Structural Properties,Theory Functional Calculations (DFT), Natural Bond Orbital and Energies for the fluorocarbon compounds

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Abstract: The structural and electronic properties of wurtzite $C_{20}H_{11}F_{13}ClN_3O_3S$ structure have been theoretically investigated within the framework of the density functional theory method(1). B3LYP/3-21G calculation results indicated that some selected bond length and bond angles values for the $C_{20}H_{11}F_{13}ClN_3O_3S$ In this paper, the optimized geometries and frequencies of the stationary point and the minimum-energy paths of two new compounds with $C_{20}H_{11}F_{13}ClN_3O_3S$ chemical formula are calculated by using the DFT methods with 3-21G basis set. The detail group points of compound is C_1.

Keywords: Electronic structure, Fluorocarbon compounds, DFT Calculations, Vibrational analysis, B3LYP level.

1. Introduction

Sulfa drugs are still today among the drugs first used (together with ampicillin and gentamycin)as chemotherapeutic agents in bacterial infections by Escherichia coli in humans (2).Sulfonamides are antimicrobial agents widely employed in animal production and their residues in food could be an important risk to human health. In the dairy industry, large quantities of milk are monitored daily for the presence of sulfonamides. Fluoroalkanes can serve as oil-repellent/water-repellent fluoropolymers, solvents, liquid breathing research agents, and powerful greenhouse gases. Fluorocarbon liquids are colorless. They have high density, up to over twice that of water, due to their high molecular weight. Recently, perfluorochemicals (PFCs) are of specialpublic concern as environmental contaminantsbecause they are globally distributed, persistent, andbioaccumulative for higher chain homologues. During this study we report the optimized geometries, assignments and electronic structure calculations for the compound. The structure of the compound has been optimized by using the DFT (B3LYP) method with the 3-21G basis sets, using the Gaussian 09 program.Density functional theory methods were employed to determine the optimized structures of $C_{20}H_{11}F_{13}ClN_3O_3S$ and Initial calculations were performed at the DFT level and split- valence plus polarization 3-21G basis sets were used.

2. Experimental

2.1 Chemicals and reagents

The optimized structural parameters were used in the vibrational frequency calculations at the DFT level to characterize all stationary points as minima. All computational are carried out using Gaussian 09w program. Harmonic vibrational frequencies (v) in cm^{-1} and infrared intensities (int) in Kilometer per mole of all compounds were performed at the same level on the respective fully optimized geometries. Energy minimum molecular geometries were located by minimizing energy, with respect to all geometrical coordinates without imposing any symmetrical constraints.

