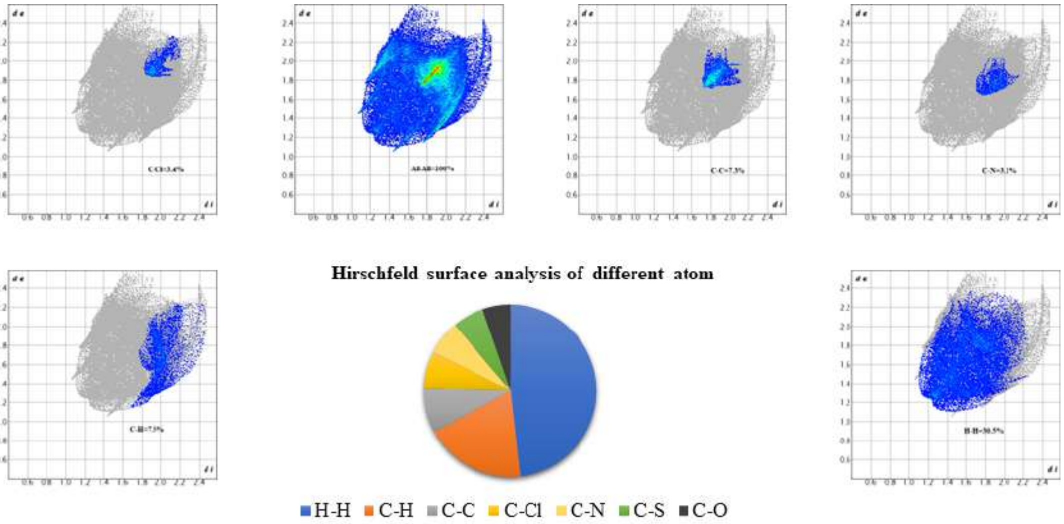
The complex's Hirschfeld surface [27; 28] was created using the Schiff bases **(S1-S2)** asymmetric unit given in Figure **6** and **7**. Two-dimensional fingerprint plots, which may be dissected to quantify the individual contributions of each intermolecular interaction involved in the structure, can also be used to investigate the intermolecular interactions.[29; 30] Respectively These graphs illustrate the % intermolecular contributions for various interatomic contacts to the Hirschfeld surface as well as the percentage contributions of an atom in the Hirschfeld surface with all other atoms present outside the surface to define its function in crystal packing.[31]

Theoretical analysis of the crystal packing of Schiff bases **(S1–S2)** was revealed that the H-H connections appear to be the largest contributor, quantified as 33.7 and 30.5 respectively. Because of their significant percentage contribution to intermolecular interactions, hydrogen atoms play a key role in the overall stabilization of the structure of these compounds. The oxygen atom of the C=O group was shown to have the least impact on intermolecular interactions, in the packing of the crystals. The overall two-dimensional fingerprint plots were generated based on the crystallographic information file (CIF) using the Crystal Explorer program are shown in following Figure **5** and **6.**



S1

Figure 5. Two-dimensional fingerprint plots for Schiff base (S1).



S2

Figure 6. Two-dimensional fingerprint plots for Schiff base (S2).

3.6. Frontier Molecular Orbitals (FMOs):

These Schiff bases have been declared stable because of the negative magnitude of E_{HOMO} and $E_{LUMO.}$ Schiff base's **(S1-S2)** HOMO LUMO energy gap measured are 3.61 and 4.27 eV given in **Figure 7**. The significant energy gap value suggested to the Schiff base **S2** (4.27 eV) was hard and less polarizable, as well as high chemical stability and low reactivity, and resistance towards deformation of the electron cloud of chemical

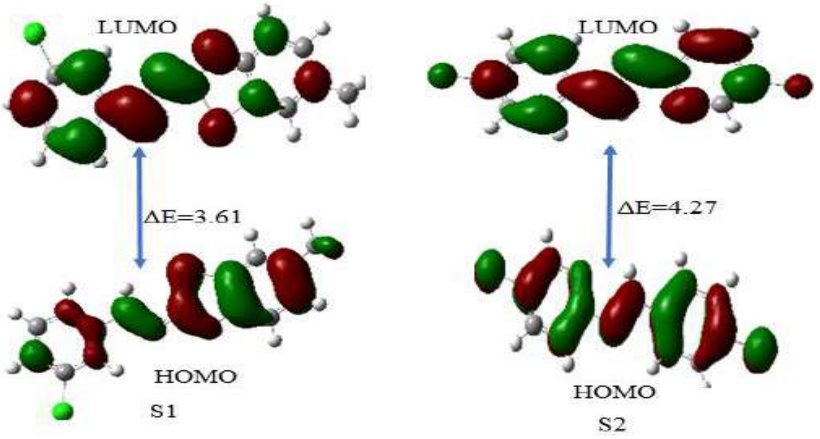


Figure 7. HOMO LUMO orbital of Schiff bases (S1-S2).

