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Synthesis, spectroscopic characterizations and quantum chemical computational studies of 6-fluoro-N-(4-substitutedbenzylidene)-1H-indazol-3-amine

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ABSTRACT

In the present investigation five number of Schiff base derivatives was synthesized and characterized by FT-IR, and spectra. To identify the stable structure of the molecule meticulous conformational analysis was performed. The optimized geometrical parameters obtained by DFT calculations using B3LYP/6-31G(d,p) level method. The calculated HOMO and LUMO energies show that the charge transfers occur with in the molecule. Mulliken charges were also calculated using B3LYP/6-31G(d,p) level method. Besides, molecular electrostatic potential (MEP) were performed by the DFT method.

INTRODUCTION

Schiff bases which contain an imine(-N=CH-) group attracts much interest in synthetic chemistry. Some donor atoms such as N, O,S in Schiff bases have structural similarities with natural biological systems and imports in elucidating the mechanism of transformations and racemisation reactions due to presence of imine (-N=CH-) group [1].Schiff base compounds possess potent antitubercular[2,3], anticancer [4,5], anti-inflammatory [6,7], antioxidant [8,9], antimalarial [10], antiviral [11,12]and anticonvulsant [13] activity. Also, it was reported that some of these compounds possess potent antibacterial, antifungal, herbicidal and clinical activities [14, 15].Furthermore, Indazolone and its derivatives have been widely studied due to their broad range of biological activities, such ascell apoptosis[16], rheumatoid arthritis[17], antiproliferative effect[18], Occular hypertension and glaucoma[19], psychotic activity[20], hypotensive activity[21], obesity[22], tumorcell cytotoxic assay[23],anti-hyperlipidemic activity[24], Trichomonacidal activity[25], Analgesic and antipyretic activity[26],antiprotozoal activity[27], antidiabetic activity[28],anti-inflammatory activity[29], antiarthritic effect[30],local anaesthetic activity[31],platelet anti aggregating effect[32], anti spermatogenic activity[33],antihypertensive[34]activities.

In the present work, we prepared five Schiff base derivatives of Indazole moiety. In order to achieve this objective, FT-IR and NMR spectroscopic studies along with DFT HOMO (highest occupied molecular orbital)LUMO (lowest unoccupied molecular orbital) analysis have been performed by applying density functional theory calculations based on Becke3–Lee–Yang–Parr (B3LYP) with 6-31G(d,p) as basis set.

MATERIALS AND METHODS

All the chemicals and solvents used were of AR grade obtained from Sigma Aldrich, Lobachemie (India).The melting points were taken in an open capillary tube and are uncorrected. Infrared spectra (KBr, 4000-400 cm^{-1}) have been recorded on SHIMADZU Fourier transform spectrophotometer. The NMR spectra were recorded in Bruker AMX 500 NMR spectrometer operating at 400 MHz has been utilized for recording ^1H NMR spectra in $CDCl_3$

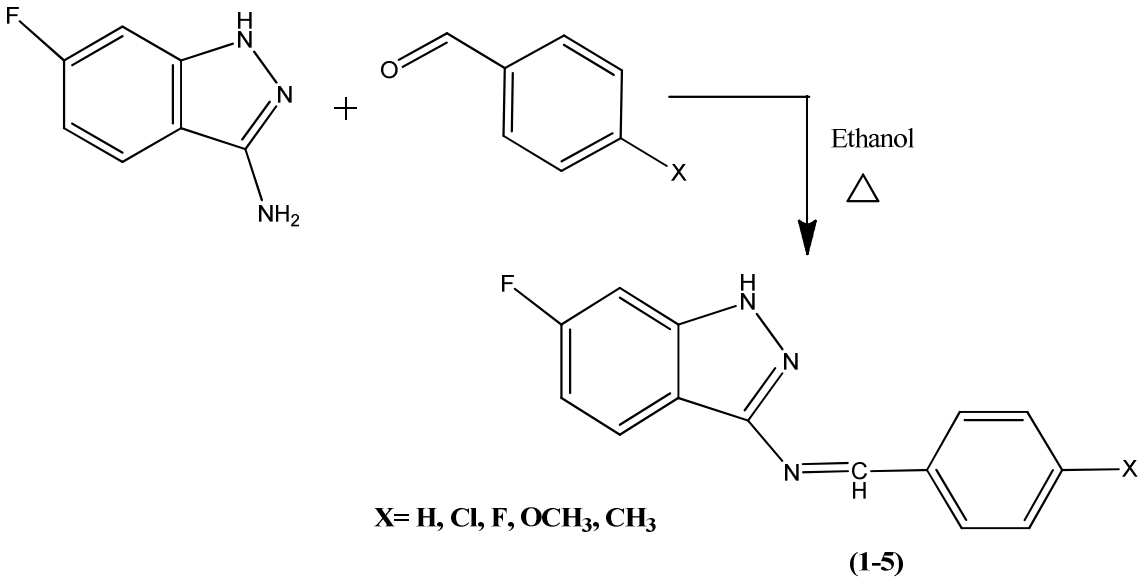
solvent using TMS as internal standard. The purity of the compounds was checked by TLCon pre-coated Silicagel (HF254, 200 mesh) aluminium platesas adsorbent and Iodine chamber as visualizing agent.

Computational Details

Full geometry optimization of Schiff bases was performed by using the density functional B3LYP method [35–37] with the standard 6-31 G(d,p) basis set. Computations were carried out with the Gaussian 03 package [38]. The harmonic vibrational frequencies were calculated at the same level of theory for the optimized structures. Vibrational band assignments were made using the Gauss-View molecular visualization program [39].The electronic properties such as HOMO and LUMO energies were determined by TD-DFT approach. To investigate the reactive sites of the title compound the MEP wereevaluated using the B3LYP/6-31 G(d,p) method.

RESULTS AND DISCUSSION

To a mixture of 6-fluoro-1H-indazol-3-amine (0.1 mol.) and substituted aromatic benzaldehyde, (0.1 mol.) in ethanol, 1ml of glacial acetic acid added then the resultant mixture was refluxed for (5-6 hours), progress of the reaction was monitored by TLC. After the completion of the reaction, the obtained product was poured into crushed ice stirred well; solid obtained was recrystallized from suitable solvent. Their physical constant data are given in Table-1 and synthetic scheme -1.



Schem:1. Synthesis of Schiff base derivatives

4.1 Synthesis of N-benzylidene-6-fluoro-1H-indazol-3-amine

Mol. Formula: $C_{14}H_{10}N_3F$; Mol. Wt: 239.09; m.pt: 153-154^{0}C; IR (KBr) (cm^{-1}): 3059 (AromaticC-H stretching), 1587 (HC=N), 1246 (C-F stretching);^{1}H NMR(400 MHz, $CDCl_3$, δ,(ppm): 6.61-8.08 (m, Ar-H), 8.10 (s, 1H,CH=N), 9.84 (s, 1H,N-H).

4.2 Synthesis of N-(4-chlorobenzylidene)-6-fluoro-1H-indazol-3-amine

Mol. Formula: $C_{14}H_9N_3ClF$; Mol. Wt: 273.05; m.pt: 127-128^{0}C;IR (KBr) (cm^{-1}): 3053((Aromatic C-Hstretching),1585 (HC=N), 1253 (C-F stretching), 3358 (N-H stretching; ^{1}H NMR(400 MHz, $CDCl_3$, δ,(ppm): 6.61-8.08 (m, Ar-H), 8.12 (s, 1H,CH=N), 9.48 (s, 1H,N-H).

4.3 Synthesis of 6-fluoro-N-(4-fluorobenzylidene)-1H-indazol-3-amine

Mol. Furmula: $C_{14}H_9N_3F_2$; Mol. Wt: 257.08; m.pt: 177-178^{0}C; IR (KBr) (cm^{-1}): 3057((Aromatic C-Hstretching),1598(HC=N), 3358(N-H stretching), 1257 (C-F stretching):^{1}H NMR(400 MHz, $CDCl_3$, δ,(ppm): 6.58-7.68 (m, Ar-H), 8.07 (s, 1H,CH=N), 9.95 (s, 1H,N-H).

4.4 Synthesis of 6-fluoro-N-(4-methoxybenzylidene)-1H-indazol-3-amine

Mol. Formula : $C_{15}H_{12}N_3OF$; Mol.wt : 269.10; m.pt: 101-102^{0}C; IR (KBr) (cm^{-1}): 3059((Aromatic C-Hstretching), 2947(Aliphatic-C-H stretching), 3367(N-H stretching), 1595(HC=N), 1249(C-F stretching):^{1}H NMR(400 MHz, $CDCl_3$, δ,(ppm): 6.60-8.27 (m, Ar-H), 8.37 (s, 1H,CH=N), 10.59 (s, 1H,N-H).

4.5 Synthesis of 6-fluoro-N-(4-methylbenzylidene)-1H-indazol-3-amine

Mol. Formula : $C_{15}H_{12}N_3F$; Mol.wt : 253.10; m.pt: 135-136^{0}C; IR (KBr) (cm^{-1}): 3062((Aromatic C-Hstretching), 2941(Ali-C-H stretching), 1595(HC=N), 3365(N-H stretching), 1246(C-F stretching):^{1}H NMR(400 MHz, $CDCl_3$, δ,(ppm): 6.60-8.27 (m, Ar-H), 8.37 (s, 1H,CH=N), 9.97 (s, 1H,N-H).

