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Molecular structure and vibrational spectra of 2- [2-(ethylamino-4-chlorophenylaminothiazol)-5-oyl] benzothiazoleby experimental and computation techniques

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Abstract
2-[2-(Ethylamino-4-chlorophenylaminothiazol)-5-oyl] benzothiazole is found to have antifungal and antibacterial activities promoting effect. The, 2-[2-(ethylamino-4-chlorophenylaminothiazol)-5-oyl] benzothiazole derivatives are the subject of considerable pharmaceutical and chemical interest. Theoretical information on the optimized geometry, and IR intensities were obtained by means of Density Functional Theory (DFT) using standard B3LYP/6-31G basis sets with Gaussian, 09 software package. The calculated geometries such as bond lengths, bond angle, dihedral angle atomic charges and intensities of Vibrational bonds of the titled compound were investigated. The IR spectra are obtained and assigned by vibrational analysis and found to be reliable compared with the experimental results. HOMO-LUMO energy gap shows the chemical stability of the molecule.

Keywords: gaussian, DFT, B3LYP, mullikencharges, HOMO, LUMO

1. Introduction

Benzothiazole derivatives are fascinating chemical products used in the field of medicine as they have been found to possess a wide spectrum of biodynamic properties [4]. Benzothiazole analogs of dendrodoine derivatives have attracted a great deal of interest due to their biological and commercial importance [5]. The study of benzothiazoles is, therefore, of practical and theoretical importance [6]. A density functional theory of different benzothiazole derivatives have been calculated by using DFT/B3LYP method.

In recent years, among the computational methods calculating the electronic structure of molecular systems, experimental values of molecular geometry [2, 3], Vibrational frequencies, atomic charges, dipole moment, thermo dynamical properties etc [1]. Inpite of the existing studies, t here are still lack of information about structural and energetic properties of 2-[2-(ethylamino-4-chlorophenylaminothiazol)-5-oyl]
benzothiazole has been computationally investigated by using Density Functional Theory (DFT).

Patil *et al.* reported the DFT study on dihydroxyphenyl benzothiazole by using B3LYP/6-31G (d). The main objective of this paper is to present, more accurate vibrational assignments, bond lengths, bond angles, atomic charges and HOMO-LUMO of 2-[2-(ethylamino-4-chlorophenylaminothiazol)-5-oyl] benzothiazole using DFT/ B3LYP method. A systematic study on vibrational spectra and structure of 2-[2-(Butylamino-4-phenylaminothiazol)-5-oyl] benzothiazole.

2. Computational details

The DFT computation of 2-[2-(ethylamino-4-chlorophenylaminothiazol)-5-oyl] benzothiazole has been performed using Gaussian ’09 program package at the Becke-3Lee-Yang-Parr(B3LYP) level with standard 6-31G basis set. The optimized structural parameters are used in the vibrational frequency calculations at DFT level. At the optimized geometry of the title molecule no imaginary frequency modes are obtained, so there is a true minimum potential energy surface is found.

The assignments of the normal modes of vibration for the titled compound have been made by visual inspection of the individual mode using the Gauss view software[7].The optimized structure of 2-[2-(ethylamino-4-chlorophenylaminothiazol)-5-oyl] benzothiazole is given in figure 1. The optimized structural parameter calculated by B3LYP level with 6-31 basis set are given in Table 1.

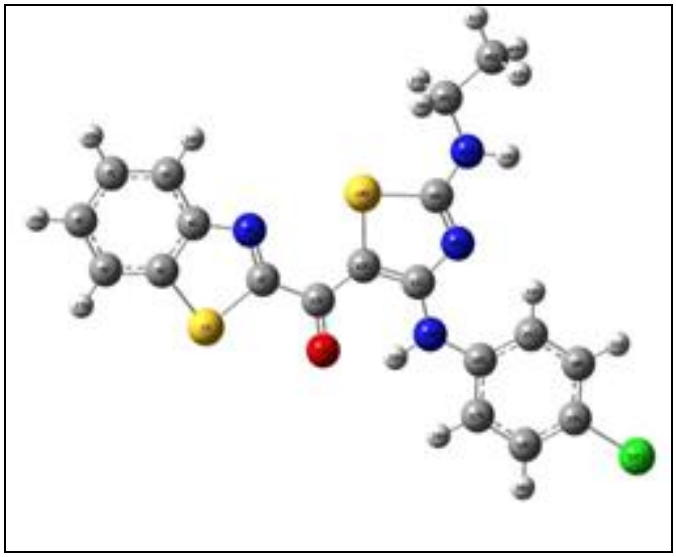


Fig 1: Optimized structure of 2-[2-(ethylamino-4-chlorophenylaminothiazol)-5-oyl] benzothiazole