2.2 NBO (Natural Bond Orbital) study of structures

NBO Calculated Hybridizations are significant parameters for our investigation. The structure of the compound has been optimized by using the DFT (B3LYP) method with the 3-21G basis sets, using the Gaussian 09w program. Density functional theory methods were employed to determine the optimized structures of $C_{20}H_{11}F_{13}ClN_3O_3S$ (Table 1, Figure 1).
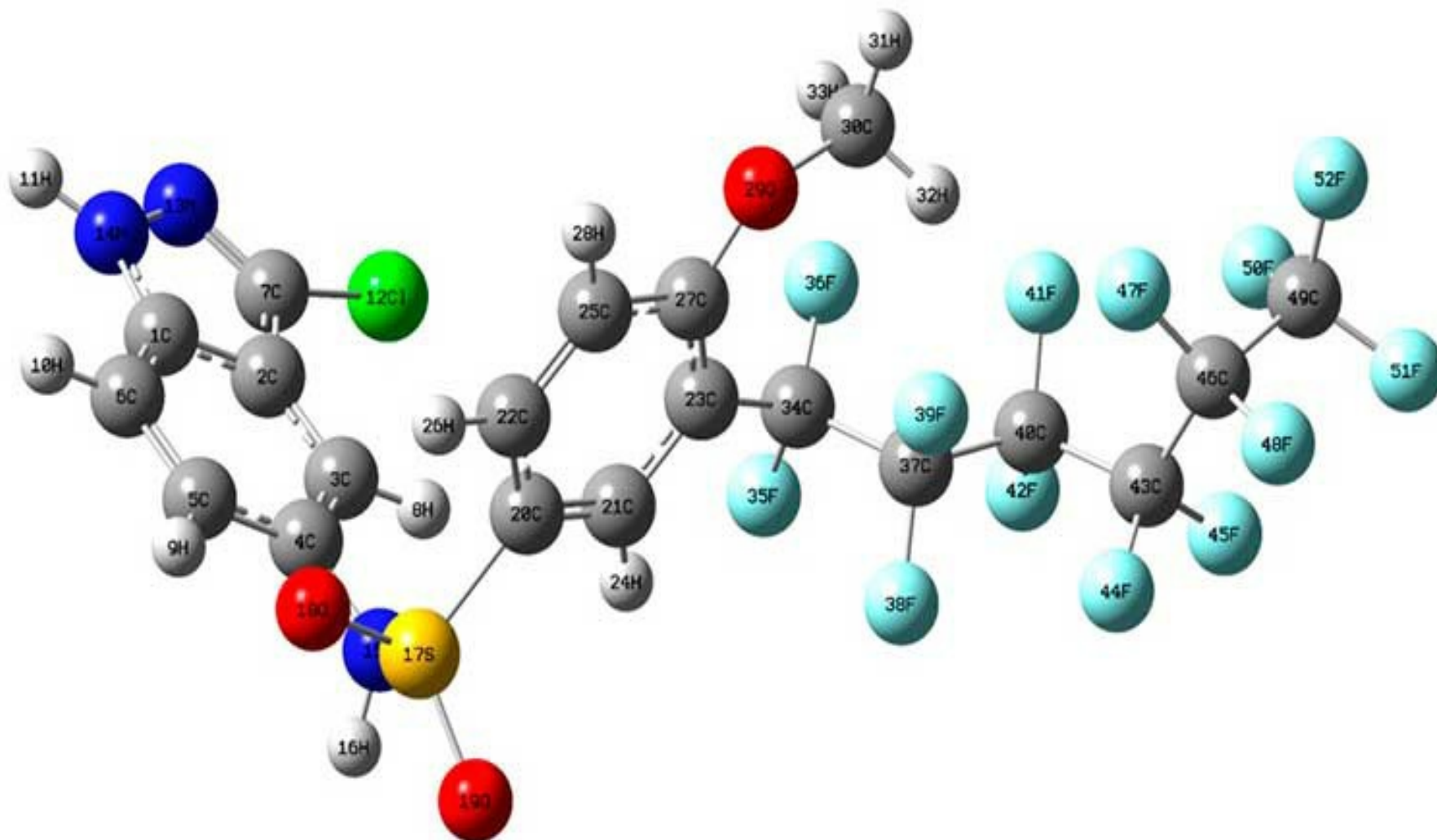
Figure 1. Optimized geometries of $C_{20}H_{11}F_{13}ClN_3O_3S$ at B3LYP/3-21Glevel of theory.

Table 1. Geometrical parameters optimized for $C_{20}H_{11}F_{13}ClN_3O_3S$ some selected bond lengths (Å) and angles (∘).

