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Vibational Spectroscopic, Molecular Structure and HOMO, LUMO Studies of Sulfanilamide by Density Functional Method

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Abstract: The molecular geometry and molecular vibrations of Sulfanilamide have been investigated with the aid of quantum chemical calculations, using functional theory (DFT/B3LYP/6-311++G(d,p)/CC-pvdz/Aug-cc-Pvdz) method. The optimized geometrical parameters obtained by all methods show good agreement with experimental X-ray data correction factors, which bring computational frequencies in closer agreement with the experimental data, which have been calculated for predominant vibrational motions of the normal modes at each level of theory. A detailed interpretation of the infrared spectra of Sulfanilamide was also reported. The calculated HOMO and LUMO energies show the occurrence of charge transfer in the molecule. The theoretical spectrogram for FTIR spectra of the title molecule has been constructed.

Introduction

Aryl and heteroarysulfonamides are an important class of therapeutic agents in current medicinal science[1,2]. Compounds comprising a sulfonamide backbone have a wide range of biological activities as antibacterial[3], anti-inflammatory[4], Hypoglcaemic[5] and anti-tumor[1] activities. Aniline and its derivatives are used in the production of dyes, pesticides and antioxidants[6,7]. In aniline, the amino group affects the planarity of the molecule and inclusion of an additional substituent group in aniline leads to further changes in the charge distribution in the molecule, and consequently affects the structural and vibrational parameters[7]. Extensive experimental[8] and theoretical investigations have been focused on elucidating the structure and normal vibrations of aniline derivatives. IR and Raman spectra of 3-chloro-4-methylaniline have been reported by Yurdakul and co-workers[9]. The infrared spectra of 2,4-dichloroaniline and 2,5-dichloroaniline have been studied by Srivastava[10] but assignments of the normal modes are not given. The infrared spectra of solid 3,4-dichloroaniline and 2,6-dichloroaniline have also been studied by Dotes *et al*[11]. Vibrational assignments based on FT-IR in the vapour, solution, liquid phases and the Raman spectra in the liquid state were reported for aniline[12]. They were also obtained in the gas phase from microwave spectroscopy[13,14] and in the solid state from X-ray crystallography[15]. Vibrational spectra of the 2,6-dibromo-4-nitroaniline and 2-(methylthio)aniline have been studied by applying the DFT calculations based on Becke3-Lee-Yang-Parr (B3LYP) level with 6-3IG* basis sets by Krishna Kumar *et al.*[16]. Honda *et al.*[17]. studied the NH stretching vibrations of aniline and its derivatives (including p-fluoroaniline) by using the IR-UV double- resonance spectroscopy. Shankar *et al.*[18]. Studied 2-chloro-6-methylaniline with polarized Raman and infrared spectra. Barluenga *et al*[19]. synthesized and studied ^{1}H and ^{13}C NMR spectra of 2-chloro-N-methylaniline. Rai *et al.*[20]. performed IR, Raman spectral measurements and DFT calculations of chlorine substituted anilines. Overtone spectra of 2-ethylaniline, N-methylaniline, N-ethylaniline, N,N-dimethylaniline and N,N-diethyl aniline have been studied in region 2500-1500 cm^{-1} by Rai *et al.*[21]. Recently, Kavitha *et al.*[22]. Studied the Raman and IR spectra and quantum chemical calculations for 4-nitroaniline. Furthermore, *ab-initio* MO-techniques are used to study the electronic properties of the sulfenamide derivatives [ArNHSR][23], and the substituents effect on the geometry energetic and relative stability was discussed.

Literature survey reveals that neither the complete Raman and IR spectra nor the quantum chemical calculations for sulfanilamide have been reported so far. The main objective of the present study is to give a complete description of the molecule geometry and molecular vibrations of title compound. For that purpose, quantum chemical computations were carried out on sulfanilamide using Density Functional Theory (DFT). Density Functional Theory calculations are reported to provide excellent vibrational frequencies of organic compounds if the calculated frequencies are scaled to compensate for the approximate treatment of electron correlation, for basis set deficiencies.