1. MOLECULAR GEOMETRY

The optimized structure parameters of substituted N-benzylidene-6-fluoro-1H-indazol-3-aminecalculated by DFT-B3LYP levels with 6-31 G (d, p) basis set are listed in the Table 2. Sincethe crystal structure of the exact title Schiff base is not available till now, the optimizedstructure can only be compared with similar Schiff base of N-[(E)-Quinoxalin-2-ylmethylidene]-1Hindazol-5-aminefor which crystal structure has been solved along with complete optimized bond lengths and bond angles[40].

The carbon–carbon bonds in benzene are not of equal length which is justified by thepresenceof fused indazol ring. However, the differences between the six C–C distances are small.The compound 1 shows N(9)-N(10) bond length is 1.3577Å, with the two C(7)-N(8) and C(7)-N(9) lengths being equal to 1.3781 Å and 1.3341Å (16), as well as the N(8)-C(12) bond being 1.2851Åand the C-N bond length is 1.2851 Å.Compound 2shows thechloro substituted phenyl ringC(18)- Cl(19) bond length is 1.7564 Å and two C(7)-N(8) and C(7)-N(9) bond lengths being equal to 1.377Å and 1.3353 Å. The observed N (8)-C (12) bond distance 1.2854 Å and N (9)-N (10) bond length is 1.3554 Å. The chloro substituent C(4)-F(11) observed 1.3524 Å.

Compound 3 shows the fluoro substituted phenyl ringC(18)-F(19) observed 1.347 Å. The two C (7)- N (8) and C(7)-N(9) bond lengths are equal to 1.3773 Å and 1.335 Å and N(8)-C(12)bond length is 1.2858 Å . The bond distance ofN(9)-N(10), N(10)-H(23) and C(4)-F(11) of compound 3 is 1.3566 Å, 1.007 Å and 1.3528 Å respectively.Compound 4 have shown C(7)-N(8) and C(7)-N(9) bond lengths being equal to 1.377 Å and1.377 Å and N(8)-C(12) and N(9)-N(10) bond length is 1.2876 Å and 1.3588 Å. Compound 4withN(9)-N(10), N(10)-H(24) and C(4)-F(11) bond length is 1.3588 Å, 1.0068 Å and 1.3535 Å respectively. Compound 5 shows the two C(7)-N(8) and C(7)-N(9)bond lengths are equal to1.3781Å and 1.334Å and N(8)-C(12) bond length is1.2859Å. The bond distance of N (9)-N(10), N(10)-H(23) and C(4)-F(11) of compound 5 is 1.3584Å, 1.0069Å and 1.3532Å respectively.

2. HOMO–LUMO Analysis

Highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO) are very important parameters for quantum chemistry. We can determine the way in which the molecule interacts with other species; hence, they are called the frontier orbital's[41] . HOMO, which can be thought the outermost orbital containing electrons, tends to give these electrons such as an electron donor. On the other hand; LUMO can be thought the innermost orbital containing free places to accept electrons.

The electronic absorption and HOMO and LUMO energies were calculated respectively using DFT methods with 6-31 G(d,p) basis set and are listed in the Figure 2 . The HOMO represents the ability to donate an electron, LUMO as an electron acceptor represents the ability to obtain an electron.

The low value of HOMO–LUMO gap 0.14397 eV (Fig. 2) in 4-Chloro substituent, benzaldehyde 0.14705 eV, 4-Methyl substituent 0.1471 eV, 4-Methoxy substituent 0. 14673 eV and 4-Fluro substituent 0.1471 eVwhile comparing to reflects the chemically reactive nature. The decrease in the HOMO and LUMO energy gap explains the eventual charge transfer interaction taking place within the molecule which is responsible for the activity of the molecule. Consequently, the lowering of the HOMO–LUMO band gap is essentially a consequence of the large stabilization of the LUMO due to the strong electron-acceptor ability of the electron-acceptor group. The compound 4-Chloro substituent have minimum energy compared all the four substituted Schiff base derivatives.

3. MULLIKEN CHARGE DISTRIBUTION

The calculations of effective atomic charges plays an important role in the application of quantum mechanical calculations to molecular systems, because of atomic charge changes effect of dipole moment, molecular polarizability, electronic structure, acidity– basicity behavior and more a lot of properties of molecular systems[42]The charge distribution of the molecule has calculated on the basis of Mulliken using B3LYP/6-31G(d,p) level calculation. This calculation depicts the charges of the every atom in the molecule. Distribution of positive and negative charges is the vital to increasing or decreasing of bond length between the atoms. The survey of literature reveals that effective atomic calculations gave an important role in the application of chemical calculation to molecular system because of atomic charges effect dipole moment, molecular polarizability, electronic structure, acidity–basicity behaviour and more lot of properties of molecular system[43]In the present study, compound 1 shows

the positive charge distribution in the carbon atoms C_1, C_2, C_4, C_6, C_7, C_{16}, C_{18},C_{19} and C_{25} and the negative charge distribution in the other atoms N_{11}, N_{12}, N_{13}, F_{15} and C_{20}.

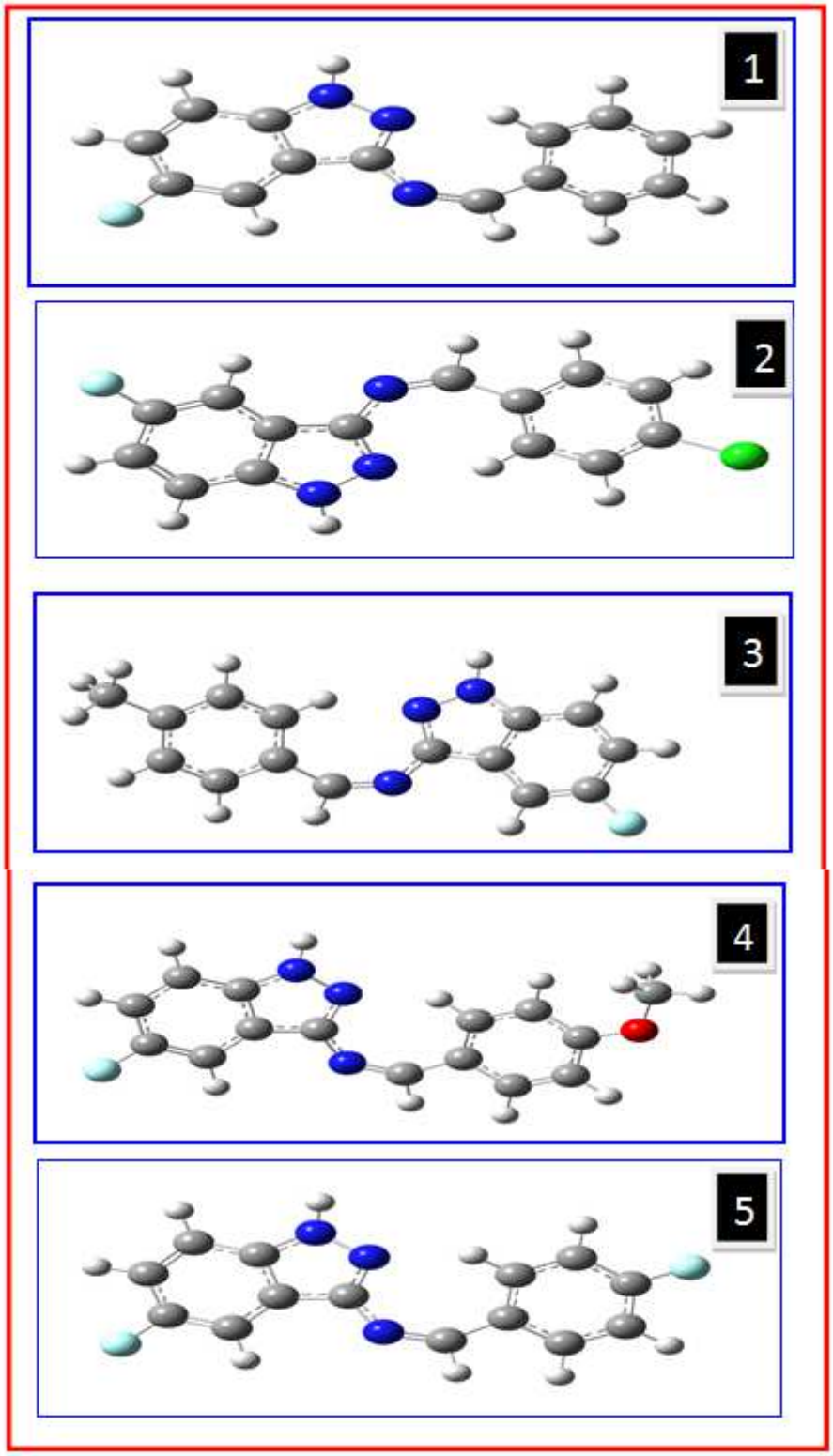


Figure1: Optimized molecular structures of schiff base derivatives (1-5)

The Compound 2 shows the positive charge distribution in the carbon atoms C_1, C_2, C_4, C_6, C_7, C_{16}, C_{18}, C_{19}, C_{21} and C_{23} and negative charge distribution in the other atoms N_{11}, N_{12}, N_{13}, F_{15}, C_{20} and C_{25}. The positive charge distribution in the carbon atoms C_1, C_2, C_4, C_6, C_7, C_{16}, C_{18}, C_{19} and C_{25} and negative charge distribution in the other atoms N_{11}, N_{12}, N_{13}, F_{15}, C_{20}, C_{21}, C_{23} and F_{28} shows Compound 3. The Compound 4 shows positive charge

distribution in the carbon atoms C_1, C_2, C_4, C_6, C_7, C_{16}, C_{18}, C_{19}, C_{25} and C_{29} and negative charge distribution in the other atoms C_3, C_5, N_{11}, N_{12}, N_{13}, F_{15}, C_{20}, C_{21}, C_{23} and O_{28}. The positive charge distribution in the carbon atoms C_1, C_2, C_4, C_6, C_7, C_{16}, C_{18}, C_{19} and C_{25} and negative charge distribution in the other atoms C_3, C_5, N_{11}, N_{12}, N_{13}, F_{15}, C_{20}, C_{21}, C_{23} and F_{28} shows in Compound 5.