	Bond length		Bond length		Bond length
C_7-Cl_{12}	1.7959	H_{31}-F_{52}	0.9053	C_{43}-F_{44}	1.35
N_{13}-N_{14}	1.4114	H_{33}-F_{39}	1.3936	C_{43}-F_{45}	1.35
N_{15}-S_{17}	1.7765	C_{34}-F_{35}	1.35	C_{46}-F_{47}	1.35
S_{17}-O_{18}	105992	C_{37}-F_{39}	1.35	C_{46}-F_{48}	1.35
S_{17}-O_{19}	1.5874	C_{40}-F_{42}	1.35	C_{49}-F_{50}	1.35
O_{29}-C_{30}	1.4639	F_{41}-F_{52}	1.717	C_{49}-F_{51}	1.35
C_{30}-F_{52}	1.4049	F_{41}-F_{50}	1.4323	F_{41}-C_{49}	1.7674
	Bond Angles		Bond Angles		Bond Angles
N_{15}-S_{17}-O_{19}	102.3412	F_{35}-C_{34}-F_{36}	109.4712	H_{32}-C_{46}-F_{48}	150.7584
C_2-C_7-Cl_{12}	124.3832	F_{38}-C_{37}-F_{39}	109.4712	F_{47}-C_{46}-F_{48}	109.4713
O_{29}-C_{30}-F_{52}	111.7984	F_{41}-C_{40}-F_{42}	109.4712	F_{41}-C_{49}-F_{51}	151.1907
Cl_{12}-C_7-N_{13}	121.5988	C_{40}-F_{41}-F_{50}	108.903	F_{50}-C_{49}-F_{52}	109.4713
C_7-N_{13}-N_{14}	103.8277	C_{40}-F_{41}-F_{52}	124.9545	F_{51}-C_{49}-F_{52}	109.4712
C_{30}-H_{32}-F_{47}	134.5953	F_{50}-F_{41}-F_{52}	88.3745	C_{30}-F_{52}-F_{41}	73.4312
N_{15}-S_{17}-O_{18}	114.0423	F_{44}-C_{43}-F_{45}	109.4712	H_{31}-F_{52}-F_{41}	51.3647

Natural Bond Orbital's (NBOs) are localized few-center orbital's that describe the Lewis-like molecular bonding pattern of electron pairs in optimally compact form. More precisely, NBOs are an orthonormal set of localized "maximum occupancy" orbital's whose leading N/2 members (or N members in the open-shell case) give the most accurate possible Lewis-like description of the total N-electron density. This analysis is carried

out by examining all possible interactions between "filled" (donor) Lewis-type NBOs and "empty" (acceptor) non-Lewis NBOs, and estimating their energetic importance by 2nd-order perturbation theory. Since these interactions lead to donation of occupancy from the localized NBOs of the idealized Lewis structure into the empty non-Lewis orbitals (and thus, to departures from the idealized Lewis structure description), they are referred to as "delocalization" corrections to the zeroth-order natural Lewis structure.

Natural charges have been computed using natural bond orbital (NBO) module implemented in Gaussian 09w. The. These quantities are derived from the NBO population analysis. The former provides an orbital picture that is closer to the classical Lewis structure. The NBO analysis involving hybridizations of selected bonds are calculated at B3LYP methods and 3-21G level of theory (Tables 2, 3).

Table2. The NBO Calculated Hybridizations for $C_{20}H_{11}F_{13}ClN_3O_3S$ at the B3LYP/3-21G.

B3LYP	Atom	Bond	B3LYP	Atom	Bond
$S^1p^{4.55},S^1p^{2.73}$	$N_{13}\text{-}N_{14}$	N-N	$S^1p^{2.83},S^1p^{6.03}$	$C_7\text{-}Cl_{12}$	C-Cl
$S^1p^{2.22},S^1p^{8.76}$	$S_{17}\text{-}O_{18}$	S-O	$S^1p^{4.51},S^1p^{4.18}$	$N_{15}\text{-}S_{17}$	N-S
$S^1p^{4.19},S^1p^{3.18}$	$C_4\text{-}F_{35}$	C-F	$S^1p^{2.58},S^1p^{8.76}$	$S_{17}\text{-}O_{19}$	S-O
$S^1p^{2.59},S^1p^{4.76}$	$O_{29}\text{-}C_{30}$	O-C	$S^1p^{2.57},S^1$	$N_{15}\text{-}H_{16}$	N-H
$S^1p^{3.98},S^1p^{3.12}$	$C_{37}\text{-}F_{38}$	C-F	$S^1p^{4.16},S^1p^{3.16}$	$C_{34}\text{-}F_{36}$	C-F
$S^1p^{4.07},S^1p^{3.23}$	$C_{40}\text{-}F_{41}$	C-F	$S^1p^{4.19},S^1p^{3.22}$	$C_{37}\text{-}F_{39}$	C-F
$S^1p^{3.97},S^1p^{3.19}$	$C_{43}\text{-}F_{44}$	C-F	$S^1p^{4.00},S^1p^{3.14}$	$C_{40}\text{-}F_{42}$	C-F