Experimental

The fine samples of sulfanilamide (Aldrich, 99.5%) was obtained and used as such for the spectral measurements. The FT-IR spectrum of this compound was recorded at room temperature in the region 400 – 4000 cm^{-1} on a Nicolet Magna 520 FT-IR spectrometer using KBr pellet technique with scanning speed of 30 cm^{-1} min^{-1} and the spectral resolution of 4.0 cm^{-1}. The observed experimental FT-IR and the theoretical predicted IR spectra at B3LYP/6-311++G(d,P), B3LYP/cc-pvdz and B3LYP/Aug-cc-pvdz are shown in Fig. 2. UV-vis spectrum was recorded on Shimadz UV-1601 PC spectrophotometer.

Method of Calculation

The optimized structure parameters of sulfanilamide calculated by Density Function Theory (DFT) levels on a personal computer using Gaussian-03 program package for Windows Molecular modeling system[24] running on a Windows XP workstation in Two 3.2 GHZ Quad-Core Intel Xeon Processors, 16-GB Memory. The optimized structural parameters were used in the vibrational frequency calculations at DFT level to characterize all stationary point as minima utilized three diferent basis set approaches namely B3LYP/6-311++G(d,P), B3LYP/cc-pvdz and B3LYP/Aug-cc-pvdz for the computation of molecular structural are listed in Table 1 in accordance with the atom numbering scheme given in Fig 1. Table 1 compares the calculated bond lengths and angles for sulfanilamide with those experimentally available data[25,26].

Results and Discussion

4-1 Molecular geometry

The gas phase optimized structure parameters of Sulfanilamide calculated by B3LYP and TDDFT methods using different basis set are listed in Table 1 in accordance with the optimized structure and atom numbering of compounds is shown in Fig 1. Since the crystal structure of this compound is not available, the optimized structure can only be compared with the other similar systems for which the structure has been optimized[25,26]. From the theoretical values, we can find that most of the optimized bond angles are slightly larger than the experimental values due to the theoretical calculations belonging to isolated molecules in gaseous phase and the experimental resultsing molecules belong to solid state. Several researchers have explained the changes in the bond length of the C-H bond for the substituent molecules, which are due to a change in the charge distribution on the carbon atom of benzene ring[27-30].

The substituent may be of the electron withdrawing type (Cl, F, Br, NO_2 *etc.*) or electron donating type (NH_2, CH_3, C_2H_5, etc). the carbon and hydrogen atoms are bonded with σ-bond in benzene ring and the substitution of SO_2NH_2 reduces the electron density at the ring carbon atom. Therefore, the substitution with the SO_2NH_2 at the para-position which shares its p electron with the ring leads to some changes of the bond lengths and bond angles in the aromatic ring. The DFT methods predict bond lengths which are systematically too long, particularly the C–H and N–H bond lengths [31].

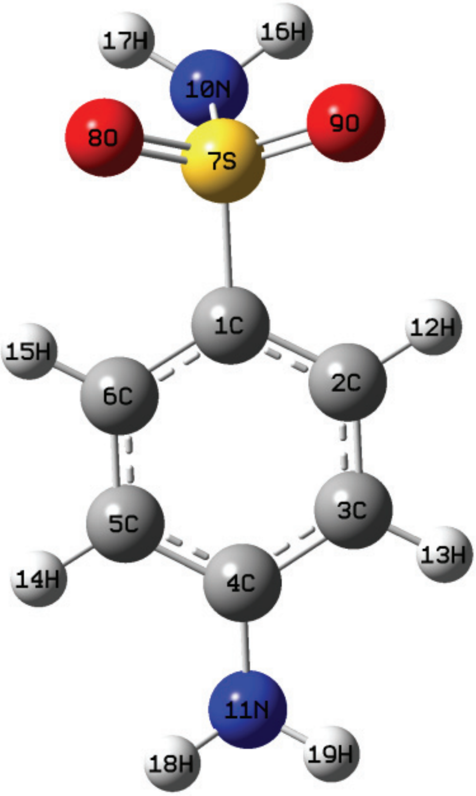


Fig. 1. Geometry of the Sulfanilamide optimized at the B3LYP/6-311++G(d,p).

Table 1. Geometrical parameters optimized in sulfanilamide molecule.