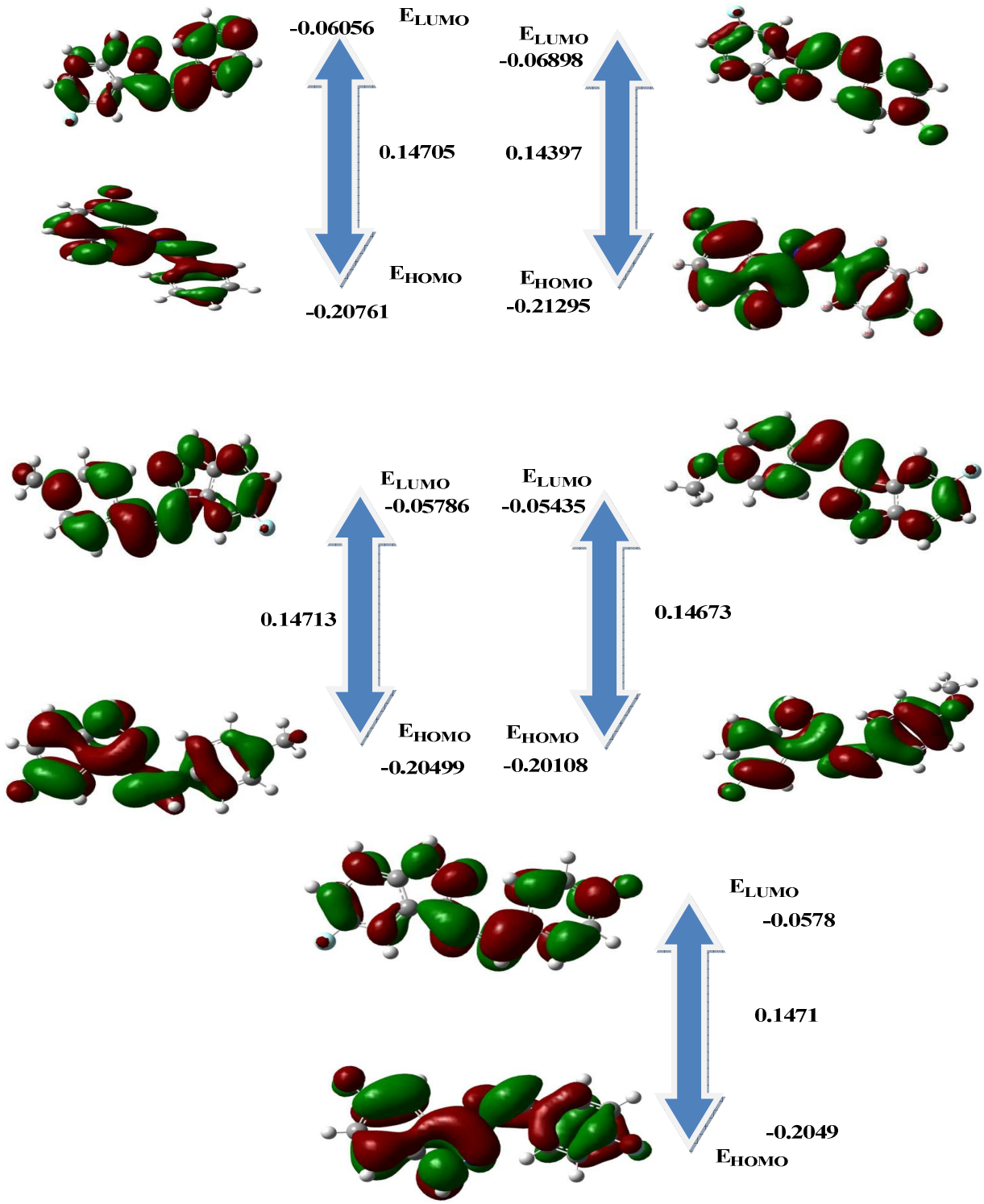
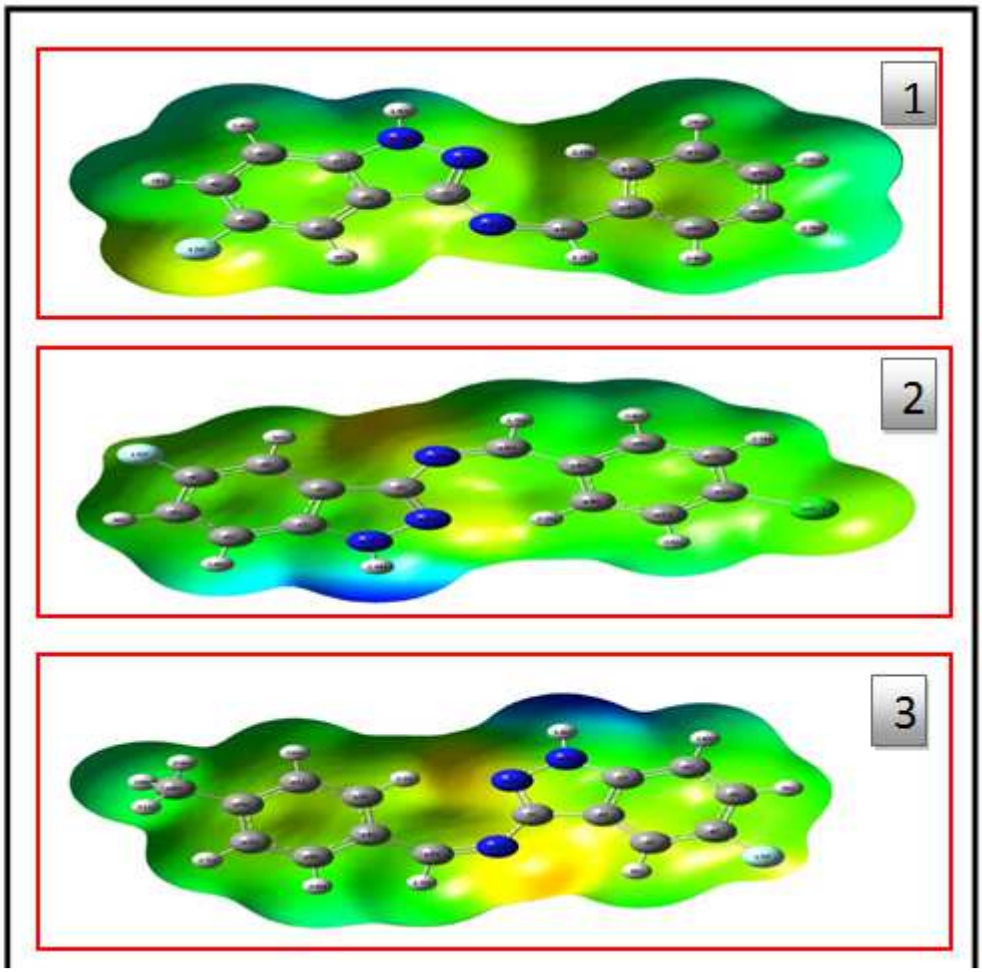


Figure 2: 3D HOMO and LUMO plots of the Schiff base derivatives (1-5)

From the results of Mulliken charge distribution the nitrogen, fluoro and oxygen atoms have more negative charge. The C_7, C_4 and C_1 atoms have more positive charge in all the Schiff base compounds. The atomic charge values are listed in Table 6. Mullikens atomic charge plot has shown in Fig. 4.

4. Molecular Electrostatic Potential

The electron density isosurfaces on which the electrostatic potential surface has been mapped are shown in Fig. 3 for two conformers of title compound. The different values of the electrostatic potential at the surface are represented by different colors ; red represents regions of most negative electrostatic potential, blue represents regions of most positive electrostatic potential and green represents regions of zero potential[44].The molecular electrostatic potential (MESP) is widely used as a reactivity map displaying most probable regions for the electrophilic attack of charged point-like reagents on organic molecules [33]. MESP contour map provides a simple way in predicting the interaction of different geometries. The electrostatic potential has been used primarily for predicting sites and relative reactivities towards electrophilic attack and in studies of biological recognition and hydrogen bonding interactions [34–40]. In order to predict the reactive sites for electrophilic and nucleophilic attacks of the title molecule, MESP was calculated at the B3LYP/6-311G(d,p) optimized geometry. The negative (red and yellow) regions of MESP were related to electrophilic reactivity and the positive (blue color) ones to nucleophilic reactivity shown in Fig. 3. As depicted in Fig. 3, this molecule has two possible sites for electrophilic attack. The negative regions are mainly over the F and the partial region between N and N atoms.