These data shows the hyper conjugation of electrons between ligand atoms with central metal atom. These conjugations stand on the base of p-d π-bonding. The NBO calculated hybridization for $C_{20}H_{11}F_{13}ClN_3O_3S$ shows that all of compounds have SP^X hybridization and non planar configurations. The total hybridization of these molecules are SP^X that confirmed by structural. The amount of bond hybridization showed the in equality between central atoms angles (Table 2) shown distortion from normal VSEPR structures and confirmed deviation from VSEPR structures. (Figure 2).

$E_{LUMO}=-0.04005$

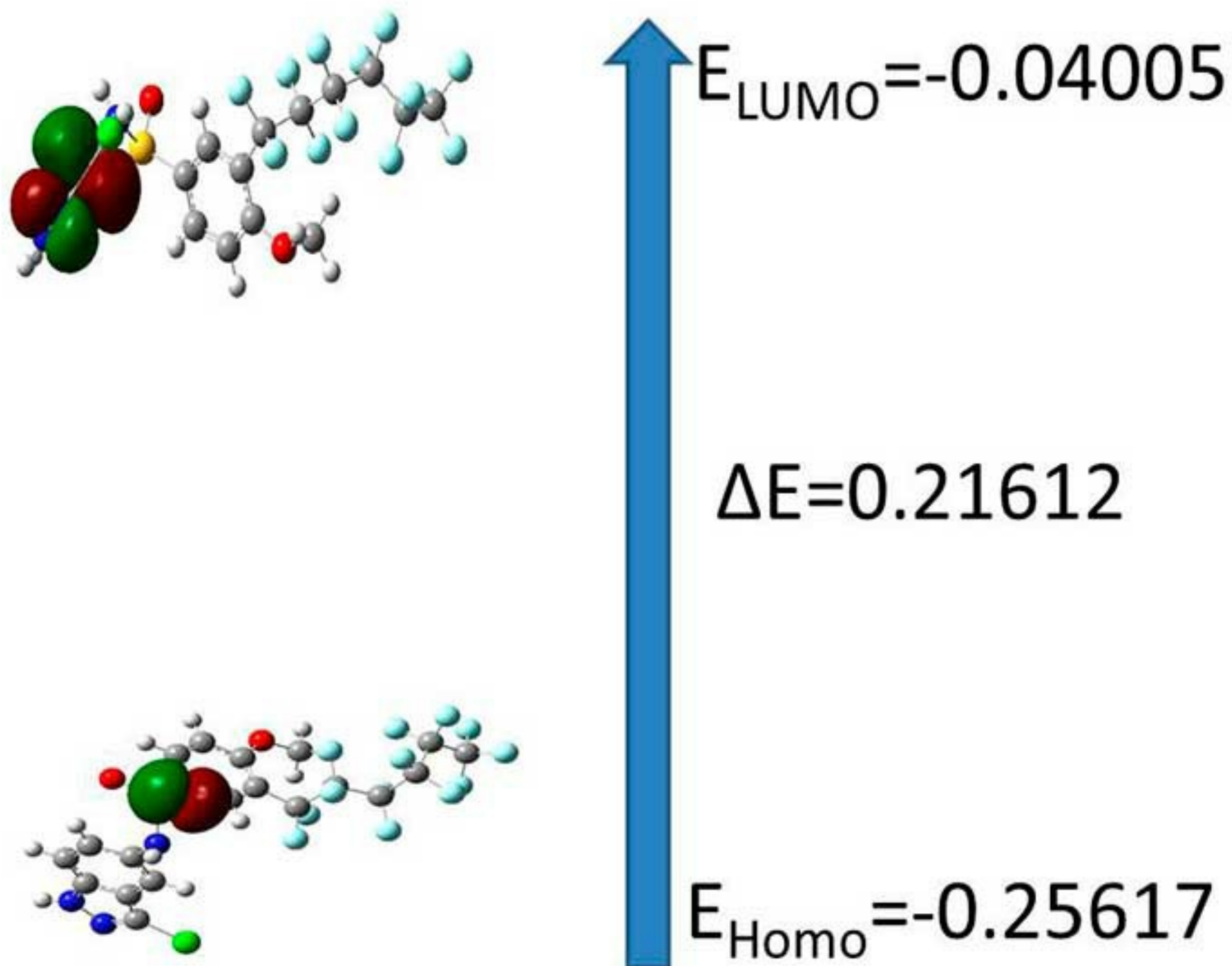$\Delta E=0.21612$

$E_{Homo}=-0.25617$

