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DFT and Vibrational spectroscopic study on 2-[2-(ethylamino-4-methylphenylaminothiazol)-5-oyl] benzothiazole

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Abstract: *Thecompound 2-[2-(ethylamino-4-methylphenylaminothiazol)-5-oyl]benzothiazole was characterized by IR spectral data. The geometry of the molecule was investigated and optimized with the help of B3LYP/6-311G density functional theory (DFT) method using 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. The calculated Homo and LUMO energy gaps also confirm that charge transfer occurs within the molecule.*

Keywords: *Gaussian, DFT, B3LYP, Mullikencharges, HOMO, LUMO.*

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I. 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.[1] Benzothiazole analogs of dendrodoine derivatives have attracted a great deal of interest due to their biological and commercial importance.[2] The study of benzothiazoles is, therefore, of practical and theoretical importance.[3] A density functional theory of different benzothiazole derivatives have been calculated by using DFT/B3LYP method. Benzothiazole derivatives have long been therapeutically used for the treatment of various diseases. However, in recent years, 2-aminobenzothiazoles have emerged as an important pharmacophore in the development of antitumor agents. Benzothiazole is a privileged bicyclic ring system. It contains a benzene ring fused to a thiazole ring. The small and simple benzothiazole nucleus is present in compounds involved in research aimed at evaluating new products that possess interesting biological activities like- antimicrobial, antitubercular, antitumour, antimalarial, anticonvulsant, anthelmintic, analgesic and anti-inflammatory activity Patil *et al.* reported the DFT study on dihydroxyphenyl benzothiazole by using B3LYP/6-31G (d)[4]. 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-methylphenylaminothiazol)-5-oyl]benzothiazole using DFT/B3LYP method. A systematic study on vibrational spectra and structure of 2-[2-(ethylamino-4-methylphenylaminothiazol)-5-oyl]benzothiazole.

II. Computational Details

The DFT computation of 2-[2-(ethylamino-4-methylphenylaminothiazol)-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 .The optimized structure of 2-[2-(ethylamino-4-methylphenylaminothiazol)-5-oyl]benzothiazol is given in **figure 1**.The optimized structural parameter calculated by B3LYP level with 6-31G basis set are given in **Table 1**.

Figure1-Optimized structure of 2-[2-(ethylamino-4-methylphenylaminothiazol)-5-oyl]benzothiazole

