FT-IR and Computational Study of Sulphaguanidine

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ABSTRACT

The vibrational wavenumbers of sulphaguanidine were calculated using Gaussian03 software at different levels and compared with experimentally observed data. The predicted infrared intensities, Raman activities and first hyperpolarizability are reported. The calculated geometrical parameters (DFT) are in agreement with that of similar derivatives. The potential energy scan studies for different torsion angles are also reported. The splitting of NH stretching wavenumber in the infrared spectrum indicates the weakening of the NH bond.

Key words: FT-IR, Computation, Sulphaguanidine.

INTRODUCTION

Sulfonamides form a significant class of compounds in medicinal and pharmaceutical chemistry with several biological applications[1-4]. There has been growing interest in using organic materials for nonlinear optical (NLO) devices, functioning as second harmonic generators, frequency converters, electro-optical modulators, etc. because of the large second order electric susceptibilities of organic materials. The organic compound showing high hyperpolarizability are those containing an electron-donating group and an electron withdrawing group interacting through a system of conjugated double bonds. In the case of sulfonamides, the electron withdrawing group is the sulfonyl group[5]. To our knowledge, no theoretical HF or density functional theory (DFT) calculations, or detailed vibrational infrared analyses, have been performed on the title compound.

EXPERIMENTAL

All the chemicals were procured from Sigma-Aldrich, USA. The FT-IR spectrum was recorded using a Bruker IFS 28 spectrometer in KBr pellets, number of scans 16, resolution 2 cm^{-1}.

Computational details

Calculations of the title compound were

carried out with Gaussian03 software program[6] using the HF/6-31G* and B3LYP/6-31G* basis sets to predict the molecular structure and vibrational wavenumbers. The DFT hybrid B3LYP functional tends also to overestimate the fundamental modes; therefore scaling factors have to be used for obtaining a considerably better agreement with experimental data. Therefore, a scaling factor of 0.9613 and 0.8929 were uniformly applied to the DFT and HF calculated wavenumbers[7]. Potential energy surface scan studies have been carried out to understand the stability of planar and non-planar structures of the molecule. The profiles of potential energy surface for torsion angles $N_{20}-C_{19}-N_{17}-S_{14}$, $N_{22}-C_{19}-N_{17}-S_{14}$ and $C_{19}-N_{17}-S_{14}-C_3$ are calculated. The energy is minimum for -143.5° (-1040.33670), 38.4° (-1040.33511) and -172.8° (-1040.33577 Hartree) for the above torsion angles. The assignment of the calculated wavenumbers is aided by the animation option of MOLEKEL program, which gives a visual presentation of the vibrational modes[8,9].

RESULTS AND DISCUSSION

The observed IR bands with their relative intensities and calculated (scaled) wavenumbers and assignments are given in Table 1. The anti-symmetric and symmetric stretching modes of SO_2 group appear in the region 1360-1310 and 1165-1135 cm^{-1}, respectively[10]. The observed bands at