Table 1: Optimized geometrical parameters of 2-[2-(ethylamino-4-chlorophenylaminothiazol)-5-oyl] benzothiazole at B3LYP with 6-31G level

Parameters	Bond lengths(Å)	Parameters	Bond angles(◦)	Parameters	Dihedral angle(◦)
	Calculated		Calculated		Calculated
S1-C2	1.8416	C2-S1-C5	86.4296	C5-S1-C2-N3	-0.0075
S1-C5	1.8146	S1-C2-N3	115.4563	C5-S1-C2-C13	-180.0049
C2-N3	1.3006	S1-C2-C13	117.7843	C2-S1-C5-C4	0.0062
C2-C13	1.4715	N3-C2-C13	126.7594	C2-S1-C5-C9	180.0039
N3-C4	1.3971	C2-N3-C4	112.8813	S1-C2-N3-C4	0.0066
C4-C5	1.4186	N3-C4-C6	114.99	C13-C2-N3-C4	180.0037
C4-C6	1.4038	N3-C4-C6	124.8925	S1-C2-C13-C12	180.0015
C5-C9	1.3964	C5-C4-C6	120.1174	S1-C2-C13-O14	180.0037
C6-C7	1.3923	S1-C5-C4	110.2428	N3-C2-C13-C12	0.0044
C6-C24	1.0837	S1-C5-C9	128.7071	N3-C2-C13-O14	180.0067
C7-C8	1.4099	C4-C5-C9	121.0502	C2-N3-C4-C5	-0.0044
C7-C25	1.0847	C4-C6-C7	118.7922	C2-N3-C4-C6	-180.0033
C8-C9	1.3976	C4-C6-H24	119.3009	N3-C4-C5-S1	-0.0044
C8-C26	1.0851	C7-C6-H24	121.9069	N3-C4-C5-C9	-180.0023
C9-C27	1.084	C6-C7-C8	120.7222	C6-C4-C5-S1	-180.0026
S10-C12	1.8384	C6-C7-H25	119.7852	C6-C4-V5-C9	-0.0004
S10-H34	1.8297	C8-C7-H25	119.4927	N3-C4-C6-H24	0.0018
C11-C21	1.4192	C7-C8-C9	121.1065	N3-C4-C6-C7	180.002
C11-N15	1.3598	C7-C8-H26	119.5608	C5-C4-C6-C7	0.0
C11-H35	1.3751	C9-C8-H26	119.3327	C5-C4-C6-H24	-180.0003
C12-C13	1.4147	C5-C9-C8	118.2116	S1-C5-C9-C8	180.003
C15-O14	1.2874	C5-C9-H27	121.1095	S1-C5-C9-H27	0.0019
N15-C16	1.4071	C8-C9-H27	120.7246	C4-C5-C9-C8	0.004
N15-C28	1.0295	C12-S10-C34	86.3388	C4-C6-C7-H25	-179.999
C16-C17	1.4109	C12-C11-N15	120.7246	H24-C6-C7-C8	180.007
C16-C21	1.408	C12-C11-N35	116.8622	H24-C6-C7-H25	-180.0004
C17-C18	1.3941	N15-C11-N35	122.4132	C6-C7-C8-C9	-0.0004
C17-C29	1.0857	S10-C12-C11	109.0035	C6-C7-C8-H26	180.0002
C18-Cl30	1.0829	S10-C12-C13	126.5923	H25-C7-C8-C9	-180.0001
C19-C20	1.3916	C11-C12-C13	124.4042	H25-C7-C8-H26	0.005
C19-Cl22	1.8295	C2-C13-C12	120.6238	C7-C8-C9-C5	0.0
C20-C21	1.3983	C2-C13-O14	117.5411	C7-C8-C9-H27	180.0011
C20-H31	1.0833	C12-C13-O14	121.8351	H26-C8-C9-C5	-180.0006
C21-H32	1.0796	C11-N15-C16	131.1259	H26-C8-C9-H27	0.0005
N23-H33	1.012	C11-N15-H28	111.282	C34-S10-C12-C11	0.0034
N23-C34	1.3449	C16-N15-H28	117.5921	C34-S10-C12-C13	-179.9997
N23-C36	1.4691	N15-C16-C17	116.2259	C12-S10-C34-N23	179.9952
H34-N35	1.3252	N15-C16-C21	124.6175	C12-S10-C34-N35	-0.0041
C36-H37	1.0983	C17-C16-C21	119.1566	N15-C11-C12-S10	180.0007
C36-C39	1.5292	C16-C17-C18	120.8578	N15-C11-C12-C13	0.0037
C39-H40	1.0959	C16-C17-H29	119.5855	N35-C11-C12-S10	-0.0025
		C18-C17-H29	119.5567	N35-C11-C12-C13	180.0005
		C17-C18-C19	118.8969	C12-C11-N15-C16	180.0025
		C17-C18-H30	120.4856	C12-C11-N15-H28	0.0022
		C19-C18-H30	120.6176	N35-C11-N15-C16	0.0057
		C18-C19-C20	121.4196	N35-C11-N15-H28	180.0056
		C18-C19-Cl22	119.2265	C12-C11-N35-C34	-0.0006
		C20-C19-Cl22	119.3539	N15-C11-N35-C34	180.0038
		C19-C20-C21	119.7597	S10-C12-C13-C2	0.006
		C19-C20-H31	120.2385	S10-C12-C13-O14	180.0036
		C21-C20-H31	120.0017	C11-C12-C13-C2	180.0025
		C16-C21-C20	119.9094	C11-C12-C13-O14	0.0001
		C16-C21-H32	119.5106	C11-N15-C16-C21	-0.002
		H33-N23-C34	120.58	C11-N15-C16-C17	-180.0016
		H33-N23-C36	116.1442	H28-N15-C16-C17	-0.0014
		C34-N23-C36	118.9921	H28-N15-C16-C21	-180.0018
		S10-C34-N23	124.8636	N15-C16-C17-C18	0.0001
		S10-C34-N35	121.047	N15-C16-C17-H29	0.00002
		N23-C34-N35	115.9574	C21-C16-C17-C18	0.0005
		C11-N35-C34	111.8381	C21-C16-C17-H29	-179.9995
		N23-C36-H37	109.2556	N15-C16-C21-C20	179.9999
		N23-C36-H38	109.256	N15-C16-C21-H32	-0.0002
		N23-C36-C39	110.3824	C17-C16-C21-C20	-0.0005
		H37-C36-C39	107.2905	C17-C16-C21-H32	179.9994
		C36-C39-H40	110.2963	C16-C17-C18-C19	-0.0001
		C36-C39-H41	110.2967	C16-C17-C18-H30	-180.0001