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

Parameters	**Bond lengths(Å)**	**Parameters**	**Bond angles(◦)**	**Parameters**	**Dihedral angle(◦)**
	Calculated		**Calculated**		**Calculated**
S1-C2	1.843	C2-S1-C5	86.4287	C5-S1C2-C3	0.0012
S1-C5	1.8147	S1-C2-N3	115.4168	C5-S1-C2-C13	180.0009
C2-C3	1.3005	S1-C2-C13	117.6262	C2-S1-C5-C4	0.0012
C2-C13	1.4719	N3-C2-C13	126.9569	C2-S1-C5-C9	179.9994
N3-C4	1.3973	C2-N3-C4	112.9016	S1-C2-N3-C4	0.0008
C4-C5	1.4185	N3-C4-C5	115.0085	C13-C2N3-C4	179.9996
C4-C6	1.4036	N3-C4-C6	124.8727	S1-C2-C13-C12	180.0063
C5-C9	1.3964	C5-C4-C6	120.1188	S1-C2-C13-O14	0.0096
C6-C7	1.3925	S1-C5-C4	110.2444	N3-C2-C13-C12	0.0066
C6-C23	1.0837	S1-C5-C9	125.7332	N3-C2-C13-O14	-180.0092
C7-C8	1.4097	C4-C5-C9	121.0224	C2-N3-C4-C5	0.0003
C7-C24	1.0848	C4-C6-C7	118.8159	C2-C3-C4-C6	179.9997
C8-C9	1.3977	C4-C6-C23	119.2716	N3-C4-C5-S1	0.0012
C8-C25	1.0851	C7-C6-C23	121.9125	N3-C4-C5-C9 C6-	180.0006
S10-C12	1.0841	C6-C7-C8	120.7053	C4-C5-S1	180.0006
S10-H33	1.8393	C6-C7-C24	119.7904	C6-C4-C5-C9	0.0
C11-N15	1.8306	C8-C7-C24	119.5043	C3-C4-C6-C7	180.0007
C11-H34	1.4215	C7-C8-C9	121.0914	N3-C4-C6-C23	0.0005
C13-O14	1.3564	C7-C8-C25	119.5746	C5-C4-C6-C7	0.0
N15-C16	1.3768	C9-C8-C25	119.334	C5-C4-C6-C23	180.0002
C16-C17	1.4129	C5-C9-C8	118.2462	S1-C5-C9-C8	180.0007
C16-C21	1.2884	C5-C9-C26	121.0936	S1-C5-C9-C26	0.0005
C17-C18	1.4111	C8-C9-C26	120.6602	C4-C5-C9-C8	0.0
C17-C28	1.0292	C12-S10-H33	86.4876	C4-C5-C9-C26	180.0003
C18-C19	1.4082	C12-C11-N15	120.8143	C4-C6-C7C8	0.0
C18-H29	1.4077	C12-C11-H34	116.7198	C4-C6-C7-C24	180.0001
C19-C20	1.3941	N15-C11-H34	122.466	C23-C6-C7-C8	180.0002
C19-H42	1.0863	S10-C12-C11	109.0333	C23-C6-C7-C24	0.0001
C20-C21	1.4044	S10-C12-C13	126.5666	C6-C7-C8-C9	0.0 180.0001
C20-H30	1.0863	C11-C12-C13	124.4001	C6-C7-C8-C25	180.0
C21-H31	1.4055	C2-C13-C12	120.6225	C24-C7-C8-C9	0.0001
N22-H32	1.5127	C2-C13-O14	117.4357	C24-C7-C8-C25	0.0001
N22-H33	1.3961	C12-C13-O14	121.9418	C7-C8-C9-C5	180.0003
N22-H35	1.0871	C11-N15-C16	131.3301	C7-C8-C9-C26	179.9999
H33-H34	1.0798	C11-N15-C27	111.3732	C25C8-C9C5	0.0002
H35-H36	1.0119	C16-N15-C27	117.2967	C25-C8-C9-C26	0.0079
H35-H37	1.346	N15-C16-C17	116.2873	H33-S10-C12-C11	180.0084
H35-H38	1.4684	N15-C16-C21	124.8164	H33-S10-C12-C13	180.0048
H38-H39	1.3234	C17-C16-C21	118.8963	C12-S10-H33-C22	0.0072
H38-H40	1.0984	C16-C17-C18	120.564	C12-S10-H33-H34	180.0074
H38-H41	1.0984	C16-C17-C28	16,17,28)	N15-C11-C12-S10	0.0079
H42-C43	1.5293	C18-C17,C28	119.4842	N15-C11-C12-C13	0.008
H42-N44	1.096	C17-C18-C19	119.9518	H34-C11-C12-S10	180.0085
H42-H45	1.0939	C17-C18-H29	121.2673	H34-C11-C12-C13	180.002
H38-H40	1.096	C19-C18-H29	119.2117	C12-C11-C15-C16	0.0065
H35-H36	1.0977	C18-C19-C20	19,18,29)	C12-C11-N15,27)	0.0012
H42-H43	1.0977	C18-C19H42	119.521	H34-C11-N15-C16	180.0058
H33-H34	1.0947	C20-C19-H42	117.5413	H34-C11-N15-C27	0.0028
		C19-C20-C21	121.3992	C12-C11-H34-H33	180.0021
		C19-C20-H30	121.0595	N15-C11-C34-H33	0.0028
		C21-C20-H30	122.1025	S10-C12-C13-C2	180.0138
		C16-C21-C20	119.2394	S10-C12-C13-O14	180.0034
		C16-C21-H31	118.6581	C11-C12-13-C2	0.0132
		C20-C21-H31	119.6287	C11-C12-C13O14	180.0016

		H32-N22-H33	119.4334	C11-N15-C16-C17	0.0014
		H32-N22-H35	120.9379	C11-N15-C16-C21	0.0032
		H33-N22-H35	116.0796	C27-N15-C16-C17	180.0034
		S10-H33-N22	119.0495	C27-N15-C16-C21	180.0002
		S10-H33-H34	124.8709	N15-C16-C17-C18	0.0002
		C2-H33-H34	120.9533	N15-C16-C17-C28	0.0
		C11-H34-H33	116.0523	C21-C16-C17-C18	180.0
		N22-H35-H36	122.9944	C21-C16-C17-C28	180.0002
		N22-H35-H37	111.897	N15-C16-C21-C20	0.0004
		N22-H35-H38	109.311	N15-C16-C21-H31	0.0
		H36-H35-H37	109.3114	C17-C16-C21-C20	179.9998
		H36-H35-H38	110.3945	C17-C16-21,H31	-0.0001
		H37-H35-H38	107.2507	C16-C17-C18-C19	179.9999
		H35-H38-H39	110.255	C16-C17-C18-C29	-180.0001
		H35-H38-H40	110.2551	C28-C17-C18-C19	-0.0001
		H35-H38-H41	111.134	C28-C17-C18-H29	0.0002
		H39-H38-H40	110.1175	C17-C18-C19-C20	-179.9992
		H39-H38-H41	111.1341	C17-C18-C19-H42	179.9998
		H40-H38-H41	107.8669	H29-C18-C19-20	0.0008
		C19-H42-C43	108.6021	H29-C18-C19-H42	0.0001
		C19-H42-N44	107.8668	C18-C19-C20-C21	179.9998
		C19-H42-H45	111.5448	C18-C19-C20-H30	179.9992
		C43-H42-N44	111.5448	H42-C19-C20-C21	0.0009
		C43-H42-H45	111.2741	H42-C19-C20-H30	120.1767
		N44-H42-H45	107.0217	C18-C19-H42-C43	120.2034
				C18-C19-H42-N44	-0.0131
				C18-C19-H42-H45	(-59.8226
				C20-C19-H42-C43	59.7973
				C20-C19-H42-N44	179.9876
				C20-C19-H42-H45	0.0
				C19-C20-C21-C16	179.9998
				C19-C20-C21-H31	179.9998
				H30-C20-C21-C16	0.0001
				H30-C20-C21H31	180.0003
				H32-N22-H33-S10	0.0023
				H32-N22-H33-H34	0.0029
				H35-N22-H33-S10	-179.9997
				H35-N22-H33-H34	121.4471
				H32-N22-H35-H36	121.4392
				H32-N22-H35-H37	0.0041
				H32-N22-H35-H38	58.5556
				H33-N22-H35-H36	58.5581
				H33-N22-H35,H37	179.9986
				H33-N22,H35-H38	0.0041
				S10-H33-H34-C11	180.0016
				N22-H33-H34-C11	60.5346
				N22-H35-H38-H39	179.9998
				N22-H35-H38-H40	-60.5351
				N22-H35-H38-H41	-60.3469
				H36-H35-H38-H39	59.1182
				H36-H35-H38-H40	178.5833
				H36-H35-H38-H41	-178.5835
				H37-H35-H38-H39	59.1183
				H37-H35-H38-H40	60.3468
				H37-H35-H38-H41	