1305, 1130 cm^{-1} in the IR spectrum were assigned to the SO_2 stretching modes. The DFT calculations give the anti-symmetric and symmetric stretching modes at 1314, 1135 cm^{-1}. Although the region of the SO_2 scissors (560 ± 40 cm^{-1}) and that of SO_2 wagging vibration (500 ± 55 cm^{-1}) partly overlap, the two vibrations appear separately[10]. The scissoring mode is observed at 555 cm^{-1} in the IR spectrum. The wagging mode is observed at 511 cm^{-1} in the IR spectrum. The DFT calculations give these modes at 538 and 508 cm^{-1}. Hangen *et al.*[11] reported the SO_2 stretching vibrations at 1314, 1308, 1274, 1157, 1147, 1133 cm^{-1} and SN stretching modes at 917, 920, 932, 948 cm^{-1} for sulfonamide derivatives. Chohan *et al.*[12] reported SO_2 stretching modes at 1345, 1110 cm^{-1} and SN and CS stretching modes at 833 cm^{-1} for sulfonamide derivatives. The twisting SO_2 mode is expected[10] in the region 440 ± 50 cm^{-1} and the rocking mode at around 350 cm^{-1}. For the title compound, the band observed at 412 cm^{-1} in the IR spectrum is assigned as the twisting mode of SO_2 moiety. The DFT calculations give these modes at 416 and 399 cm^{-1}. Rodriguez *et al.*[13] reported the SO_2 bands in the range 1242-1394, 590-632 and 460-470 cm^{-1}. The SN stretching vibration[10] is expected in the region 905 ± 30 cm^{-1}. The band calculated at 830 cm^{-1} is assigned as SN stretching mode and the band at 849 cm^{-1} in the IR spectrum is assigned as this mode. The C-S stretching mode is observed at 658 cm^{-1} (DFT)[10].
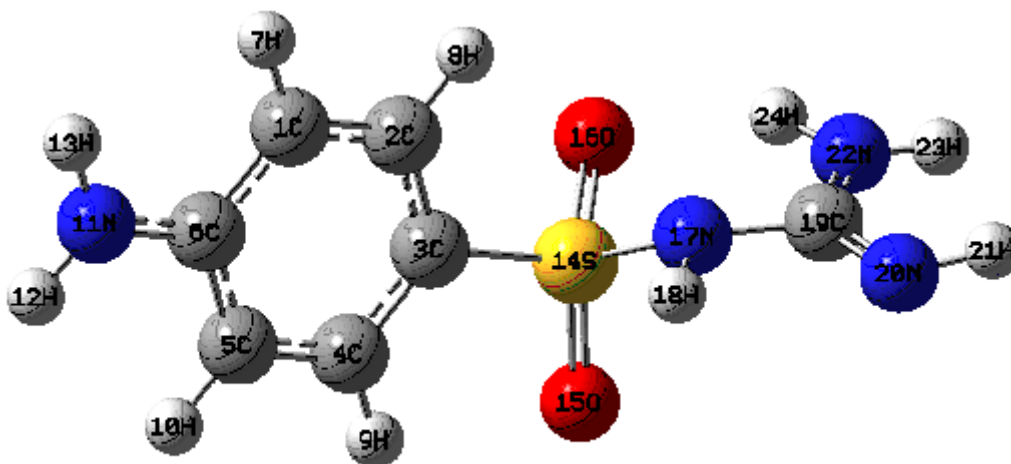
**Table 1: Calculated vibrational wavenumbers (scaled),
measured infrared band positions and assignments**