Parameters	B3LYP/6-311++G(d,P)	B3LYP/cc-pvdz	B3LYP/Aug-cc-pvdz	X-ray
Bond length				
C1-C2	1.394	1.398	1.398	1.375
C1-C6	1.395	1.398	1.398	1.386
C1-S7	1.784	1.789	1.792	1.767
C2-C3	1.386	1.390	1.391	1.391
C2-H12	1.083	1.091	1.089	0.930
C3-C4	1.406	1.412	1.410	1.397
C3-H13	1.085	1.093	1.091	0.930
C4-C5	1.406	1.412	1.410	1.377
C4-N11	1.385	1.386	1.388	1.412
C5-C6	1.386	1.390	1.391	1.390
C5-H14	1.085	1.093	1.091	0.930
C6-H15	1.083	1.091	1.089	0.930
S7-O8	1.463	1.485	1.489	1.437
S7-O9	1.463	1.485	1.489	1.434
S7-N10	1.700	1.721	1.723	1.601
N10-H16	1.015	1.024	1.019	0.870
N10-H17	1.015	1.024	1.019	0.830
N11-H18	1.008	1.014	1.010	0.960
N11-H19	1.008	1.014	1.010	0.750
Bond angle (^{o})				
C2-C1-C6	120.5	120.7	120.9	121.1
C2-C1-S7	119.8	119.6	119.5	119.8
C6-C1-S7	119.8	119.6	119.5	119.5
C1-C2-C3	119.7	119.6	119.5	119.5
C2-C3-C4	120.7	120.7	120.6	120.9
C3-C4-C5	118.7	118.7	118.9	118.9
C3-C4-N11	120.6	120.7	120.6	121.2
C4-C5-C6	120.7	120.7	120.6	119.4
C1-S7-O8	107.9	108.1	108.2	107.4
C1-S7-O9	107.8	108.1	108.2	107.7
O8-S7-O9	122.3	122.5	122.1	119.3
O8-S7-N10	106.5	106.6	106.5	106.5
O9-S7-N10	106.6	106.6	106.5	106.5
Dihedral angles (^{o})				
C2-C1-S7-O8	156.7	156.1	156.7	165.9
C2-C1-S7-O9	22.8	21.7	22.6	36.0
C2-C1-S7-N10	-90.3	-91.1	-90.4	-78.4
C6-C1-S7-O8	-23.1	-21.8	-22.6	-17.2
C6-C1-S7-O9	-156.9	-156.4	-156.8	-147.1
C6-C1-S7-N10	90.1	90.9	90.3	98.5
C2-C3-C4-N11	177.8	177.3	177.4	177.9
C5-C6-C4-N11	-177.8	-177.3	-177.4	-177.9

The large deviation from experimental C–H and N–H bond lengths may arise from the low scattering factors of hydrogen atoms in the X-ray diffraction experiment. In this study, the C-H bond lengths were calculated by B3LYP/6-311++G(d,P) method as1.083, 1.085, 1.085 and 1.083 for the ring, Table. 1. The experimental value of C–H bond lengths is 0.93A, while the value in the theoretical result is bigger than (1A). The obtained bond lengths of C=C fall in the range from 1.375 to 1.397 for Sulfanilamide molecule, these bond lengths were found in the range 1.386–1.406A, by using B3LYP/6-311++G(d,P) method. Calculated values of C=C with the three methods reported in Table 1. are longer than experimental bond lengths. As seen in Table 1, the S–N bond was predicted longer than according to the other bond lengths. Similarly, in this study, the S–O bond lengths are predicted well with experiment at all levels as reported in Table 1. The optimized parameters obtained by B3LYP methods using different basis sets are approximately similar to those observed experimentally. Substitution with the amine group and SO_2 leads to some changes of the bond angles in the aromatic ring. The C2–C1–C6 angle at the position of the SO_2 substituent and C3–C4–C5 angle at the position of the amine substituent are bigger (121.1 and 118.9^o, respectively) and the others are smaller than typical hexagonal angle of 120^o. The calculated angles of benzene ring are more reliable with experimental data than Sulfanilamide molecule.