		C36-C39-H42	111.1439	H29-C17-C18-C19	179.9999
		H40-C39-H41	110.1033	H29-C17-C18-H30	-0.0004
		H40-C39-H42	111.1448	C17-C18-C19-C20	-0.004
		H41-C39-H42	107.8547	C17-C18-C19-Cl22	179.9996
		H41-C36-C39	108.6188	H30-C18-C19-C20	179.9996
				H30-C18-C19-Cl22	-0.0004
				C18-C19-C20-H21	0.0004
				C18-C19-C20-H31	180.0003
				Cl22-C19-C20-H21	-179.9995
				Cl22-C19-C20-H31	0.0003
				C19-C20-H21-C16	0.0
				C19-C20-H21-H32	-179.9999
				H31-C20-H21-C16	-179.9998
				H31-C20-H21-H32	0.0003
				H33-N23-C34-S10	179.9854
				H33-N23-C34-N35	-0.0154
				C36-N23-C34-S10	0.0198
				C36-N23-C34-N35	-1799809
				H33-N23-C36-H37	121.4659
				H33-N23-C36-H38	-121.436
				H33-N23-C36-C39	0.0153
				C34-N23-C36-H37	-58.5694
				C34-N23-C36-H38	58.5694
				C34-N23-C36-C39	179.98
				S10-C34-N35-C11	0.0035
				N23-C34-N35-C11	-179.9958
				N23-C36-C39-H40	60.55
				N23-C36-C39-H41	179.9971
				N23-C36-C39-H42	-60.5551
				H37-C36-C39-H40	-60.2812
				H37-C36-C39-H41	59.1658
				H37-C36-C39-H42	178.6137
				H38-C36-C39-H40	-178.618
				H38-C36-C39-H41	-178.618
				H38-C36-C39-H42	60.2769