HF/6-31G*			B3LYP/6-31G*			$\upsilon_{(IR)}$ (cm^{-1})	Assignments
υ (cm^{-1})	IR Intensity	Raman Activity	υ (cm^{-1})	IR Intensity	Raman Activity		
3568	44.72	60.76	3617	27.03	74.80		$\upsilon_{as}NH_2$
3543	99.63	58.03	3585	66.34	84.90		$\upsilon_{as}NH_2$
3450	104.88	184.30	3497	99.88	268.15	3496 s	υ_sNH_2
3429	87.24	34.56	3407	44.79	52.82	3438 s	υ_sNH_2
3381	118.79	99.42	3357	119.39	200.96	3388 s	υNH
3364	16.32	243.51	3340	11.19	355.37	3346 s, 3215 m	υNH
3044	7.14	78.40	3116	3.44	80.53		υCH
3039	1.86	62.50	3113	7.18	55.44		υCH
3015	11.45	84.85	3082	14.13	110.37		υCH
3014	11.19	81.51	3081	13.38	96.72		υCH
1681	563.53	23.40	1659	306.24	70.27		υCN
1661	167.54	10.96	1649	146.95	18.39		δNH_2
1655	239.81	20.12	1642	229.57	51.47	1620 s	δNH_2
1599	251.27	112.49	1593	219.96	97.04	1572 m	υPh
1579	22.87	1.90	1568	7.54	1.07	1534 s	υPh
1505	139.84	1.52	1496	70.25	13.79	1492 m	υPh
1437	10.11	0.58	1431	5.69	0.62	1434 w	υPh
1411	275.69	2.19	1394	163.13	23.02		δNH
1365	67.23	4.37	1348	1.18	0.57		δNH
1333	9.29	0.70	1321	94.38	2.52		$\upsilon Ph, \delta CH$
1300	152.82	11.46	1314	20.27	1.21	1305 w	$\upsilon_{as}SO_2$
1253	2.68	0.29	1285	75.74	11.24	1236 s	$\upsilon C_6\text{-}N_{11}$
1188	69.54	4.45	1187	51.30	3.45	1176 s	$\rho NH_2, dCH$
1130	6.34	0.37	1135	9.48	1.14	1130 s	υ_sSO_2
1124	17.94	5.68	1111	14.92	12.70	1086 s	$\upsilon NH_2, \delta CH$
1084	277.03	7.94	1050	39.32	17.81	1050 s	$\upsilon C_{19}\text{-}N_{17}$
1062	62.78	27.06	1047	265.07	37.39		$\upsilon C_{19}\text{-}N_{22}$
1047	3.62	1.40	1027	1.68	0.18		δCH
1033	2.07	0.15	992	5.13	10.28	1010 w	γCH
1024	5.44	0.52	973	0.07	0.20	964 w	δSNC
998	3.48	3.78	946	1.27	0.17	941 w	γCH
965	139.32	8.60	918	106.70	25.93		γCH
873	136.53	1.05	900	63.60	5.55		$\delta Ph(X)$
851	3.69	3.39	830	41.17	1.68	849 w	υSN
832	21.18	15.70	820	77.02	16.44	823 s	Ring breathing
810	5.71	24.97	811	17.33	19.57	810 s	γCH
802	73.79	7.32	807	20.43	4.28		γCH
786	229.22	9.49	769	61.61	18.34		ωNH_2
749	133.37	8.64	731	170.92	62.87	747 w	ωNH_2
735	16.28	1.21	703	2.70	1.98		$\delta Ph(X)$
679	26.63	12.39	689	44.05	33.06	687 s	γPh
653	173.70	1.73	658	183.66	12.91		υCS
638	0.32	6.31	634	0.86	4.81		γNH

Table 1: Cont.

616	27.10	7.54	617	28.48	7.05	604 s	γNH
563	37.04	20.86	538	39.69	64.53	555 s	δSO$_2$
540	39.39	0.79	524	83.61	0.99	542s	δPh
526	159.86	1.81	508	79.71	2.09	511 w	ωSO$_2$
486	407.94	6.72	464	282.26	26.97	463 w	γPh(X)
468	207.88	1.77	442	230.46	4.70		δPh(X)
443	29.27	4.17	426	70.48	9.52		γPh
425	1.30	0.20	416	1.99	1.14	412 w	τSO$_2$
410	2.20	2.13	407	11.70	3.41		δCX(X)
385	12.53	6.62	401	0.48	2.04		δCX(X)
377	0.26	1.86	399	9.02	8.38		ρSO$_2$
351	9.52	4.76	340	10.41	10.82		ρNH$_2$
332	4.92	2.57	307	5.10	30.45		ρNH$_2$
288	22.40	6.41	285	9.22	11.57		γCX(X)
262	3.50	2.22	246	5.01	9.35		δCNS
241	46.89	6.69	238	30.01	7.56		γCNS
222	2.79	6.90	215	1.43	13.32		γCX(X)
149	1.84	0.57	144	3.71	0.59		δNC=N
140	2.93	2.74	136	0.49	3.81		tNH$_2$
91	1.28	2.60	92	0.43	3.12		tNH$_2$
60	3.17	4.31	58	3.23	2.77		tNCNH$_2$
51	2.16	5.21	51	2.00	9.48		tPh
30	0.52	9.66	28	0.35	11.60		tSO$_2$

υ-stretching, δ-in-plane bending, γ-out-of-plane bending, τ-twist, t- torsion; Ph-phenyl ring; X-substituent sensitive; subscripts; as, asymmetric; s, symmetric.