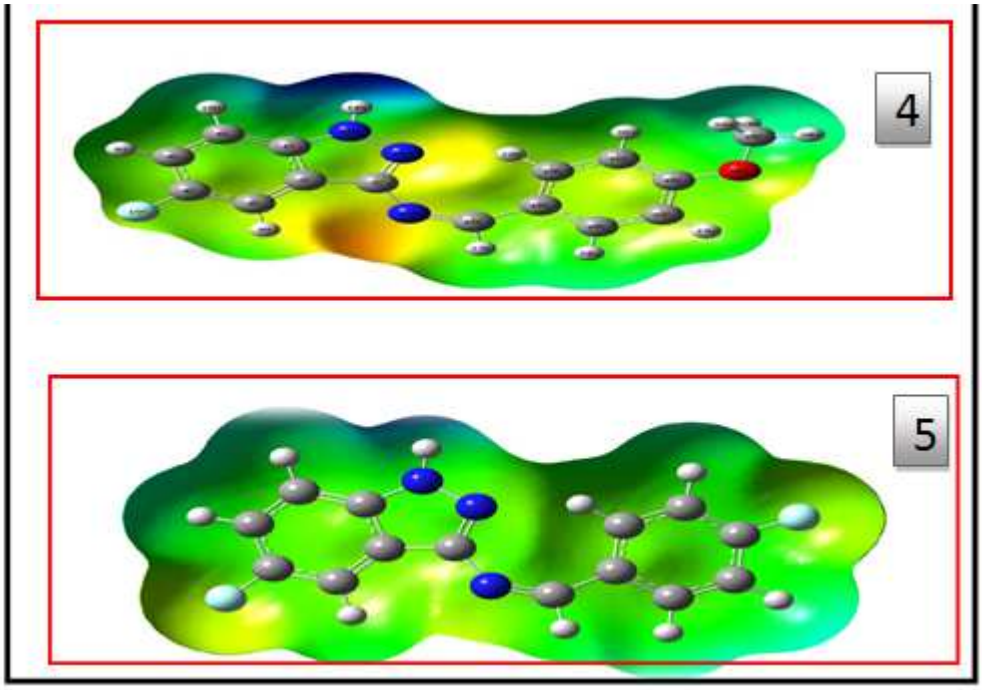
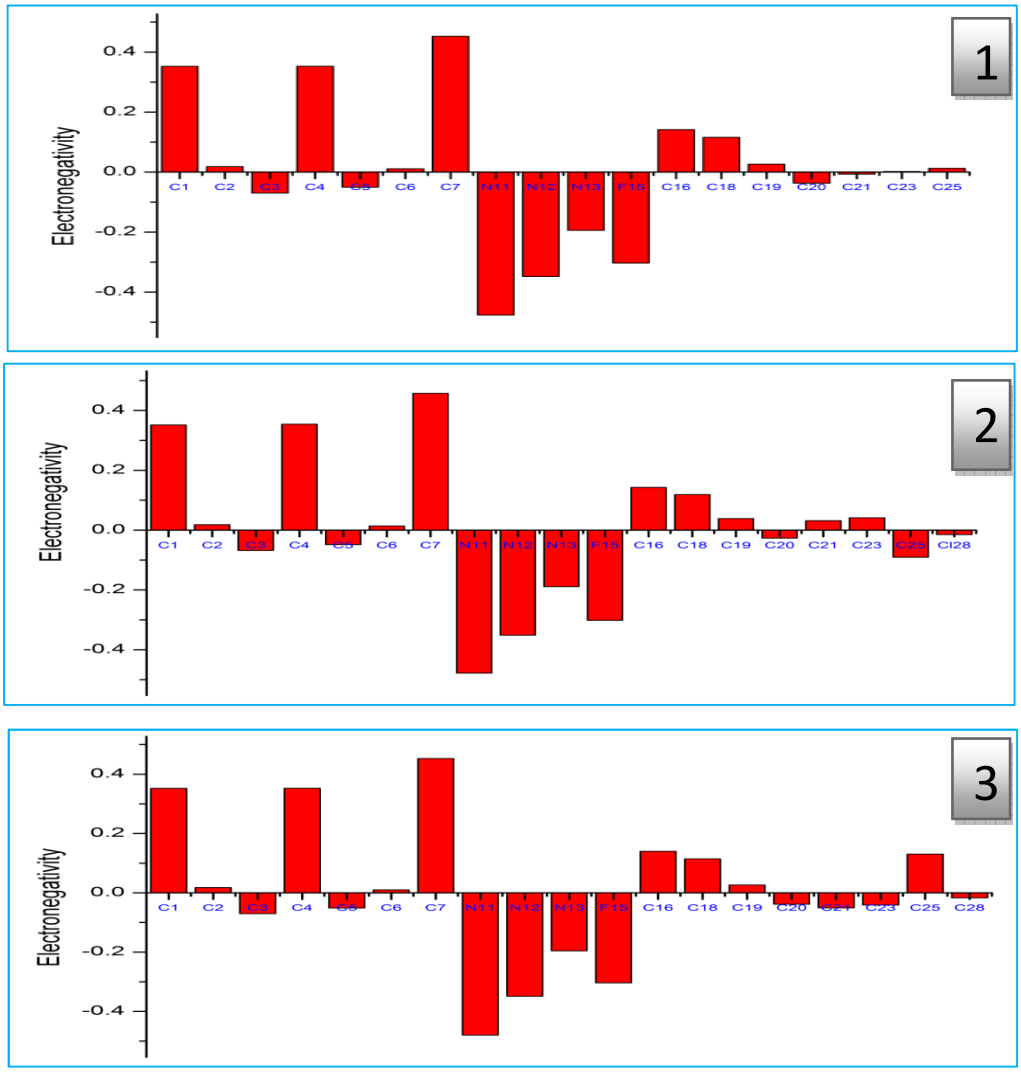


Figure - 3: Molecular electrostatic potentials of Schiff base derivatives(1-5)



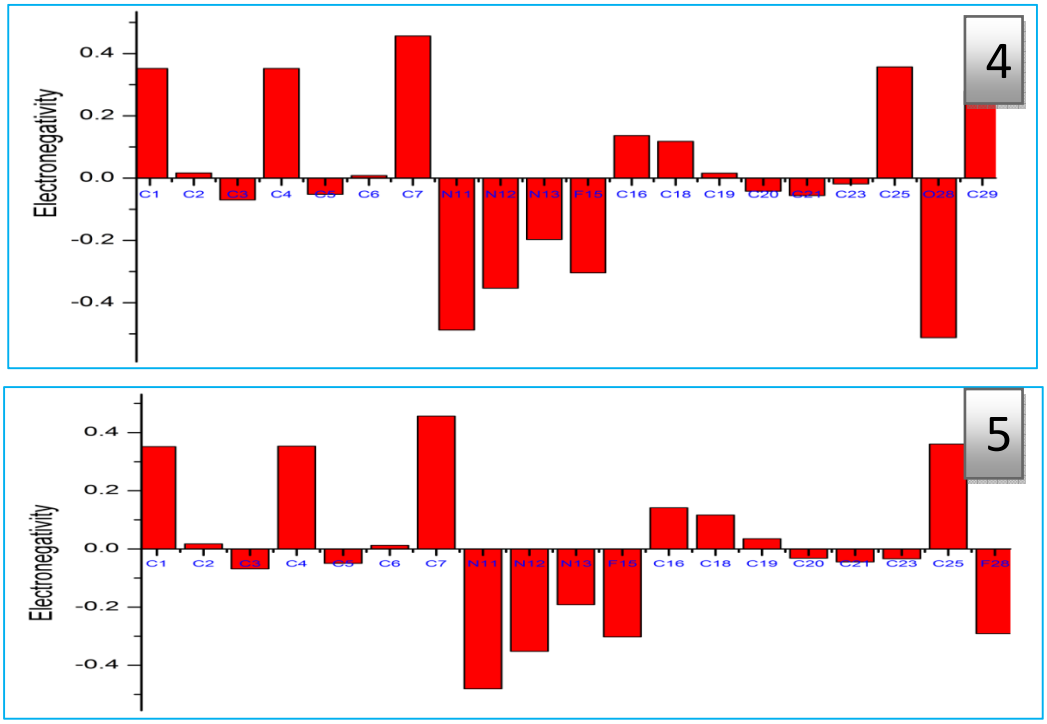


Figure 4: Mulliken plots of the Schiff base derivatives (1-5)

Table 1.Physical constants of substituted (*E*)-N-benzylidene-3,5-dichloropyridin-4-amines

compound	Substituents	Molecular Formula	Molecular Weight	Melting Point
1	H	$C_{14}H_{10}N_3F$	239.09	
2	Cl	$C_{14}H_9N_3ClF$	273.05	
3	F	$C_{14}H_9N_3F_2$	257.08	
4	OCH_3	$C_{15}H_{12}N_3OF$	269.10	
5	CH_3	$C_{15}H_{12}N_3F$	253.10	

Table 2: Optimized geometrical parameters (bond length, bond, angle, dihedral angle) of Schiff base derivatives (1-5) obtained by B3LYP method