3. Results and discussion

3.1 Molecular geometry

The optimized structure of 2-[2-(ethylamino-4-chlorophenylaminothiazol)-5-oyl] benzothiazole is given in figure 1. The optimized structural parameter calculated by B3LYP level with 6-31G basis set are given in Table1.The self-consistent field (SCF) energy of 2-[2-(ethylamino-4-chlorophenylaminothiazol)-5-oyl] benzothiazole at B3LYP level with the basis set 6-31G is found to be -2283.5322 a. u; with dipole moment 7.7905 Debye. The bond lengths of C4-C5, C5-C6, C6-C7, C7-C8, C8-C9 and C9-C4 shows double bond character (aromatic bond). similarly, the bond lengths of C16-C17,C17-C18,C18-C19,C19-C20,C20-C21 and C21-C22 shows double bond characters (aromatic bond).The bond angle (C12-S10-C34) is very less (86.3388°) than the bond angle (C11-N15-C16)131.1259° which is due to the fact that electronegativity of nitrogen is greater than sulphur.

3.2 Vibrational assignments

In order to obtain the spectroscopic signature of the title compound, we performed a frequency calculation analysis[8-9].Vibrational frequency were calculated by using B3LYP/6-31G, method. 2-[2-(ethylamino-4-chlorophenylaminothiazol)-5-oyl] benzothiazole molecules consists of 42 atom therefore it got 120 normal modes of vibrations. The scaling factor of 0.96 is used for getting theoretical vibrational frequency. Comparison of the frequencies calculated at DFT method using 6-31G basis set with experimental values reveal that the B3LYP method shows very good agreement with the literature observation.

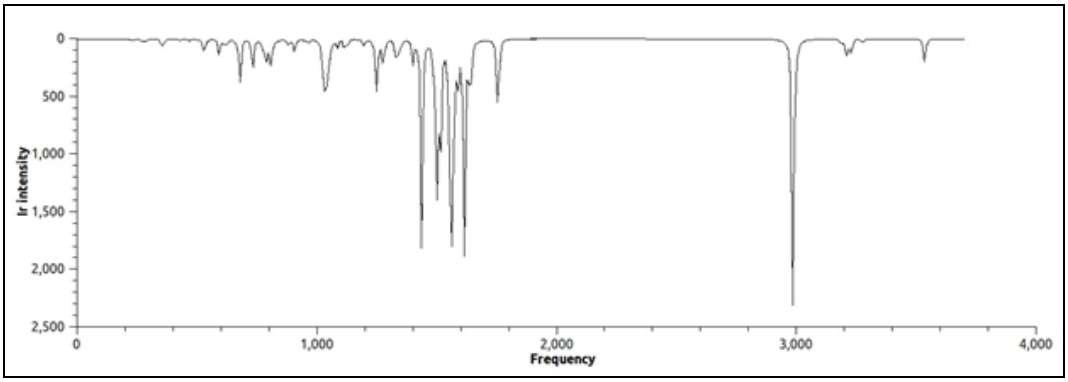


Fig 2: Calculated IR spectrum of 2-[2-(ethylamino-4-chlorophenylaminothiazol)-5-oyl] benzothiazole

Table 2: Selected theoretical vibrational assignments along with their intensities of 2-[2-(ethylamino-4-chlorophenylaminothiazol)-5-oyl] benzothiazole calculated at B3LYP/6-31G level