The N-H stretching vibrations generally give rise to bands[14,15] at 3500-3300 cm^{-1}. The NH stretching bands are observed at 3388, 3346 cm^{-1} in the IR spectrum and at 33357, 3340 cm^{-1} (DFT) theoretically. In the present study, the NH stretching band has split into a doublet, 3346 and 3215 cm^{-1} in the IR spectrum owing to the Davydov coupling between neighboring units. A similar type of splitting observed in acetanilide[16,17] and N-methylacetamide[18] in the stretching band is attributed to the Davydov splitting. The splitting of about 131 cm^{-1} in the IR spectrum is due to strong intermolecular hydrogen bonding. Furthermore, the N-H stretching wavenumbers are red shifted by 125 cm^{-1} in the IR spectrum with a strong intensity from the computed wavenumbers, which indicates the weakening of the N-H bond[19]. In N-monosubstituted amides, the in-plane bending frequency and the resonance stiffened C-N band stretching frequency fall close together and therefore interact. The NH deformation band of guanidine structural motif is expected in the region[10,20] 1395 ± 25 cm^{-1}. The DFT calculations give this modes at 1394 and 1348 cm^{-1}. The out-of-plane NH deformation is expected in the region[10] 650 ± 50 cm^{-1} and bands at 634 and 617 cm^{-1} (DFT) are assigned as this mode. Wang and Ma[21] reported NH stretching bands in the region, 3365-3374 cm^{-1} and guanidine C=N stretching bands in the region 1598-1638 cm^{-1}. According to Henry *et al.*[22] IR spectrum exhibits typical features for Schiff base possessing several bands of υNH vibration with maxima in the range 3380-3270 cm^{-1} and bands due to υC=N at 1635 cm^{-1}. The C=N stretching skeletal bands[23-25] were observed in the range 1627-1566 cm^{-1}. DFT calculations give the υC=N mode at 1649 cm^{-1}. The C-N stretching vibration[10] is moderately to strongly active in the region 1275 ± 55 cm^{-1}. Primary aromatic amines with nitrogen directly on the ring absorb at 1330-1200 cm^{-1} because of the stretching of the phenyl C-N bond[20]. For the title compound, the C_6-N_{11} stretching mode is observed at 1236 cm^{-1} in the IR spectrum and at 1285 cm^{-1} theoretically. Panicker *et al.*[26] reported CN stretching mode at 1219, 1237 (IR), 1222 (Raman)

and at 1292, 1234, 1200 cm^{-1} theoretically. The CN stretching modes C_{19}-N_{17} and C_{19}-N_{22} are assigned at 1050, 1047 cm^{-1} theoretically, and at 1050 cm^{-1} in the IR spectrum, which is expected[10] in the range 950-1115 cm^{-1}. Fanchiang and Tseng[27] reported CN stretching modes at 1037 and 1120 cm^{-1}.

The NH_2 stretching modes of guanidine[10] are expected in the region 3260-3390 cm^{-1} and in the present case bands observed at 3496, 3438 cm^{-1} in the IR spectrum and bands at 3617, 3585, 3497, 3407 cm^{-1} (DFT) are assigned as NH_2 stretching modes. Topacli and Topacli[28] reported the calculated wavenumbers in the range 3670-3920 cm^{-1} for NH_2 stretching modes. The bands corresponding to the δNH_2 vibrations[10] are expected in the region 1610 ± 30 cm^{-1}. In the IR spectrum δNH_2 is observed at 1620 cm^{-1}. The calculated value are 1649, 1642 cm^{-1}. The rocking/twisting mode of NH_2 is expected in the region 1195 ± 90 cm^{-1} and the DFT calculations give this mode at 1187 and 1111 cm^{-1}. Experimentally, bands are observed at 1176 and 1111 in the IR spectrum. The wagging mode of NH_2 is expected[10] in the range 840 ± 55 cm^{-1} and is observed at 747 cm^{-1} in the IR spectrum. The DFT calculations give these modes at 769 and 731 cm^{-1}. The torsion NH_2 mode is expected in the range 355 ± 65 cm^{-1} and the bands at 340, 307 cm^{-1} (DFT) are assigned as this mode. For sulfonamide derivatives, the NH_2 modes are reported at[29] 3390, 3395, 3399 cm^{-1} and NH modes at 3253, 3230, 3255 cm^{-1}.