4-2 Vibrational Analysis

The sulfanilamide molecule has 19 atoms and therefore contains 51 normal modes of vibration. Vibrational spectral assignments have been performed on the recorded FT-IR spectrum based on the theoretical predicted wavenumbers by DFT (B3LYP/6-311++G(d,p), cc-pvdz and Au-cc-pvdz). Table 2 summarizes the experimental and calculated vibrational frequencies. According to the theory, sulfanilamide has a structure C1 point group symmetry. For C1 symmetry there would not be any relevant distribution. ChemCroft[32] graphical interface, was used to assign the calculated harmonic wavenumbers using scaled displacement vectors to identify the motion of modes. Comparison of the frequencies calculated at DFT method using different basis sets with experimental values reveals agreement with calculated vibrational modes due to inclusion of electron correlation for this method. The resulting vibrational frequencies for the optimized geometries and the proposed vibrational assignment and available experimental FT-IR are given in

Table 2. The descriptions concerning the assignment have also been listed in the last column of Table 2. The calculated modes are numbering from the biggest to the smallest frequency within each fundamental wavenumbers mode numbers in the first column of the table. The calculated IR and experimental TF-IR are shown in Fig. 2 for comparative purposes, where the calculated activity and transmittance is plotted against harmonic vibrational wave numbers cm^{-1}. It should be noted that calculations were made for a free molecule in vacuum, while experimental were performed for solid sample. In this study, we have used the scaling factor values of 0.9433, 0.9511 and 0.9444 for B3LYP/6-311++G(d,p), cc-pvdz and Au-cc-pvdz respectively[29].

Table 2.Comparison of the observed and calculated vibrational spectra of sulfonamide.

No	B3LYP/6-311++G(D,P)	B3LYP/ cc-pvdz	B3LYP/Aug-cc-pvdz	Experimental	Vibrational Assignments
1	3477	3477	3478	3478	$\upsilon_{as.}$ NH_2
2	3410	3386	3389		$\upsilon_{as.}$ SO_2-NH_2
3	3381	3377	3373	3375	$\upsilon_{sy.}$ NH_2
4	3309	3285	3283	3267	$\upsilon_{sy.}$ SO_2-NH_2
5	3120	3158	3134	3121w	υ_{sy}. C-H
6	3074	3057	3034	3080w	υ_{as} C-H
7	2987	3020	3002		$\upsilon_{sy.}$ C-H
8	2986	3019	3000		$\upsilon_{as.}$ C-H
9	1637	1661	1654	1629	υsciss.NH_2 C-C
10	1544	1553	1543	1595	Sciss. SO_2-NH_2
11	1522	1545	1527	1504	υC-C
12	1496	1484	1468		υC-C (semi-circle)
13	1443	1454	1439	1440	υC-C + υC-C
14	1379	1391	1378		υC-C
15	1283	1312	1294	1314	υC-C + ωNH_2+βC-H + $\upsilon_{as}SO_2$
16	1253	1264	1247		υC-SO_2 + βC-H
17	1241	1248	1240		υC-NH_2 + βC-H
18	1233	1227	1188	1187	$\upsilon_{sy.}$S=O + ρNH_2 + ρ$NH_2(SO_2)$+βC-H
19	1137	1132	1129	1147	βC-H
20	1086	1084	1079	1096	βC-H + ρNH2
21	1058	1066	1049		βC-C-C + βC-H
22	1029	1033.	1020		ρNH_2

No	**B3LYP/6-311++G(D,P)**	**B3LYP/ cc-pvdz**	**B3LYP/Au g-cc-pvdz**	**Experimental**	**Vibrational Assignments**
23	1015	1025	1009		βC-C-C + υS=O
24	1011	1010	990		ρNH$_2$
25	963	965	954	969	Trigonal bending
26	919	925	923		γC-H
27	906	916	902	900	γC-H
28	805	834	811	836	Ring breathing+ S-N
29	790	803	794	824	γC-H
30	780	791	783		γC-H
31	772	782	773		γC-H
32	701	689	684	685	γC-H
33	618	649	631	626	ωNH_2
34	611	616	608		ωSO$_2$ NH_2
35	605	613	607	563	βNH$_2$(SO$_2$)
36	513	517	502	540	βSO$_2$+ C-C-C
37	505	502	490		βSO$_2$+ C-C-C + ω2NH$_2$ + ωSO$_2$
38	452	468	433		ω2NH$_2$ + βO=S=O
39	436	435	419		γC-H + ωNH$_2$
40	424	420	414		tC-N +tC-S
41	395	399	396		γC-C-C
42	365	360	352		γC-NH$_2$ +γS-NH$_2$
43	330	332	329		υS-NH2+ωNH$_2$ + ωSO$_2$
44	326	326	324		tNH$_2$ + tSO$_2$
45	318	313	309		ρNH$_2$ +ρNH$_2$(SO$_2$) + tSO$_2$
46	265	265	261		βC-NH$_2$ + βC-SO$_2$
47	193	193	190		ωNH$_2$ +υS-NH$_2$
48	157	155	155		ρNH2 +τSO$_2$ +τNH$_2$
49	103	83	106		τNH$_2$
50	81	81	81		ωSO$_2$ + ωNH$_2$ + υS-NH$_2$
51	11	-40	19		tNH$_2$ + tSO$_2$