BOND LENGTH									
COMPOUND 1		**COMPOUND 2**		**COMPOUND 3**		**COMPOUND 4**		**COMPOUND 5**	
C(18)-H(28)	1.0862	C(18)-Cl(19)	1.7564	C(18)-F(19)	1.347	C(20)-H(32)	1.0969	C(19)-H(31)	1.094
C(17)-H(27)	1.086	C(17)-H(28)	1.0841	C(17)-H(28)	1.0843	C(20)-H(31)	1.097	C(19)-H(30)	1.0974
C(17)-C(18)	1.3966	C(17)-C(18)	1.3951	C(17)-C(18)	1.3912	C(20)-H(30)	1.0906	C(19)-H(29)	1.094
C(16)-H(26)	1.0863	C(16)-H(27)	1.0844	C(16)-H(27)	1.0847	O(19)-C(20)	1.4211	C(18)-C(19)	1.5089
C(16)-C(18)	1.396	C(16)-C(18)	1.3943	C(16)-C(18)	1.3904	C(18)-O(19)	1.36	C(17)-H(28)	1.087
C(15)-H(25)	1.0871	C(15)-H(26)	1.0868	C(15)-H(26)	1.0867	C(17)-H(29)	1.0848	C(17)-C(18)	1.4019
C(15)-C(17)	1.3905	C(15)-C(17)	1.3893	C(15)-C(17)	1.3891	C(17)-C(18)	1.4045	C(16)-H(27)	1.0875
C(14)-H(24)	1.0818	C(14)-H(25)	1.0821	C(14)-H(25)	1.0819	C(16)-H(28)	1.0836	C(16)-C(18)	1.4015
C(14)-C(16)	1.3937	C(14)-C(16)	1.3926	C(14)-C(16)	1.392	C(16)-C(18)	1.4012	C(15)-H(26)	1.0872
C(13)-C(15)	1.4107	C(13)-C(15)	1.4104	C(13)-C(15)	1.4114	C(15)-H(27)	1.0871	C(15)-C(17)	1.389
C(13)-C(14)	1.4083	C(13)-C(14)	1.408	C(13)-C(14)	1.4097	C(15)-C(17)	1.3826	C(14)-H(25)	1.082
C(12)-C(13)	1.4769	C(12)-C(13)	1.4762	C(12)-C(13)	1.4751	C(14)-H(26)	1.0821	C(14)-C(16)	1.392
C(12)-H(23)	1.096	C(12)-H(24)	1.0959	C(12)-H(24)	1.096	C(14)-C(16)	1.3934	C(13)-C(15)	1.4101
N(10)-H(22)	1.007	N(10)-H(23)	1.0071	N(10)-H(23)	1.007	C(13)-C(15)	1.4146	C(13)-C(14)	1.4081
N(9)-N(10)	1.3577	N(9)-N(10)	1.3554	N(9)-N(10)	1.3566	C(13)-C(14)	1.4067	C(12)-C(13)	1.4746
N(8)-C(12)	1.2851	N(8)-C(12)	1.2854	N(8)-C(12)	1.2858	C(12)-C(13)	1.4705	C(12)-H(24)	1.0962
C(7)-N(9)	1.3341	C(7)-N(9)	1.3353	C(7)-N(9)	1.335	C(12)-H(25)	1.0962	N(10)-H(23)	1.0069
C(7)-N(8)	1.3781	C(7)-N(8)	1.377	C(7)-N(8)	1.3773	N(10)-H(24)	1.0068	N(9)-N(10)	1.3584
C(6)-H(21)	1.0852	C(6)-H(22)	1.085	C(6)-H(22)	1.0851	N(9)-N(10)	1.3588	N(8)-C(12)	1.2859
C(5)-H(20)	1.0845	C(5)-H(21)	1.0844	C(5)-H(21)	1.0845	N(8)-C(12)	1.2876	C(7)-N(9)	1.334
C(5)-C(6)	1.3859	C(5)-C(6)	1.3858	C(5)-C(6)	1.3858	C(7)-N(9)	1.3347	C(7)-N(8)	1.3781
C(4)-F(11)	1.353	C(4)-F(11)	1.3524	C(4)-F(11)	1.3528	C(7)-N(8)	1.377	C(6)-H(22)	1.0852
C(4)-C(5)	1.4093	C(4)-C(5)	1.4096	C(4)-C(5)	1.4095	C(6)-H(23)	1.0852	C(5)-H(21)	1.0845
C(3)-H(19)	1.0834	C(3)-H(20)	1.0834	C(3)-H(20)	1.0834	C(5)-H(22)	1.0845	C(5)-C(6)	1.386
C(3)-C(4)	1.3795	C(3)-C(4)	1.3795	C(3)-C(4)	1.3794	C(5)-C(6)	1.3861	C(4)-F(11)	1.3532
C(2)-C(7)	1.4414	C(2)-C(7)	1.4414	C(2)-C(7)	1.4414	C(4)-F(11)	1.3535	C(4)-C(5)	1.4091
C(2)-C(3)	1.4034	C(2)-C(3)	1.4033	C(2)-C(3)	1.4034	C(4)-C(5)	1.4091	C(3)-H(20)	1.0835
C(1)-N(10)	1.3711	C(1)-N(10)	1.3716	C(1)-N(10)	1.3713	C(3)-H(21)	1.0834	C(3)-C(4)	1.3796
C(1)-C(6)	1.4038	C(1)-C(6)	1.4038	C(1)-C(6)	1.4039	C(3)-C(4)	1.3797	C(2)-C(3)	1.4034
C(1)-C(2)	1.4116	C(1)-C(2)	1.4112	C(1)-C(2)	1.4113	C(1)-N(10)	1.371	C(1)-N(10)	1.3711