The aromatic CH stretching vibrations[10] absorb weakly to moderately between 3120-3000 cm^{-1}. The B3LYP calculations give bands in the range 3081-3116 cm^{-1} as δCH stretching modes. Experimentally, no bands are observed. The benzene ring possesses six ring stretching vibrations of which the four with the highest wavenumbers occurring near 1600, 1580, 1490 and 1440 cm^{-1} are good group vibrations[10]. The fifth ring stretching vibration is active near 1315 ± 65 cm^{-1}, a region that overlaps strongly with that of the CH in-plane deformation[10]. The sixth ring stretching vibration, the ring breathing mode, appears as a weak band near 1000 cm^{-1} in mono-, 1,3-di, and 1,3,5-trisubstituted benzenes. In the otherwise substituted benzenes, however, this vibration is substituent sensitive and difficult to distinguish from other modes. The ring breathing mode for the para-substituted benzenes with entirely different substituents[30] has been reported to be strongly IR active with typical bands in the interval 780-840 cm^{-1}. For the title compound, this is confirmed by the band in the IR spectrum at 823 cm^{-1}, which finds support from the computational results (820 cm^{-1} by DFT). The ring breathing mode of para-substituted benzenes are reported at 804 and 792 cm^{-1} experimentally and at 782 and 795 cm^{-1} theoretically[31,32]. For the title compound, the phenyl ring stretching modes are observed at 1572, 1534, 1492, 1434 cm^{-1} in the IR spectrum and at 1593, 1568, 1496, 1431, 1321 cm^{-1} theoretically. For para-substituted benzenes, the δCH modes[10] are seen in the range 995-1315 cm^{-1} and in the present case the bands observed at 1176, 1086 cm^{-1} in the IR spectrum and at 1321, 1187, 1111, 1027 cm^{-1} (B3LYP) are assigned as these modes. The CH out-of-plane deformations[10] are observed between 1000 and 700 cm^{-1}. Generally, the CH out-of-plane deformations with the highest wavenumbers are weaker than those absorbing at lower wavenumbers. These γCH modes are observed at 1010, 941 cm^{-1} in the IR spectrum and at 992, 946, 811, 807 cm^{-1} theoretically. The strong CH out-of-plane deformation band occurring at 840 ±50 cm^{-1} is typical for 1,4-di-substituted benzenes[10]. For the title compound, a band is observed at 810 cm^{-1} in the IR spectrum. Again according to literature[10,20] a lower $\bar{a}$CH absorbs in the neighborhood 820 ± 45 cm^{-1}, but is much weaker or infrared inactive. The DFT calculations give a γCH at 807 cm^{-1} and no band is experimentally observed for this mode. The substituent sensitive modes of the phenyl ring are also identified and assigned.