υ: stretching ; υ_{sy}: Symmetric stretching; υ_{as}: asymmetric stretching; β: in-plane bending; γ: out of plane bending; ρ: rocking.

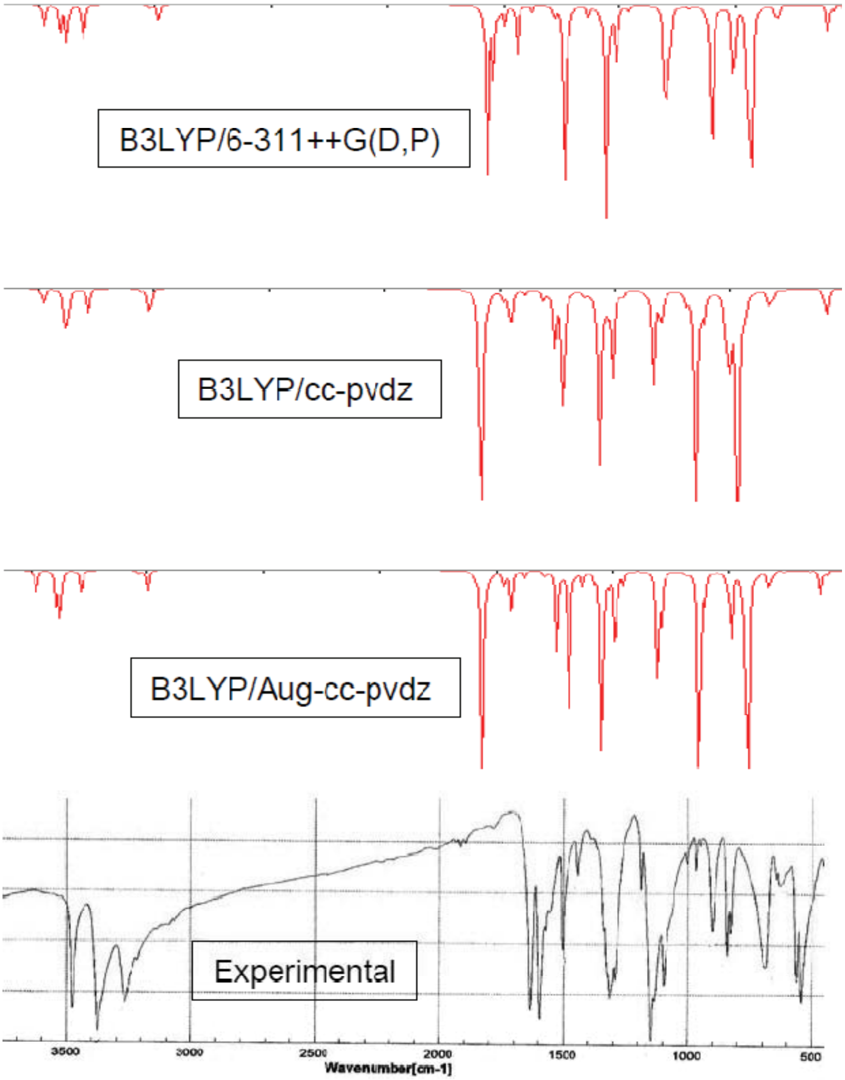


Fig. 2. Experimental and calculated IR spectra of the sulfanilamide.