BOND ANGLE									
COMPOUND 1		**COMPOUND 2**		**COMPOUND 3**		**COMPOUND 4**		**COMPOUND 5**	
H(28)-C(18)-C(17)	120.1318	Cl(19)-C(18)-C(17)	119.4063	F(19)-C(18)-C(17)	118.9424	H(32)-C(20)-H(31)	109.1637	H(31)-C(19)-H(30)	107.2182
H(28)-C(18)-C(16)	120.2011	Cl(19)-C(18)-C(16)	119.5664	F(19)-C(18)-C(16)	119.0914	H(32)-C(20)-H(30)	109.2757	H(31)-C(19)-H(29)	108.1907
C(17)-C(18)-C(16)	119.6637	C(17)-C(18)-C(16)	121.0248	C(17)-C(18)-C(16)	121.9632	H(32)-C(20)-O(19)	111.5619	H(31)-C(19)-C(18)	111.4787
H(27)-C(17)-C(18)	120.3009	H(28)-C(17)-C(18)	120.291	H(28)-C(17)-C(18)	119.8335	H(31)-C(20)-H(30)	109.2331	H(30)-C(19)-H(29)	107.2399
H(27)-C(17)-C(15)	119.9704	H(28)-C(17)-C(15)	121.0123	H(28)-C(17)-C(15)	121.9639	H(31)-C(20)-O(19)	111.5966	H(30)-C(19)-C(18)	111.03
C(18)-C(17)-C(15)	119.7282	C(18)-C(17)-C(15)	118.6964	C(18)-C(17)-C(15)	118.2023	H(30)-C(20)-O(19)	105.9271	H(29)-C(19)-C(18)	111.4766
H(26)-C(16)-C(18)	119.8324	H(27)-C(16)-C(18)	119.8612	H(27)-C(16)-C(18)	119.3656	C(20)-O(19)-C(18)	118.5176	C(19)-C(18)-C(17)	121.0179
H(26)-C(16)-C(14)	119.3429	H(27)-C(16)-C(14)	120.3753	H(27)-C(16)-C(14)	121.3438	O(19)-C(18)-C(17)	115.6751	C(19)-C(18)-C(16)	121.0947
C(18)-C(16)-C(14)	120.8215	C(18)-C(16)-C(14)	119.761	C(18)-C(16)-C(14)	119.287	O(19)-C(18)-C(16)	124.8051	C(17)-C(18)-C(16)	117.8647
H(25)-C(15)-C(17)	119.61	H(26)-C(15)-C(17)	118.9494	H(26)-C(15)-C(17)	119.0608	C(17)-C(18)-C(16)	119.517	H(28)-C(17)-C(18)	119.6059
H(25)-C(15)-C(13)	119.0447	H(26)-C(15)-C(13)	119.2056	H(26)-C(15)-C(13)	119.1266	H(29)-C(17)-C(18)	118.6805	H(28)-C(17)-C(15)	119.6518
C(17)-C(15)-C(13)	121.3417	C(17)-C(15)-C(13)	121.8418	C(17)-C(15)-C(13)	121.8095	H(29)-C(17)-C(15)	121.6089	C(18)-C(17)-C(15)	120.7422
H(24)-C(14)-C(16)	120.4978	H(25)-C(14)-C(16)	119.8931	H(25)-C(14)-C(16)	120.0685	C(18)-C(17)-C(15)	119.7105	H(27)-C(16)-C(18)	119.145
H(24)-C(14)-C(13)	119.3176	H(25)-C(14)-C(13)	119.4043	H(25)-C(14)-C(13)	119.2782	H(28)-C(16)-C(18)	120.7492	H(27)-C(16)-C(14)	119.016
C(16)-C(14)-C(13)	120.1708	C(16)-C(14)-C(13)	120.6937	C(16)-C(14)-C(13)	120.6434	H(28)-C(16)-C(14)	119.0115	C(18)-C(16)-C(14)	121.8366
C(15)-C(13)-C(14)	118.2585	C(15)-C(13)-C(14)	117.9691	C(15)-C(13)-C(14)	118.0807	C(18)-C(16)-C(14)	120.2347	H(26)-C(15)-C(17)	119.3918
C(15)-C(13)-C(12)	115.1161	C(15)-C(13)-C(12)	115.2334	C(15)-C(13)-C(12)	115.1962	H(27)-C(15)-C(17)	119.0365	H(26)-C(15)-C(13)	119.1025
C(14)-C(13)-C(12)	126.6245	C(14)-C(13)-C(12)	126.7972	C(14)-C(13)-C(12)	126.7228	H(27)-C(15)-C(13)	119.0241	C(17)-C(15)-C(13)	121.4989
C(13)-C(12)-H(23)	111.2424	C(13)-C(12)-H(24)	111.1188	C(13)-C(12)-H(24)	111.1075	C(17)-C(15)-C(13)	121.9357	H(25)-C(14)-C(16)	120.3123
C(13)-C(12)-N(8)	135.9579	C(13)-C(12)-N(8)	136.1264	C(13)-C(12)-N(8)	136.2009	H(26)-C(14)-C(16)	119.5987	H(25)-C(14)-C(13)	119.3489
H(23)-C(12)-N(8)	112.6924	H(24)-C(12)-N(8)	112.675	H(24)-C(12)-N(8)	112.6106	H(26)-C(14)-C(13)	119.2222	C(16)-C(14)-C(13)	120.3283
H(22)-N(10)-N(9)	118.6629	H(23)-N(10)-N(9)	118.7147	H(23)-N(10)-N(9)	118.7206	C(16)-C(14)-C(13)	121.1657	C(15)-C(13)-C(14)	117.7165
H(22)-N(10)-C(1)	128.1846	H(23)-N(10)-C(1)	128.1881	H(23)-N(10)-C(1)	128.1927	C(15)-C(13)-C(14)	117.4213	C(15)-C(13)-C(12)	115.3337
N(9)-N(10)-C(1)	112.8018	N(9)-N(10)-C(1)	112.8455	N(9)-N(10)-C(1)	112.8157	C(15)-C(13)-C(12)	115.4787	C(14)-C(13)-C(12)	126.947
N(10)-N(9)-C(7)	106.3509	N(10)-N(9)-C(7)	106.3924	N(10)-N(9)-C(7)	106.3971	C(14)-C(13)-C(12)	127.0985	C(13)-C(12)-H(24)	111.2068
C(12)-N(8)-C(7)	131.6135	C(12)-N(8)-C(7)	132.1652	C(12)-N(8)-C(7)	131.9822	C(13)-C(12)-H(25)	111.0764	C(13)-C(12)-N(8)	136.0575
N(9)-C(7)-N(8)	128.1276	N(9)-C(7)-N(8)	128.4876	N(9)-C(7)-N(8)	128.4872	C(13)-C(12)-N(8)	136.4307	H(24)-C(12)-N(8)	112.6352
N(9)-C(7)-C(2)	110.237	N(9)-C(7)-C(2)	110.1505	N(9)-C(7)-C(2)	110.1478	H(25)-C(12)-N(8)	112.4126	H(23)-N(10)-N(9)	118.6577
N(8)-C(7)-C(2)	121.397	N(8)-C(7)-C(2)	121.2029	N(8)-C(7)-C(2)	121.1949	H(24)-N(10)-N(9)	118.6889	H(23)-N(10)-C(1)	128.1525
H(21)-C(6)-C(5)	121.0042	H(22)-C(6)-C(5)	121.0369	H(22)-C(6)-C(5)	121.0268	H(24)-N(10)-C(1)	128.1478	N(9)-N(10)-C(1)	112.7921
H(21)-C(6)-C(1)	121.9785	H(22)-C(6)-C(1)	122.0087	H(22)-C(6)-C(1)	121.9962	N(9)-N(10)-C(1)	112.7859	N(10)-N(9)-C(7)	106.3547
C(5)-C(6)-C(1)	117.0174	C(5)-C(6)-C(1)	116.9543	C(5)-C(6)-C(1)	116.977	N(10)-N(9)-C(7)	106.4035	C(12)-N(8)-C(7)	131.4489
H(20)-C(5)-C(6)	121.1218	H(21)-C(5)-C(6)	121.1256	H(21)-C(5)-C(6)	121.1276	C(12)-N(8)-C(7)	131.6525	N(9)-C(7)-N(8)	128.1733
H(20)-C(5)-C(4)	118.3968	H(21)-C(5)-C(4)	118.3805	H(21)-C(5)-C(4)	118.3836	N(9)-C(7)-N(8)	128.5318	N(9)-C(7)-C(2)	110.2224
C(6)-C(5)-C(4)	120.4814	C(6)-C(5)-C(4)	120.4938	C(6)-C(5)-C(4)	120.4889	N(9)-C(7)-C(2)	110.1112	N(8)-C(7)-C(2)	121.3724
F(11)-C(4)-C(5)	117.4009	F(11)-C(4)-C(5)	117.3795	F(11)-C(4)-C(5)	117.3839	N(8)-C(7)-C(2)	121.1687	H(22)-C(6)-C(5)	121.01
F(11)-C(4)-C(3)	119.3096	F(11)-C(4)-C(3)	119.3084	F(11)-C(4)-C(3)	119.3093	H(23)-C(6)-C(5)	120.9936	H(22)-C(6)-C(1)	121.9733
C(5)-C(4)-C(3)	123.2894	C(5)-C(4)-C(3)	123.3121	C(5)-C(4)-C(3)	123.3067	H(23)-C(6)-C(1)	121.9899	C(5)-C(6)-C(1)	117.0167
H(19)-C(3)-C(4)	121.4548	H(20)-C(3)-C(4)	121.4955	H(20)-C(3)-C(4)	121.5018	H(22)-C(5)-C(6)	121.1259	H(21)-C(5)-C(6)	121.124
H(19)-C(3)-C(2)	121.9232	H(20)-C(3)-C(2)	121.9235	H(20)-C(3)-C(2)	121.9048	H(22)-C(5)-C(4)	118.3938	H(21)-C(5)-C(4)	118.3946
C(4)-C(3)-C(2)	116.6211	C(4)-C(3)-C(2)	116.5804	C(4)-C(3)-C(2)	116.5928	F(11)-C(4)-C(5)	117.3989	F(11)-C(4)-C(5)	117.4016
C(7)-C(2)-C(3)	134.3858	C(7)-C(2)-C(3)	134.3497	C(7)-C(2)-C(3)	134.3306	F(11)-C(4)-C(3)	119.3215	F(11)-C(4)-C(3)	119.3103
C(7)-C(2)-C(1)	105.0802	C(7)-C(2)-C(1)	105.1176	C(7)-C(2)-C(1)	105.133	C(5)-C(4)-C(3)	123.2795	C(5)-C(4)-C(3)	123.2881
C(3)-C(2)-C(1)	120.534	C(3)-C(2)-C(1)	120.5326	C(3)-C(2)-C(1)	120.5363	H(21)-C(3)-C(4)	121.5193	H(20)-C(3)-C(4)	121.4611
N(10)-C(1)-C(6)	132.4217	N(10)-C(1)-C(6)	132.3853	N(10)-C(1)-C(6)	132.4018	H(21)-C(3)-C(2)	121.8515	H(20)-C(3)-C(2)	121.9126
N(10)-C(1)-C(2)	105.5217	N(10)-C(1)-C(2)	105.488	N(10)-C(1)-C(2)	105.5	N(10)-C(1)-C(6)	132.4376	N(10)-C(1)-C(6)	132.4186
C(6)-C(1)-C(2)	122.0564	C(6)-C(1)-C(2)	122.1265	C(6)-C(1)-C(2)	122.098	N(10)-C(1)-C(2)	105.5032	N(10)-C(1)-C(2)	105.5202

DIHEDRAL ANGLE									
COMPOUND 1		**COMPOUND 2**		**COMPOUND 3**		**COMPOUND 4**		**COMPOUND 4**	
C(15)-C(17)-C(18)-C(16)	0.2552	C(15)-C(17)-C(18)-C(16)	0.2954	C(15)-C(17)-C(18)-C(16)	0.3006	C(18)-O(19)-C(20)-H(30)	179.4655	C(16)-C(18)-C(19)-H(29)	-30.2504
C(15)-C(17)-C(18)-H(28)	179.5805	C(15)-C(17)-C(18)-Cl(19)	179.7202	C(15)-C(17)-C(18)-F(19)	179.6591	C(18)-O(19)-C(20)-H(31)	-61.7581	C(16)-C(18)-C(19)-H(30)	89.2532
H(27)-C(17)-C(18)-C(16)	-179.463	H(28)-C(17)-C(18)-C(16)	-179.522	H(28)-C(17)-C(18)-C(16)	-179.473	C(18)-O(19)-C(20)-H(32)	60.6567	C(16)-C(18)-C(19)-H(31)	-151.269
H(27)-C(17)-C(18)-H(28)	-0.1379	H(28)-C(17)-C(18)-Cl(19)	-0.0977	H(28)-C(17)-C(18)-F(19)	-0.114	C(16)-C(18)-O(19)-C(20)	0.8148	C(17)-C(18)-C(19)-H(29)	151.5197
C(14)-C(16)-C(18)-C(17)	-0.3988	C(14)-C(16)-C(18)-C(17)	-0.4432	C(14)-C(16)-C(18)-C(17)	-0.4441	C(17)-C(18)-O(19)-C(20)	-179.797	C(17)-C(18)-C(19)-H(30)	-88.9767
C(14)-C(16)-C(18)-H(28)	-179.723	C(14)-C(16)-C(18)-Cl(19)	-179.867	C(14)-C(16)-C(18)-F(19)	-179.802	C(15)-C(17)-C(18)-C(16)	-0.4022	C(17)-C(18)-C(19)-H(31)	30.5009
H(26)-C(16)-C(18)-C(17)	178.9489	H(27)-C(16)-C(18)-C(17)	178.9813	H(27)-C(16)-C(18)-C(17)	178.8686	C(15)-C(17)-C(18)-O(19)	-179.825	C(15)-C(17)-C(18)-C(16)	-0.0559
H(26)-C(16)-C(18)-H(28)	-0.3759	H(27)-C(16)-C(18)-Cl(19)	-0.4426	H(27)-C(16)-C(18)-F(19)	-0.4889	H(29)-C(17)-C(18)-C(16)	179.454	C(15)-C(17)-C(18)-C(19)	178.2295
C(13)-C(15)-C(17)-C(18)	0.6875	C(13)-C(15)-C(17)-C(18)	0.6096	C(13)-C(15)-C(17)-C(18)	0.6247	H(29)-C(17)-C(18)-O(19)	0.0308	H(28)-C(17)-C(18)-C(16)	-179.923
C(13)-C(15)-C(17)-H(27)	-179.593	C(13)-C(15)-C(17)-H(28)	-179.573	C(13)-C(15)-C(17)-H(28)	-179.607	C(14)-C(16)-C(18)-C(17)	0.4907	H(28)-C(17)-C(18)-C(19)	-1.6377
H(25)-C(15)-C(17)-C(18)	179.9948	H(26)-C(15)-C(17)-C(18)	179.9621	H(26)-C(15)-C(17)-C(18)	179.9827	C(14)-C(16)-C(18)-O(19)	179.8576	C(14)-C(16)-C(18)-C(17)	-0.0889
H(25)-C(15)-C(17)-H(27)	-0.2858	H(26)-C(15)-C(17)-H(28)	-0.2214	H(26)-C(15)-C(17)-H(28)	-0.2493	H(28)-C(16)-C(18)-C(17)	-178.726	C(14)-C(16)-C(18)-C(19)	-178.373
C(13)-C(14)-C(16)-C(18)	-0.3968	C(13)-C(14)-C(16)-C(18)	-0.3092	C(13)-C(14)-C(16)-C(18)	-0.3331	H(28)-C(16)-C(18)-O(19)	0.6407	H(27)-C(16)-C(18)-C(17)	179.3427