The geometrical parameters given by the theoretical results obtained are almost comparable with the reported structural parameters of similar derivatives. For benzene sulfonamide derivatives, Loughrey *et al.*[33] reported the bond lengths, S_{14}-O_{15}=1.4337, S_{14}-O_{16}=1.4256, S_{14}-N_{17}=1.6051, S_{14}-C_3=1.7737, C_6-N_{11}=1.4212Å, whereas the corresponding values in the present case are, 1.6376, 1.6482, 1.8364, 1.8463, 1.3747Å. For the title compound the DFT calculations give the bond angles C_3-S_{14}-O_{15}=108.1, C_3-S_{14}-O_{16}=111.6, S_{14}-N_{17}-H_{18}=111.8, O_{15}-S_{14}-O_{16}=118.3, O_{15}-S_{14}-N_{17}=114.3, O_{16}-S_{14}-N_{17}= 104.0, N_{17}-S_{14}-C_3=98.9, C_6-N_{11}-

$H_{12,13}$=121.1, 121.2, S_{14}-C_3-C_4=118.1, S_{14}-C_3-C_2=119.4, C_4-C_3-C_2=122.5, C_3-C_4-C_5=118.7, C_4-C_5-C_6=120.6, C_5-C_6-C_1=119.0, N_{11}-C_6-C_1=120.5, N_{11}-C_6-C_5=120.6, C_6-C_1-C_2=120.6°. The corresponding reported values are 106.5, 107.4, 110.0, 119.5, 106.1, 107.7, 109.3, 118.8, 120.5, 119.1, 120.4, 119.9, 120.3, 119.3, 122.4, 118.2, 120.4°[33]. Loughrey *et al.*[33] reported the torsion angles O_{15}-S_{14}-C_3-C_4, O_{15}-S_{14}-C_3-C_2, O_{16}-S_{14}-C_3-C_4, O_{16}-S_{14}-C_3-C_2, N_{17}-S_{14}-C_3-C_4, N_{17}-S_{14}-C_3-C_2, S_{14}-C_3-C_4-C_5, C_2-C_3-C_4-C_5, S_{14}-C_3-C_2-C_1, C_4-C_5-C_6-N_{11}, N_{11}-C_6-C_1-C_2, as -142.0, 38.5, -12.8, 167.7, 103.8, -75.7, 143.9, -39.2, 177.6, -179.9, -0.4, 179.2, 178.1, -178.6, whereas the corresponding values for the title compound are, -0.0, -177.0, 131.7, -46.0, -119.3, 63.1, -178.8, -1.2, 178.8, -180.0, -180.0°. Petrov *et al.*,[34] reported the molecular structure and conformations of benzenesulfonamide by gas electron diffraction and quantum chemical calculations and according to their results, the bond lengths, CS, SN, SO vary in the range 1.7756-1.793, 1.663-1.6925, 1.4284-1.445Å, the bond angles, CSN, CSO, NSO, HNS, HNH, vary in the range, 103.9-107.1, 107.6-107.8, 105.5-107.7, 111-113.7, 112.6-113.6°. These values are in agreement with the corresponding values for the title compound. Labisbal *et al.*[35] reported the bond lengths, SO=1.4269-1429, SN=1.6202, SC=1.7582, N_{22}-C_{19}=1.4103, N_{20}-C_{19}=1.2723, N_{17}-C_{19}=1.3483Å whereas the corresponding values for the title compound are 1.6376-1.6482, 1.8364, 1.8463, 1.3688, 1.2924, 1.4238Å. The values of bond angles O_{15}-S_{14}-O_{16}=118.6, O_{16}-S_{14}-N_{17}=108.9, O_{15}-S_{14}-N_{17}=104.9, $O_{15,16}$-S_{14}-C_3 =107.9-108.3, N_{17}-S_{14}-C_3 =107.9, C_{19}-N_{17}-S_{14} =123.0° reported by Labisbal *et al.*[35] are in agreement with the corresponding values of the title compound.

The calculated first hyperpolarizability of the title compound is 6.87 × 10^{-30} esu, which comparable with the reported values of similar derivatives, but experimental evaluation of this data is not readily available. Kucharski *et al.*[36] reported the first hyperpolarizability of certain sulfonamide amphiphiles by calculation and hyper-Rayleigh scattering in the range 0.2156-0.189 × 10^{-30} esu. We conclude that the title compound is an attractive object for future studies of nonlinear optical properties.

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