The modes related to the NH_2 group have been extensively investigated and analyzed[33-35]. The fundamental modes involving the amino group are stretching and bending of N-H bond, torsion and inversion. The title compound under investigation possesses two NH_2 groups and hence we expect two asymmetric N-H and two symmetric N-H stretching vibrations. It is stated that the N-H stretching vibrations occur in the region 3500- 3300 (cm^{-1})[36]. Honda *et al.*[17] in their studies of the jet-cooled neutral molecules of aniline, the asymmetric and symmetric NH_2 stretching vibrations were assigned the bands at 3508 and 3412 cm^{-1} respectively, while in *p*-fluroaniline, the corresponding bands were observed at lower frequencies, 3499 and 3414 (cm^{-1})[17,37]. Alvareza[38,39] assigned two strong bands in the IR spectrum of the liquid sulfamoil fluoride and sulfamoil chloride substances at 3418 cm^{-1} , 3312 cm^{-1} and 3386 cm^{-1}, 3282 cm^{-1}. They were assigned to the NH_2 antisymmetric and symmetric fundamental stretching modes, respectively. The asymmetric stretching mode appears to be calculated at the higher wavenumber 3477cm^{-1} than the symmetric mode 3381cm^{-1} at B3LYP/6-331++G(d,p) method, mode 1 and 3, Table 2. In the FT-IR spectrum the asymmetric and symmetric NH_2 stretching vibrations were assigned to the bands at 3478 cm^{-1} and 3375 cm^{-1} respectively. On the other hand the vibrational frequencies described by modes 2 and 4 assigned to the N-H symmetric and asymmetric stretching modes, respectively for NH_2 related to SO_2 (SO_2-NH_2). According to our calculations the SO_2-NH_2 antsymmetrical and symmetrical stretching modes are positioned at 3410 $cm^{-1}$and 3309 cm^{-1} respectively by B3LYP/6-311++G(d, p) method having mode nos 2 and 4 Table 2. In this study, for both NH_2 asymmetric and symmetric modes FT-IR are in agreement with the calculated values.

In addition, the two NH_2 groups have scissoring deformation (δ NH_2), rocking deformation (ρ NH_2), wagging deformation (ω NH_2) and torsion deformation (τ NH_2) modes. The internal deformation vibrations known as NH_2 scissoring frequency mode obtained at 1637 cm^{-1} by B3LYP/6-311++G(d, p) method having mode well within the range (1650-1590 cm^{-1}) reported for aniline by Jesson Thompson[40] and this observation is conforming with the experimental value of 1629 cm^{-1} in FT-IR spectrum vibrational mode 9. The vibrational mode 10 identified with SO_2NH_2 scissoring is also in good agreement with literature values[26,41,42]. The rocking mode predicted at 1086 cm^{-1} by B3LYP/6-311++G(d, p) method also shows very good agreement with experimental observation at 1096 cm^{-1} in TF-IR. The NH_2 wagging mode has been identified with the frequency at 626 cm^{-1} and this is in excellent agreement with the calculated values at mode No. 33, Table 2. The calculated frequency of the SO-NH_2 wagging vibration in mode 34 is supported by the experimental data, reported in literature values.[26,41] Likewise the twisting vibration (mode 49) is also in good agreement with literature values[43-49]. Silverstein *et al.*[43] assigned C-N stretching absorption in the region 1382-1266 cm-1 for aromatic amine. The C-N stretching is observed at 1293 (cm^{-1})[50]. Hence the bands at 1240-1248 cm^{-1} (mode 17) are assigned to C-N stretching vibration. After scaled down computed value of C-N stretching vibration also 1315-1312 cm^{-1} which is nearer to the observed value.

The hetero aromatic structure shows the presence of C–H stretching vibrations in the region 3000–3100 (cm^{-1}) which is the characteristic region for the ready identification of C–H stretching vibrations.[43-45] In this region, the bands are not affected, appreciably by the nature of the substituent. The sulfonamide has two adjacent aromatic C-H units. The C2-H, C3-H, C5-H and C6-H stretching vibration corresponds to mode 5, 6, 7 and 8, Table 2. In region 3120-2986 cm^{-1} by B3LYP/6-311++G(d,p) method shows excellent agreement with the experimental FT-IR spectrum at 3121cm^{-1} and 3080 cm^{-1}. The theoretically computed by other two methods also falls in the same region.