C(13)-C(14)-C(16)-H(26)	-179.747	C(13)-C(14)-C(16)-H(27)	-179.730	C(13)-C(14)-C(16)-H(27)	-179.632	C(13)-C(15)-C(17)-C(18)	-0.548	H(27)-C(16)-C(18)-C(19)	1.0587
H(24)-C(14)-C(16)-C(18)	178.2409	H(25)-C(14)-C(16)-C(18)	178.6004	H(25)-C(14)-C(16)-C(18)	178.5173	C(13)-C(15)-C(17)-H(29)	179.6002	C(13)-C(15)-C(17)-C(18)	0.804
H(24)-C(14)-C(16)-H(26)	-1.11	H(25)-C(14)-C(16)-H(27)	-0.8211	H(25)-C(14)-C(16)-H(27)	-0.7813	H(27)-C(15)-C(17)-C(18)	-179.846	C(13)-C(15)-C(17)-H(28)	-179.329
C(12)-C(13)-C(15)-C(17)	178.232	C(12)-C(13)-C(15)-C(17)	178.485	C(12)-C(13)-C(15)-C(17)	178.465	H(27)-C(15)-C(17)-H(29)	0.3023	H(26)-C(15)-C(17)-C(18)	179.8439
C(12)-C(13)-C(15)-H(25)	-1.0791	C(12)-C(13)-C(15)-H(26)	-0.8659	C(12)-C(13)-C(15)-H(26)	-0.8926	C(13)-C(14)-C(16)-C(18)	0.3695	H(26)-C(15)-C(17)-H(28)	-0.2889
C(14)-C(13)-C(15)-C(17)	-1.4555	C(14)-C(13)-C(15)-C(17)	-1.3257	C(14)-C(13)-C(15)-C(17)	-1.3618	C(13)-C(14)-C(16)-H(28)	179.5999	C(13)-C(14)-C(16)-C(18)	-0.5055
C(14)-C(13)-C(15)-H(25)	179.2334	C(14)-C(13)-C(15)-H(26)	179.3234	C(14)-C(13)-C(15)-H(26)	179.2807	H(26)-C(14)-C(16)-C(18)	-178.289	C(13)-C(14)-C(16)-H(27)	-179.938
C(12)-C(13)-C(14)-C(16)	-178.349	C(12)-C(13)-C(14)-C(16)	-178.623	C(12)-C(13)-C(14)-C(16)	-178.602	H(26)-C(14)-C(16)-H(28)	0.941	H(25)-C(14)-C(16)-C(18)	178.3042
C(12)-C(13)-C(14)-H(24)	2.9971	C(12)-C(13)-C(14)-H(25)	2.4618	C(12)-C(13)-C(14)-H(25)	2.5384	C(12)-C(13)-C(15)-C(17)	-178.228	H(25)-C(14)-C(16)-H(27)	-1.1281
C(15)-C(13)-C(14)-C(16)	1.2984	C(15)-C(13)-C(14)-C(16)	1.1629	C(15)-C(13)-C(14)-C(16)	1.2023	C(12)-C(13)-C(15)-H(27)	1.0696	C(12)-C(13)-C(15)-C(17)	178.0664
C(15)-C(13)-C(14)-H(24)	-177.355	C(15)-C(13)-C(14)-H(25)	-177.752	C(15)-C(13)-C(14)-H(25)	-177.657	C(14)-C(13)-C(15)-C(17)	1.3655	C(12)-C(13)-C(15)-H(26)	-0.9763
N(8)-C(12)-C(13)-C(14)	17.2206	N(8)-C(12)-C(13)-C(14)	15.1446	N(8)-C(12)-C(13)-C(14)	15.2495	C(14)-C(13)-C(15)-H(27)	-179.337	C(14)-C(13)-C(15)-C(17)	-1.3621
N(8)-C(12)-C(13)-C(15)	-162.436	N(8)-C(12)-C(13)-C(15)	-164.646	N(8)-C(12)-C(13)-C(15)	-164.56	C(12)-C(13)-C(14)-C(16)	178.2736	C(14)-C(13)-C(15)-H(26)	179.5953
H(23)-C(12)-C(13)-C(14)	-166.964	H(24)-C(12)-C(13)-C(14)	-168.467	H(24)-C(12)-C(13)-C(14)	-168.395	C(12)-C(13)-C(14)-H(26)	-3.0626	C(12)-C(13)-C(14)-C(16)	-178.151
H(23)-C(12)-C(13)-C(15)	13.378	H(24)-C(12)-C(13)-C(15)	11.7414	H(24)-C(12)-C(13)-C(15)	11.796	C(15)-C(13)-C(14)-C(16)	-1.2667	C(12)-C(13)-C(14)-H(25)	3.0282
C(7)-N(9)-N(10)-C(1)	0.7095	C(7)-N(9)-N(10)-C(1)	0.5423	C(7)-N(9)-N(10)-C(1)	0.5914	C(15)-C(13)-C(14)-H(26)	177.3972	C(15)-C(13)-C(14)-C(16)	1.2029
C(7)-N(9)-N(10)-H(22)	174.465	C(7)-N(9)-N(10)-H(23)	175.2495	C(7)-N(9)-N(10)-H(23)	175.1006	N(8)-C(12)-C(13)-C(14)	-13.7233	C(15)-C(13)-C(14)-H(25)	-177.618
C(7)-N(8)-C(12)-H(23)	-179.893	C(7)-N(8)-C(12)-H(24)	-179.763	C(7)-N(8)-C(12)-H(24)	-179.777	N(8)-C(12)-C(13)-C(15)	165.8247	N(8)-C(12)-C(13)-C(14)	16.2082
C(7)-N(8)-C(12)-C(13)	-4.1221	C(7)-N(8)-C(12)-C(13)	-3.4149	C(7)-N(8)-C(12)-C(13)	-3.4599	H(25)-C(12)-C(13)-C(14)	169.9133	N(8)-C(12)-C(13)-C(15)	-163.159
C(2)-C(7)-N(9)-N(10)	-0.9465	C(2)-C(7)-N(9)-N(10)	-0.7817	C(2)-C(7)-N(9)-N(10)	-0.8101	H(25)-C(12)-C(13)-C(15)	-10.5387	H(24)-C(12)-C(13)-C(14)	-167.844
N(8)-C(7)-N(9)-N(10)	-175.326	N(8)-C(7)-N(9)-N(10)	-176.177	N(8)-C(7)-N(9)-N(10)	-176.048	C(7)-N(9)-N(10)-C(1)	-0.8041	H(24)-C(12)-C(13)-C(15)	12.7888
C(2)-C(7)-N(8)-C(12)	153.2172	C(2)-C(7)-N(8)-C(12)	157.9406	C(2)-C(7)-N(8)-C(12)	157.1064	C(7)-N(9)-N(10)-H(24)	-174.324	C(7)-N(9)-N(10)-C(1)	0.7951
N(9)-C(7)-N(8)-C(12)	-32.9624	N(9)-C(7)-N(8)-C(12)	-27.1142	N(9)-C(7)-N(8)-C(12)	-28.1211	C(7)-N(8)-C(12)-H(25)	-179.934	C(7)-N(9)-N(10)-H(23)	174.1451
C(4)-C(5)-C(6)-C(1)	0.0051	C(4)-C(5)-C(6)-C(1)	0.0292	C(4)-C(5)-C(6)-C(1)	0.025	C(7)-N(8)-C(12)-C(13)	3.737	C(7)-N(8)-C(12)-H(24)	-179.956
C(4)-C(5)-C(6)-H(21)	179.9705	C(4)-C(5)-C(6)-H(22)	179.9749	C(4)-C(5)-C(6)-H(22)	179.981	C(2)-C(7)-N(9)-N(10)	0.9194	C(7)-N(8)-C(12)-C(13)	-4.0494
H(20)-C(5)-C(6)-C(1)	179.9442	H(21)-C(5)-C(6)-C(1)	179.9763	H(21)-C(5)-C(6)-C(1)	179.9649	N(8)-C(7)-N(9)-N(10)	175.907	C(2)-C(7)-N(9)-N(10)	-0.9871
H(20)-C(5)-C(6)-H(21)	-0.0904	H(21)-C(5)-C(6)-H(22)	-0.0779	H(21)-C(5)-C(6)-H(22)	-0.0791	C(2)-C(7)-N(8)-C(12)	-156.703	N(8)-C(7)-N(9)-N(10)	-175.443
C(3)-C(4)-C(5)-C(6)	-0.1368	C(3)-C(4)-C(5)-C(6)	-0.1404	C(3)-C(4)-C(5)-C(6)	-0.1222	N(9)-C(7)-N(8)-C(12)	28.7995	C(2)-C(7)-N(8)-C(12)	153.3772
C(3)-C(4)-C(5)-H(20)	179.9225	C(3)-C(4)-C(5)-H(21)	179.911	C(3)-C(4)-C(5)-H(21)	179.9363	C(4)-C(5)-C(6)-C(1)	-0.008	N(9)-C(7)-N(8)-C(12)	-32.7179
F(11)-C(4)-C(5)-C(6)	179.7859	F(11)-C(4)-C(5)-C(6)	179.7954	F(11)-C(4)-C(5)-C(6)	179.8018	C(4)-C(5)-C(6)-H(23)	-179.98	C(4)-C(5)-C(6)-C(1)	0.0179
F(11)-C(4)-C(5)-H(20)	-0.1548	F(11)-C(4)-C(5)-H(21)	-0.1532	F(11)-C(4)-C(5)-H(21)	-0.1397	H(22)-C(5)-C(6)-C(1)	-179.953	C(4)-C(5)-C(6)-H(22)	179.9766
C(2)-C(3)-C(4)-C(5)	0.1197	C(2)-C(3)-C(4)-C(5)	0.1007	C(2)-C(3)-C(4)-C(5)	0.0834	H(22)-C(5)-C(6)-H(23)	0.0744	H(21)-C(5)-C(6)-C(1)	179.9524
C(2)-C(3)-C(4)-F(11)	-179.801	C(2)-C(3)-C(4)-F(11)	-179.833	C(2)-C(3)-C(4)-F(11)	-179.839	C(3)-C(4)-C(5)-C(6)	0.1173	H(21)-C(5)-C(6)-H(22)	-0.089
H(19)-C(3)-C(4)-C(5)	179.7851	H(20)-C(3)-C(4)-C(5)	179.8269	H(20)-C(3)-C(4)-C(5)	179.8109	C(3)-C(4)-C(5)-H(22)	-179.936	C(3)-C(4)-C(5)-C(6)	-0.1298
H(19)-C(3)-C(4)-F(11)	-0.1362	H(20)-C(3)-C(4)-F(11)	-0.1077	H(20)-C(3)-C(4)-F(11)	-0.1117	F(11)-C(4)-C(5)-C(6)	-179.803	C(3)-C(4)-C(5)-H(21)	179.934
C(1)-C(2)-C(7)-N(8)	175.6701	C(1)-C(2)-C(7)-N(8)	176.5278	C(1)-C(2)-C(7)-N(8)	176.3841	F(11)-C(4)-C(5)-H(22)	0.1441	F(11)-C(4)-C(5)-C(6)	179.7766
C(1)-C(2)-C(7)-N(9)	0.848	C(1)-C(2)-C(7)-N(9)	0.7408	C(1)-C(2)-C(7)-N(9)	0.7408	C(2)-C(3)-C(4)-C(5)	-0.0945	F(11)-C(4)-C(5)-H(21)	-0.1596
C(3)-C(2)-C(7)-N(8)	-4.4429	C(3)-C(2)-C(7)-N(8)	-3.5853	C(3)-C(2)-C(7)-N(8)	-3.7218	C(2)-C(3)-C(4)-F(11)	179.8238	C(2)-C(3)-C(4)-C(5)	0.0948
C(3)-C(2)-C(7)-N(9)	-179.265	C(3)-C(2)-C(7)-N(9)	-179.372	C(3)-C(2)-C(7)-N(9)	-179.365	H(21)-C(3)-C(4)-C(5)	-179.786	C(2)-C(3)-C(4)-F(11)	-179.81
C(1)-C(2)-C(3)-C(4)	0.022	C(1)-C(2)-C(3)-C(4)	0.0424	C(1)-C(2)-C(3)-C(4)	0.0459	H(21)-C(3)-C(4)-F(11)	0.1328	H(20)-C(3)-C(4)-C(5)	179.7794
C(1)-C(2)-C(3)-H(19)	-179.641	C(1)-C(2)-C(3)-H(20)	-179.682	C(1)-C(2)-C(3)-H(20)	-179.68	C(1)-C(2)-C(7)-N(8)	-176.137	H(20)-C(3)-C(4)-F(11)	-0.1253
C(7)-C(2)-C(3)-C(4)	-179.851	C(7)-C(2)-C(3)-C(4)	-179.830	C(7)-C(2)-C(3)-C(4)	-179.836	C(1)-C(2)-C(7)-N(9)	-0.7185	C(1)-C(2)-C(7)-N(8)	175.7301