Scaled frequency (cm^{-1})	Intensity (km)Mol^{-1}	Assignments
3468	77.4917	N23-H33 (str)
3154	59.7216	N15-H28 (str)
3148	10.1374	C20-H31, C21-H32 (str) sym
3113	3.0606	C17-H29,C18-H30 (str) sym
3109	18.5786	C6-H24, C7-H25, C8-H26, C9-H27 (str) sym
3104	4.7005	C20-H31, C21-H32 (str) asym
3100	23.3132	C6-H24, C7-H25, C8-H26, C9-H27 (str) asym
3088	12.2125	C6-H24, C7-H25, C8-H26, C9-H27 (str) asym
3076	6.1604	C17-H29,C18-H30 (str) asym
3074	1.9468	C6-H24, C7-H25, C8-H26, C9-H27 (str) asym
3019	17.9589	C39-H40-H41-H42 (str) asym
3003	32.2489	C36-H37-H38, C39-H40-H41-H42 (str) asym
2943	14.1744	C36-H37-H38, C39-H40-H41-H42 (str) asym
2931	22.4130	C36-H37-H38, C39-H40-H41-H42 (str) asym
2911	11.5029	C36-H37-H38 (str) sym
1636	689.1749	C-C (str), N15-H28 (ip bend),C-O (str)
1590	3.1042	C-O (str), C-N (str), C-C (str), C-S (str), C-S (ip bend), C-H (ip bend)
1585	45.0264	C20-H31, C21-H32, C17-H29, C18-H30 (ip bend), C-N, C-Cl (str)
1579	383.8277	C-N(str), C-N (ip bend), C-O(str), C-S (ip bend)
1560	182.1204	C-C (str), C-Cl (ip bend), C-N, C-H (ip bend)
1551	45.0433	C-N(str), C-N (ip bend), C-O(str), C-S (ip bend)
1510	218.1532	C6-H24, C7-H25, C8-H26, C9-H27 (ip bend)
1507	82.7863	N3-C2(str), C13-O14(str), C-C (str), C-S (str),C-H (ip bend), C-S (ip bend)
1496	822.5550	C-N (str), C-O (str), C36-H37-H38 (ip bend)
1485	113.1807	C-C (str), C-O, C-N, C-Cl, C-S (str), C-H, C-N, C-S (ip bend)
1484	148.7682	C36-H37-H38, C39-H40-H41-H42 (ip bend)
1480	10.3357	C-C (str), C-O, C-N, C-Cl, C-S (str), C-H, C-N, C-S (ip bend)
1455	15.5242	C39-H40-H41-H42 (ip bend)
1432	117.2802	C6-H24, C7-H25, C8-H26, C9-H27 (ip bend)
1427	26.5016	N23-H33, C36-H37-H38, C-S (ip bend), C-N, C-O (str)
1421	313.0141	C-N (ip bend), C6-H24, C7-H25, C8-H26, C9-H27 (ip bend)
1422	568.5021	C-N (ip bend), C-N (str), C-Cl (ip bend), C-H (ip bend)
1411	13.5915	C13-O14 (str), N35-C11 (str), N15-H28 (ip bend), C-H(ip bend),C-S (str)
1404	32.2820	C-N (ip bend), C36-H37-H38, C39-H40-H41-H42 (ip bend)
1391	152.3048	C-N (str), C-N (ip bend), C-S (str), C6-H24, C7-H25, C8-H26, C9-H27 (ip bend)
1345	92.1186	C-C (str), C20-H31, C21-H32, C17-H29, C18-H30 (ip bend)
1422	1.7932	C-C (str), C20-H31, C21-H32, C17-H29, C18-H30 (ip bend)
1320	4.4466	S10-C34(str), C-O (ip bend), C-H (ip bend), C-N (ip bend)
1310	0.7895	S10-C34(str), C-O (ip bend), C-H (ip bend), C-N (ip bend)
1285	15.0423	C36-H37-H38, C39-H40-H41-H42 (ip bend)
1279	0.2962	C-S(str), C-O (str), C-C (str), C-N (str), C-N (ip bend)
1272	79.5615	C-S(str), C-O (str), C-C (str), C-N (str), C-N (ip bend)
1256	182.9410	C6-H24, C7-H25, C8-H26, C9-H27 (ip bend), C-N (ip bend)
1236	53.4691	C20-H31, C21-H32, C17-H29, C18-H30 (ip bend)
1218	7.9387	C6-H24, C7-H25, C8-H26, C9-H27 (ip bend), C-N (ip bend)
1186	1.3246	C36-H37-H38, C39-H40-H41-H42 (ip bend)
1171	41.1283	C36-H37-H38, C39-H40-H41-H42 (ip bend)
1152	2.6791	C6-H24, C7-H25, C8-H26, C9-H27 (ip bend), C-N (ip bend)
1149	3.0758	C20-H31, C21-H32, C17-H29, C18-H30 (ip bend)
1118	3.1727	C-S (str), C-C (str), C-N (ip bend), C-O (ip bend), C-H (ip bend)
1115	4.9492	C19-Cl22 (str), C20-H31, C21-H32, C17-H29, C18-H30 (ip bend)
1090	59.9099	C6-H24, C7-H25, C8-H26, C9-H27 (ip bend)
1066	1.6184	N23-H33 (ip bend), C36-H37-H38, C39-H40-H41-H42 (ip bend)
1035	7.1141	N23-H33 (ip bend), C36-H37-H38, C39-H40-H41-H42 (ip bend)
1029	2.9838	S10-C12 (str), C6-H24, C7-H25, C8-H26, C9-H27 (ip bend)
1012	2.8518	C20-H31, C21-H32, C17-H29, C18-H30 (ip bend)
1008	39.0396	C6-H24, C7-H25, C8-H26, C9-H27 (ip bend)
1002	0.0280	C21-H32, C20-H31 (ip bend)
984	3.9175	N15-H28, C17-H29, C18-H30 (op bend)
977	18.8762	C6-H24, C7-H25, C8-H26, C9-H27 (op bend)
954	2.0500	C36-H37-H38, C39-H40-H41-H42 (op bend)
944	12.9485	N15-H28(op bend), C18-H30 (op bend)
917	136.7299	C-N, C-O (op bend), C-S (str), C-N (str)
913	112.7808	C6-H24, C7-H25, C8-H26, C9-H27 (op bend)
867	0.2127	C21-H32, C20-H31 (op bend)
863	31.4308	C-N, C-O (op bend), C-S (str), C-N (str)