The in-plane aromatic C–H bending modes vibrations occur in the region 1000- 1300 cm^{-1}. The bands are sharp but are weak to medium intensity. The C–H in-plane bending vibration computed at 1253, 1241 and 1233 cm^{-1} (modes 16, 17 and 18) even though found to be contaminated by C-SO_2 and SO_2 stretching vibration are in the range found in the literature[46,47] , while the experimental observations at 1314, 1387, 1147 and 1096 cm^{-1} in FT-IR shows excellent agreement with theoretical values.

The C-H out of plane deformation modes of benzene 33, 34 are expected to occur in the region 600-1000cm^{-1}. In general the aromatic C-H vibration (stretching, in-plane and out-of-plane bending) at (mode nos. 26, 27, 29, 30, 31 and 32) calculated theoretically in different computed methods show excellent agreement with experimental values.

The symmetric and asymmetric SO_2 stretching vibrations occur in the region 1150-1125 and 1330-1295 ($cm^{-}1$)[48]. The signals appearing at 1418 and 1217 cm^{-1} can be attributed to the SO_2 antisymmetric and symmetric stretching fundamental modes respectively for sulfamoil fluoride substance[38]. For sulfanilamide asymmetric S=O stretching vibration recorded at 1314 cm^{-1} and the symmetric S=O vibration at 1187 cm^{-1}. The calculated frequencies for asymmetric vibration with

B3LYP/cc-pvdz method excellent agreement with observed values 1312 cm^{-1} (mode 15) Table 2. While B3LYP/6-311++G(d,p) and B3LYP/Aug-cc-pvdz methods estimates are lower than the typical values given in experimental study. Vibration at (mode no. 38) is assigned O=S=O bending modes.

At 836 cm^{-1} in the FT-IR spectrum the S-N stretching fundamental mode can be observed. The calculation for stretching frequencies vibration with B3LYP/cc-pvdz method also shows excellent agreement with observed value 834 cm^{-1} (mode no. 28).

The ring stretching vibrations are very much important in the spectrum of benzene and its derivatives and are highly characteristic of the aromatic ring itself. Varsanyi[45] observed five bands, 1625-1590, 1590-1575, 1540-1470, 1465-1430 and 1380-1280 cm-1. In the present work, the vibrations frequencies observed in the FT-IR spectrum at 1633, 1504 and 1440 cm^{-1} are assigned to C-C stretching vibrations. The theoretically calculated is in good agreement with xperimental observation. The ring breathing mode assigned by using ChemCraft program is well within the range 834-805 cm^{-1} (mode 28). The in-plane deformation vibration (βC-C-C) seems to be higher frequencies (modes 21 and 23) than the out-of-plane (γC-C-C) vibration (modes 37 and 41).

Absorption maxima (λ_{max}) of Sulfanilamide compound were calculated by the TD-B3LYP/6-311++G(d,p), TD-B3LYP/cc-pvdz and TD-B3LYP/Aug-cc-pvdz methods. The observed and calculated visible absorption maxima of Sulfanilamide in this study are given in Table 3. In Fig. 3, the Experimental UV–vis spectrum of Sulfanilamide was measured in chloroform solution, and it was found that the absorption bands maximized at 262.5 and 206.5 nm.

4-3 Absorption Spectra

Calculations of molecular orbital geometry show that the visible absorption maxima of sulfanilamide correspond to the electron transition from HOMO to LUMO. The λ_{max} is a function of the electron availability. The electron absorption was due to electronic transition from the ground to the first excited state, and mainly described by one electron excitation from the highest occupied molecular orbital (HOMO) to the lowest unoccupied orbital (LUMO). Figure. 4 illustrates the calculated spatial distributions of the HOMO and LUMO levels of the studied compound. As can be seen clearly, HOMO is a π orbital concentrated on the hole molecule and lone pair of electron on the O and π orbital of S=O atoms and N atom for both NH_2 groups; LUMO is of antibonding character with π*character distributed on the benzene ring.

Table 3. Experimental and theoretical electronic absorption spectra values.