C(7)-C(2)-C(3)-H(19)	0.4849	C(7)-C(2)-C(3)-H(20)	0.4443	C(7)-C(2)-C(3)-H(20)	0.4382	C(3)-C(2)-C(7)-N(8)	3.8782	C(1)-C(2)-C(7)-N(9)	0.8336
C(2)-C(1)-N(10)-N(9)	-0.1748	C(2)-C(1)-N(10)-N(9)	-0.0754	C(2)-C(1)-N(10)-N(9)	-0.1241	C(3)-C(2)-C(7)-N(9)	179.2966	C(3)-C(2)-C(7)-N(8)	-4.3942
C(2)-C(1)-N(10)-H(22)	-173.200	C(2)-C(1)-N(10)-H(23)	-174.167	C(2)-C(1)-N(10)-H(23)	-173.995	C(1)-C(2)-C(3)-C(4)	-0.0314	C(3)-C(2)-C(7)-N(9)	-179.291
C(6)-C(1)-N(10)-N(9)	179.6598	C(6)-C(1)-N(10)-N(9)	179.7641	C(6)-C(1)-N(10)-N(9)	179.7296	C(2)-C(1)-N(10)-N(9)	0.349	C(1)-C(2)-C(3)-H(20)	-179.638
C(6)-C(1)-N(10)-H(22)	6.6341	C(6)-C(1)-N(10)-H(23)	5.672	C(6)-C(1)-N(10)-H(23)	5.8588	C(2)-C(1)-N(10)-H(24)	173.1169	C(7)-C(2)-C(3)-H(20)	0.5014
C(2)-C(1)-C(6)-C(5)	0.1345	C(2)-C(1)-C(6)-C(5)	0.1122	C(2)-C(1)-C(6)-C(5)	0.1029	C(6)-C(1)-N(10)-N(9)	-179.58	C(2)-C(1)-N(10)-N(9)	-0.2688
C(2)-C(1)-C(6)-H(21)	-179.830	C(2)-C(1)-C(6)-H(22)	-179.833	C(2)-C(1)-C(6)-H(22)	-179.853	C(6)-C(1)-N(10)-H(24)	-6.8119	C(2)-C(1)-N(10)-H(23)	-172.844
N(10)-C(1)-C(6)-C(5)	-179.677	N(10)-C(1)-C(6)-C(5)	-179.705	N(10)-C(1)-C(6)-C(5)	-179.731	C(2)-C(1)-C(6)-C(5)	-0.1165	C(6)-C(1)-N(10)-N(9)	179.6535
N(10)-C(1)-C(6)-H(21)	0.3575	N(10)-C(1)-C(6)-H(22)	0.3496	N(10)-C(1)-C(6)-H(22)	0.3138	C(2)-C(1)-C(6)-H(23)	179.8556	C(6)-C(1)-N(10)-H(23)	7.0783
C(6)-C(1)-C(2)-C(3)	-0.1518	C(6)-C(1)-C(2)-C(3)	-0.1519	C(6)-C(1)-C(2)-C(3)	-0.1421	N(10)-C(1)-C(6)-C(5)	179.8026	N(10)-C(1)-C(6)-C(5)	-179.791
C(6)-C(1)-C(2)-C(7)	179.7545	C(6)-C(1)-C(2)-C(7)	179.7541	C(6)-C(1)-C(2)-C(7)	179.77	N(10)-C(1)-C(6)-H(23)	-0.2253	N(10)-C(1)-C(6)-H(22)	0.2506
N(10)-C(1)-C(2)-C(3)	179.7042	N(10)-C(1)-C(2)-C(3)	179.7081	N(10)-C(1)-C(2)-C(3)	179.7303	N(10)-C(1)-C(2)-C(3)	-179.798	N(10)-C(1)-C(2)-C(3)	179.7764
N(10)-C(1)-C(2)-C(7)	-0.3896	N(10)-C(1)-C(2)-C(7)	-0.3858	N(10)-C(1)-C(2)-C(7)	-0.3576	N(10)-C(1)-C(2)-C(7)	0.2142	N(10)-C(1)-C(2)-C(7)	-0.3268

CONCLUSION

In this study, Five Schiff base derivatives have been synthesized and characterized by FT-IR, and ^{1}H-NMR spectroscopy studies. The theoretical calculations of all the five Schiff derivatives have been performed by using the density functional theory (DFT) method with the 6-31G(d) basis set. The frontier molecular orbitals have been visualized and the HOMO–LUMO energy gap (3.4439 eV) has been calculated. These results are taken into account, we conclude that the title compounds is an attractive compound for future medicinal and pharmacological studies.

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