841	31.4308	Phenyl, thiazole, ethyl group (op bend)
826	37.4592	N15-H28, C17-H29,C18-H30 (op bend)
813	4.3740	C36-H37-H38, C39-H40-H41-H42 (op bend)
812	42.8315	C-S (str), C-N, C-H, C-O (op bend)
799	50.4548	C6-H24, C7-H25, C8-H26, C9-H27 (op bend)
764	0.8593	C13-O14, S10-C12, N3-C2 (str), C-N (op bend), C-H (op bend)
746	0.7044	C13-O14 (op bend), C2-1S (str),C12-C11 (str)
744	21.0305	C6-H24, C7-H25, C8-H26, C9-H27 (op bend)
734	0.2437	C20-H31, C21-H32, C17-H29, C18-H30 (op bend)
705	0.9751	C6-H24, C7-H25, C8-H26, C9-H27 (op bend)
688	3.0541	C24-N25 (str), C-O (str), C-S (op bend)
682	10.6947	C-S 9str), C-C (str), C-H (op bend), C19-Cl22 (str)
667	73.3751	C-S (str), C-N, C-H(op bend),C19-Cl22(str)
658	8.3487	C20-H31, C21-H32, C17-H29, C18-H30 (op bend)
632	69.3881	N23-H33 (op bend), C34-N35 (str)
631	8.3847	Phenyl, thiazole, ethyl (op bend), C19-Cl22(str), C-S (str)
607	7.0672	C-Cl (str), C-C (str), C-N, C-H, C-S (op bend)
600	21.6016	C-S (str), C-Cl (str), C-H, C-N(op bend)
588	4.3062	C-N, C-H, C20-H31,C18-H30,C17-H29 (op bend)
581	12.4265	C20-H31, C21-H32, C17-H29, C18-H30 (op bend)
512	9.0821	C20-H31, C21-H32, C17-H29, C18-H30 (op bend)
493	0.1402	N23-H33 (op bend), C34-N25 (str), C-O (str), C-S (op bend)
485	3.2982	C5-1S-C2 (str), C-H (op bend)
476	45.6746	C-Cl (str), C-N (str), C-O, C-H, C-N (op bend)
470	9.2629	N23-H33 (op bend), C34-N35 (str)
461	3.4409	S10-C12,C2-1S (str), C-N, C-H, C-O (op bend)
430	34.8049	C6-H24, C7-H25, C8-H26, C9-H27 (ip bend)

Abbreviations: sym- symmetric, asym- asymmetric, str-stretching, ip bend-in plane bending, op bend-out of plane bending.