Figure 2. The atomic orbital of the frontier molecular orbital for $C_{20}H_{11}F_{13}ClN_3O_3S$ at B3LYP/3-21G level of theory

Some thermodynamic parameters Frequencies for $C_{20}H_{11}F_{13}ClN_3O_3S$ Zero-point Energy, correction Energy, Enthalpy lengths, Gibbs free Energy are calculated and confirmed with other published theoretical data (Table 4).

Table 3. Some thermodynamic parameters Frequencies for $C_{20}H_{11}F_{13}ClN_3O_3S$ Zero-point Energy, correction Energy, Enthalpy lengths, Gibbs free Energy.

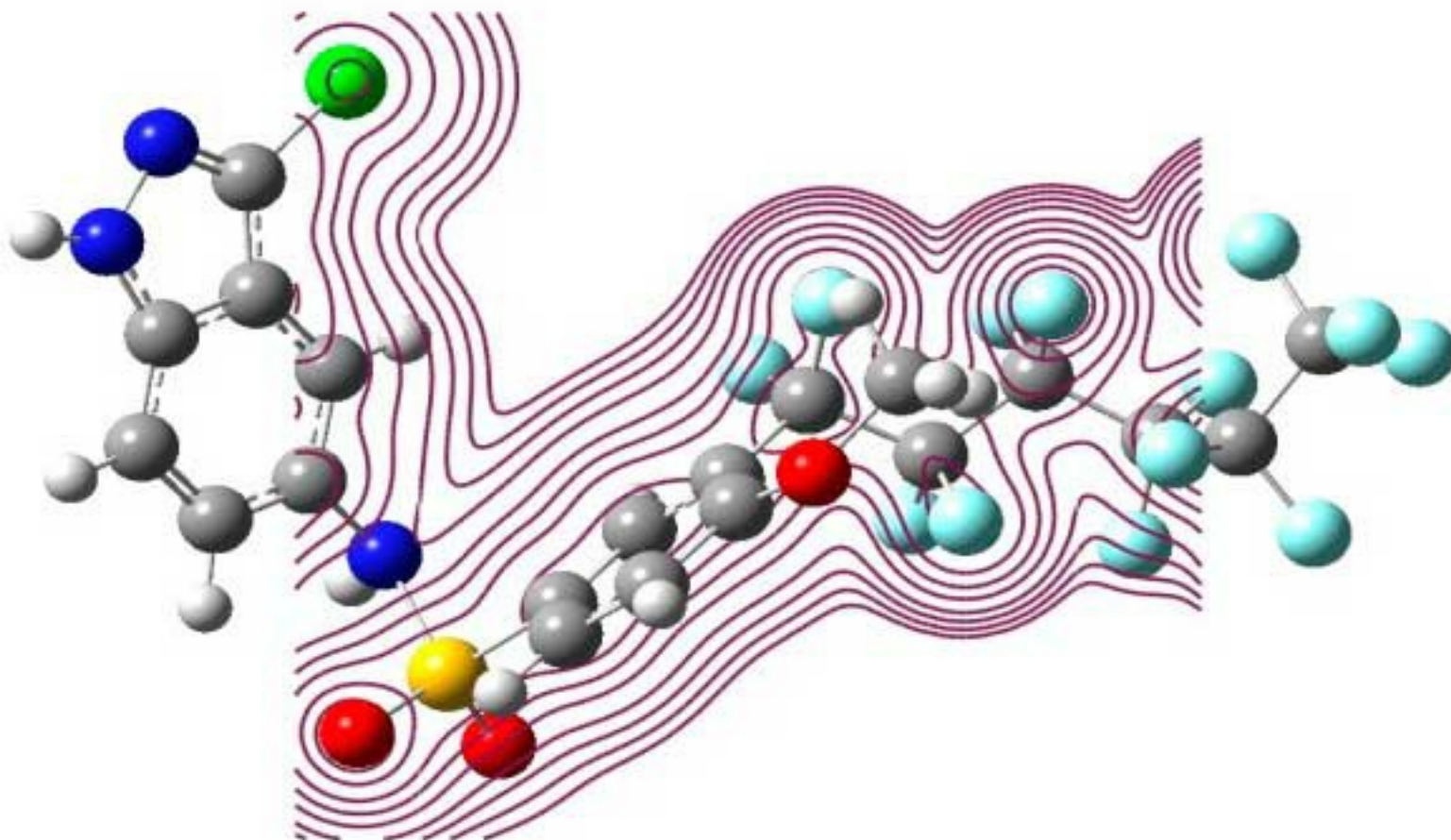| $C_{20}H_{11}F_{13}ClN_3O_3S$ |
| --- |
| Zero-point correction= 0.314221 (Hartree/Particle) |
| Thermal correction to Energy= 0.351115 |
| Thermal correction to Enthalpy= 0.352059 |
| Thermal correction to Gibbs Free Energy= 0.240518 |