3.7. Global Reactivity Parameters (GRPs):

The DFT technique gives definitions for crucial, terms related to the stability and reactivity of molecular structures. Information for quantum chemical computations can be gleaned from the energies of the FMOs,[32] HOMO, and LUMO regarding to the global reactivity parameters[33-37] such as E A (electron affinity), E I (Ionization potential), η (global hardness), X (electronegativity), ω (global electrophilicity) µ (chemical potential), were calculated using the FMOs energies for selected Schiff bases These chemical parameters can be shown in **Table 3.**

Table 3. Global reactivity parameters (eV) of permitted Schiff bases (S1-S2).

Molecular properties.	S 1	S 2
E_{HOMO}(eV)	-6.25	-6.57
E_{LUMO}(eV)	-2.63	-2.29
$\Delta E=(E_{LUMO}\text{-}E_{HOMO})$(eV)	3.61	4.27
$X=-1/2((E_{HOMO}+E_{LUMO})$	4.44	4.43
Global Hardness (η) = $1/2(E_{LOMO}\text{-}E_{HOMO})$	1.80	2.13
Chemical Potential $\mu= -X=1/2((E_{HOMO}+E_{LUMO})$	-4.44	-4.43
$IE= -E_{HOMO}$ (eV)	6.25	6.57
$EA= -E_{LUMO}$ (eV)	2.63	2.29
Global Electrophilicity $\omega=\mu^2/2\eta$	5.476	4.605

Ionization potential and electron affinity values, respectively, are used in a general sense to distinguish between a molecule's ability to donate and take electrons. It was determined that the ionization potentials of **S1-S2** were significantly higher than their electron affinities.

The chemical potential (µ) is the propensity of electrons in stable systems to escape; a negative chemical potential denotes the stability of a complex that does not spontaneously disintegrated into its constituent elements. The resistance to change in a molecule's electron distribution is measured by hardness. The term "hardness" denotes resistance to the distortion of the chemical system's electron cloud when subjected to minor disturbances. A molecule with a big HOMO LUMO gap is considered to be hard, whereas one with a small HOMO LUMO gap is considered to be soft and more reactive. Hard systems are comparatively small and significantly less polarizable than soft systems, which are big and highly polarizable. Therefore, the local hardness provides data on the intermolecular reactivity.[38; 39] In order to provide information on both electron transfer (chemical potential) and stability (hardness), electrophilicity is correlated with an electrophile's capacity to accumulate extra electronic charge and its resistance to exchanging electronic charge with the environment.

Conclusion

Since the chemistry and applications of Schiff bases have been thoroughly studied in the past, this study presents a computational method to assess the reactivity and stability characteristics of a few Schiff bases that were investigated using DFT in conjunction with B3LYP functional to reveal their chemical reactivity descriptors. Calculated bond angles and lengths obtained were well correlated with SC-XRD data. With respect to each other, and B3LYP functionals were in good agreement. The results of the NBOs research show that molecules participated in intramolecular charge transfer. The compounds' increased molecular stability is supported by the Hirschfeld surface study. A larger magnitude of NBOs-based hyper conjugative interaction values was also revealed, supporting the same molecular stability fact. According to the computed HOMO LUMO energy gap for Schiff base, which was 4.75 eV, the **S2** was less reactive than the **S1**. Schiff bases **S1** have a somewhat lower band gap than **S2** due to the certain functional groups and capacity to donate electrons. The energies of FMOs were used to compute the global reactivity parameters. The examined compounds were shown to have minimal reactivity and good agreement with NBOs and SC-XRD findings since the chemical hardness values of **S2** were found to be higher than their softness values. Combined spectroscopic methods (UV-Vis, FTIR,) were used to identify the structures of the all-Schiff bases.

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Conflict of Interest
The authors declare no conflict of interest

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