3.3 Mulliken atomic charges

Mulliken atomic charge calculation has an important role in the application of quantum chemical calculation to molecular system because of atomic charges effect dipole moment, molecular polarizability, electronic structure and more a lot of properties of molecular systems [10, 14]. The bonding capability of a molecule depends on the electronic charge on the chelating atoms. The atomic charge values have been obtained by mulliken population analysis. To validate the reliability of our results,the mulliken population analysis of 2-[2-(ethylamino-4-chlorophenylaminothiazol)-5-oyl] benzothiazole has been calculated using B3LYP/6-31G basis set. The corresponding characteristics of the atomic charge populations of the constituent atoms are presented in table 3. It was found that N (15) has more negative charge (-0.82811eV) and C (11) has more positive charge(0.53307eV).The mulliken atomic charge of all hydrogen and sulpur carries positive charge.

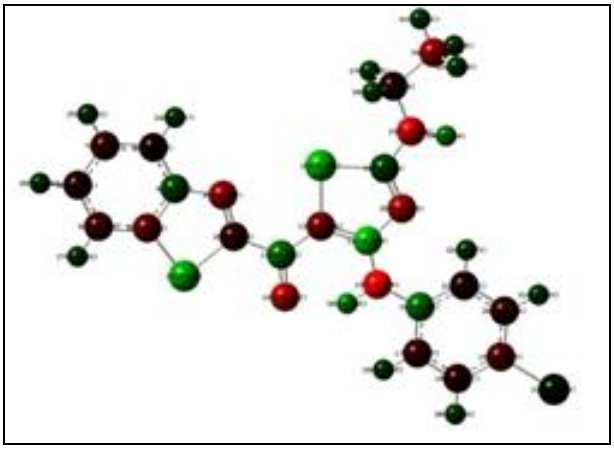
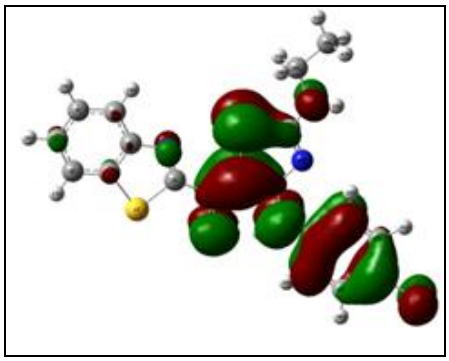


Fig 3: Mulliken charge distribution of 2-[2-(ethylamino-4-chlorophenylaminothiazol)-5-oyl] benzothiazole

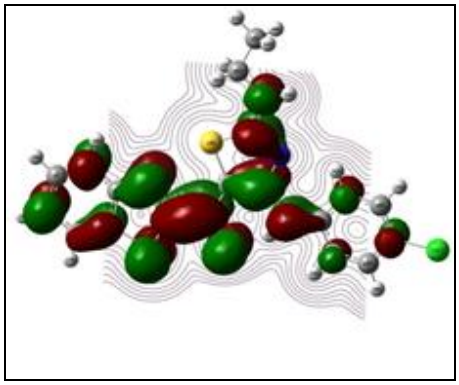
3.4 HOMO-LUMO energy gaps

The most important orbitals in a molecule are the Frontier molecular orbitals, called highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO). These orbitals determine the way the molecule interacts with other species. The lowering of the HOMOLUMO 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 [15]. ΔE reveals the chemical activity of the molecule. LUMO as an electron acceptor represents the ability to obtain an electron and HOMO represents the ability to donate an electron. The calculated energy value of HOMO is -0.8588a.u. and for LUMO is -0.1999a.u. The value of energy separation ΔE between the HOMO and LUMO is 0.6589a.u. The energy gap between HOMO and LUMO describes the chemical reactivity, optical polarisability, kinetic

stability and chemical softness-hardness of a molecule. The chemical hardness is a good indicator of the chemical stability. The molecules having a small gap are known as soft and having a large gap are known as hard molecules.



HOMO



LUMO

Fig 4: HOMO-LUMO of 2-[2-(ethylamino-4-chlorophenylaminothiazol)-5-oyl] benzothiazole

4. Conclusion

The DFT calculation on the structure and vibrational spectrum of the title compound has been carried. A complete vibrational analysis was also performed according to frequency scale factors. Intensities of each vibrational mode enable us to safely assign the fundamental bands. Finally the calculated HOMO-LUMO energies show that charge transfer occurs within the molecule which is responsible for the bioactive property of molecule. The Mulliken charge analysis explains the possibilities of hydrogen bonding.

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