2.3 Electronic density

Figure 3. Total electron density surfaces for the $C_{20}H_{11}F_{13}ClN_3O_3S$

2.4 Frontier molecular orbital

The HOMO represents the ability to donate an electron, LUMO as an electron acceptor represents the ability to obtain an electron. The HOMO and LUMO energy were calculated by B3LYP/3-21G method. This electronic absorption corresponds to the transition from the ground to the first excited state and is mainly described by one electron excitation from the highest occupied molecular or orbital (LUMO) both the highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO) are the main orbital take part in chemical stability.. Therefore, while the energy of the HOMO is directly related to the ionization potential, LUMO energy is directly related to the electron affinity. Energy difference between HOMO and LUMO orbital is called as energy gap that is an important stability for structures. In addition, 3D plots of highest occupied molecular orbitals (HOMOs) and lowest unoccupied molecular orbitals (LUMOs) are shown in Figure 2. The HOMO–LUMO energies were also calculated at the3-21G and the values are listed in Figure respectively.

IR spectrum

Infrared spectra may be obtained from samples in all phases (liquid, solid and gaseous). Liquids are usually examined as a thin film sandwiched between two polished salt plates (note that glass absorbs infrared radiation, whereas NaCl is transparent). If solvents are used to dissolve solids, care must be taken to avoid obscuring important spectral regions by solvent absorption. Perchlorinated solvents such as carbon tetrachloride, chloroform and tetrachloroethene are commonly used. Alternatively, solids may either be incorporated in a thin KBr disk, prepared under high pressure, or mixed with a little non-volatile liquid and