Experimental	Calculated/λ_{cal} (nm)					
262.5, 206.5	B3LYP/6-311++G(d,p)		B3LYP/cc-pvdz		B3LYP/Aug-cc-pvdz	
	Wave length	Oscillator strength	Wave length	Oscillator strength	Wave length	Oscillator strength
	269.4	0.020	260.2	0.023	268.0	0.017
	258.6	0.010	236.5	0.321	255.4	0.054
	249.3	0.298	203.2	0.001	247.0	0.267

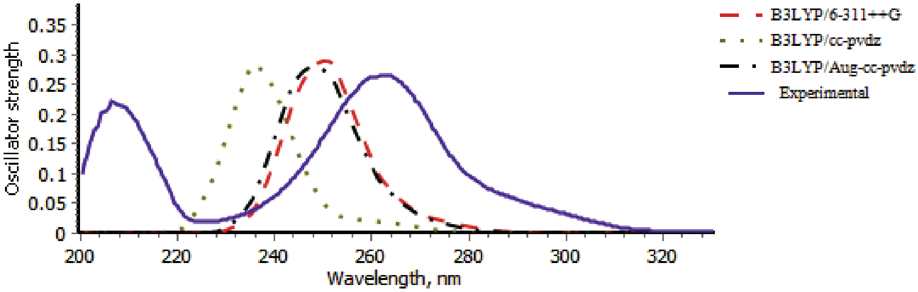
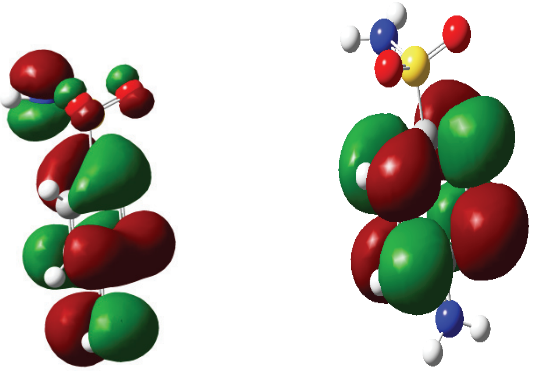


Fig. 3. Electronic absorption spectrum of sulfonamide with TD-DFT calculated transitions.



HOMO LUMO

Fig. 4. Contours of HOMO and LUMO orbitals of studied compounds.

The HOMO-LUMO energy gap of sulfanilamide was calculated by the methods were listed in Table 4, which reveal that the energy gap reflects the chemical activity of the molecule, HOMO as an electron donator and LUMO as an electron acceptor. The lower in the energy gap value of HOMO-LUMO orbital illustrated the eventual charge transfer interaction taking place within the molecule, moreover the calculated self-consistent field (SCF) energy of sulfanilamide is (-891.70725 a.u).

Table 4. HOMO-LUMO energy gap values calculated.

Parameters	B3LYP/6-311++G(d,p)	B3LYP/cc-pvdz	B3LYP/Aug-cc-pvdz
HOMO	-0.22811	-0.22091	-0.22659
LUMO	-0.03479	-0.01929	-0.03351
LUMO-HOMO	-0.19332	-0.29638	-0.21219

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دراسة الأطياف الاهتزازية، والتركيب الجزيئي، والمدارات الإلكترونية لمركب السلفونيلاميد باستخدام طريقة الكثافة الوظيفية الكمية

عبدالله بن غدران مطر السهيمي

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أبها – المملكة العربية السعودية

المستخلص. تمت دراسة التركيب الهندسي الجزيئي والأطياف الاهتزازية الجزيئية لمركب السلفونيلاميد باستخدام الطرق الكمية النظرية التالية: (DFT/B3LYP/6-311++G(d,p)/CC-pvdz/Aug-cc-Pvdz) وقد اتضح من تحليل بيانات الأشكال الهندسية في الحالة الدنيا وجود توافق كبير مع الدراسة العملية. كما وجد عند استخدام عوامل تصحيح (Correction factors) مناسبة تقارب إلى حد كبير بين النتائج النظرية والتجريبية التي تم حسابها لطيف الأشعة تحت الحمراء، ظهر ذلك عن طريق متابعة حركة الذبذبات المسيطرة في الأوضاع العادية لكل مستويات الطاقة الاهتزازية. كذلك تم حساب طاقة المدارات الإلكترونية للمركب تحت الدراسة باستخدام أعلى مدار ممتلئ (HOMO)، وكذلك أقل مدار فارغ (LUMO) وظهر من نتائج هذه الدراسة حصول انتقال للشحنة في هذا المركب.