ground to a paste (or mull) that is smeared between salt plates.but,in this paper we obtained IR spectrum theoretically by use Gaussian 09.frequencies of functional group showed in Figure 4.
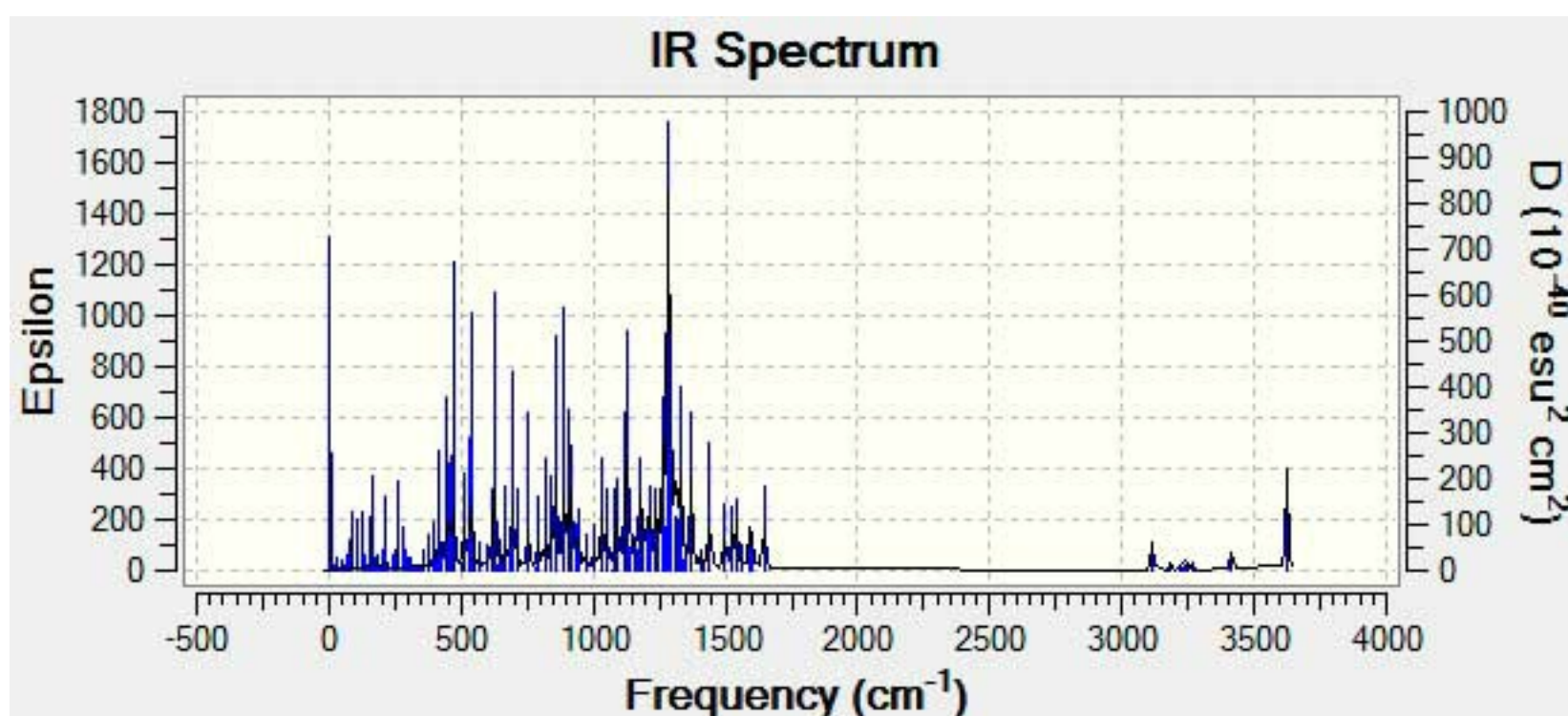
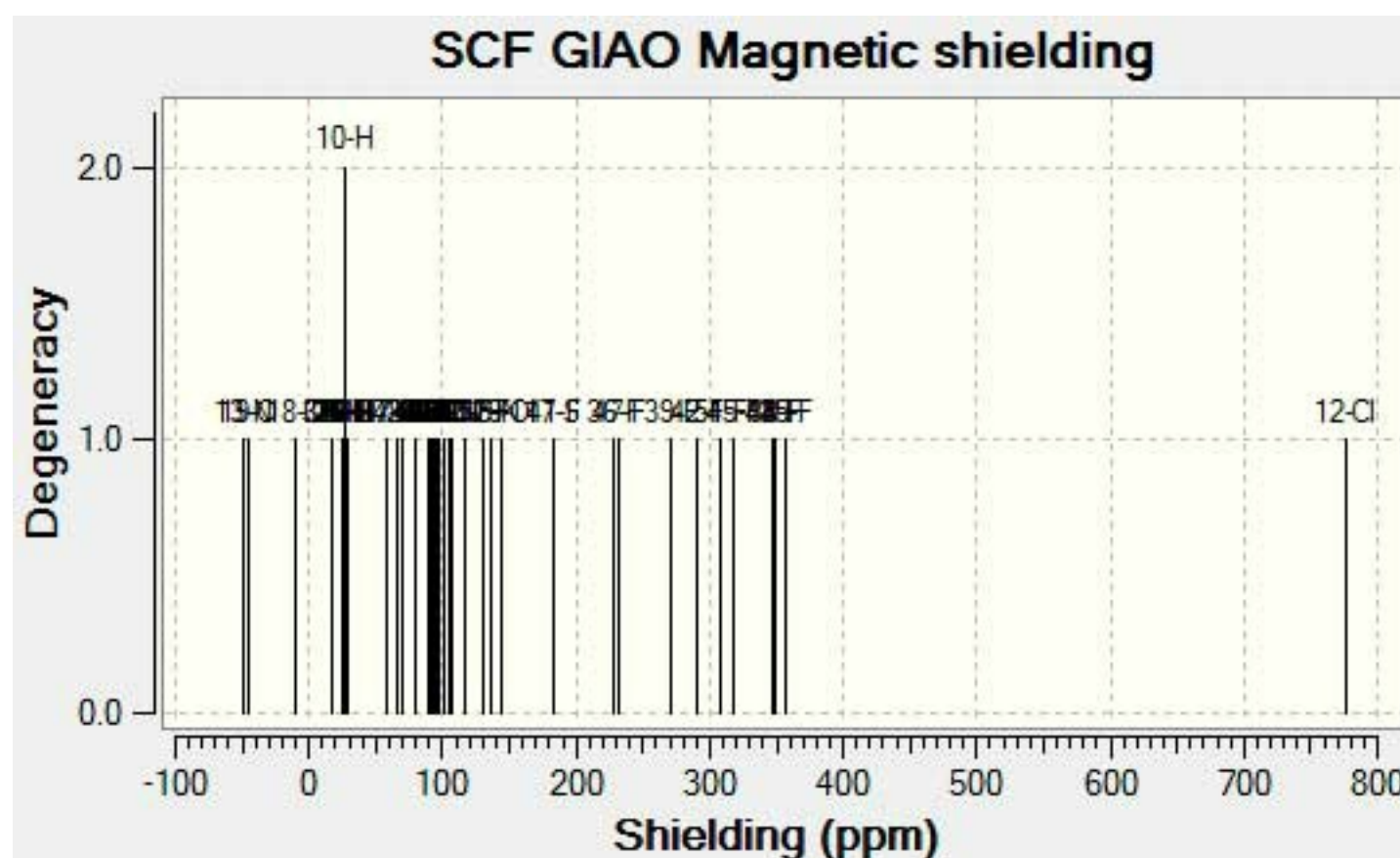Figure 4. IR spectrum for $C_{20}H_{11}F_{13}ClN_3O_3S$

NMR spectrum

Figure 5. NMR spectrum for $C_{20}H_{11}F_{13}ClN_3O_3S$

Conclusion

In this research we are interested and studied on fluorocarbon compound were chosen to theoretical studies. The optimized geometries and frequencies of the stationary point and the minimum-energy paths are calculated by using the DFT (B3LYP) methods with 3-21G basis sets. B3LYP/3-21G calculation results indicated that some selected bond length and bond angles values for the $C_{20}H_{11}F_{13}ClN_3O_3S$. The group point of compound is C_1.

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