III. Results And Discussion

Molecular geometry

The optimized structure of 2-[2-(ethylamino-4-methylphenylaminothiazol)-5oyl]benzothiazole is given in **figure 1**.The optimized structural parameter calculated by B3LYP level with 6-31G basis set are given in **Table2**.The self-consistent field(SCF) energy of 2-[2-(ethylamino-4-methylphenylaminothiazol)-5oyl]benzothiazole at B3LYP level with the basis set 6-31G is found to be -1863.2643 a.u; with dipole moment 5.9999Debye.The bond lengths of C4-C5,C5-C6,C6-C7,C7-C8,C8-C9 and C9-C5 shows double bond character(aromatic bond). similarly,the bond lengths of C15-C16,C16-C17,C17-C18,C19-C20,C20-C21 and C21-C22 shows double bond characters (aromatic bond).The bond angle (C2-S1-C5) is very less (86.4287°**)** than the bond angle (C11-N15-C27)126.9560° which is due to the fact that electronegativity of nitrogen is greater than sulphur.

Vibrational assignments

In order to obtain the spectroscopic signature of the title compound,we performed a frequency calculation analysis .Vibrational frequency were calculated by using B3LYP/6-31G,method. 2-[2-(ethylamino-4-methylphenylaminothiazol)-5oyl]benzothiazole molecules consists of 45 atom therefore it got 129 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. The hetero aromatic molecule containing an N-H group and its stretching absorption occure in the region 3500-3220cm^{-1}. Primary amine examined in dilute solution display two weak absorption bands one near 3500 cm^{-1} and the other near 3400 cm^{-1}. These bands represent, respectively the asymmetric and symmetric N-H stretching modes.In the present work, the theoretical calculation indicate the scaled frequency values at 3484 and 3448cm^{-1} is assigned to N-H stretching vibration.Primary aromatic amines normally absorb at 1615-1580 cm^{-1}.The N-H in-plane bending vibration computed by B3LYP/6-31G method good agreement with literature values. The presence of aromatic N-H out-of-plane bending vibration are appeared with in the region 767-673cm^{-1}. In the present work, the theoretical calculation indicates, the scaled frequency values at 706 and 688cm^{-1} is assigned to N-H out-of-plane bending vibration.

The assignments of methyl group vibration make a significant contribution to the titled compound. The asymmetric C-H vibration for methyl group usually occurs in the region between 2975 cm^{-1} and 2920 cm^{-1}. The theoretically computed values by B3LYP/6-31G method for C-H vibrations are found at 2992,2988,2913 cm^{-1}. Thus the theoretically computed values for C-H vibrations nearly coincide with literature values.In the title compound the methyl in-plane bending modes occur in the range 1479-1411 $cm^{-1.}$ The C-H out-of plane bending vibrations occur at 888 cm^{-1} and 774 cm^{-1}.The assignments are in agreement with the literature values.

The aromatic structure shows the presence of C-H stretching vibrations in the region 3100-3000cm^{-1} which is the characteristic region for the ready identification of the C-H stretching vibrations.The C-H stretching vibration computed by B3LYP/6-311G method good agreement with literature observations. The C-H in-plane bending vibrations were observed in the region 1420-1000cm^{-1}.These bands represents, the C-H in-plane–bending vibrations.In the present work, the theoretical calculation indicate the scaled frequency value at 1395 cm^{-1} is assigned to C-H in-plane-bending vibration. The presence of C-H out-of plane vibrations were observed in the region 999-750cm^{-1}.In the present work, the C-H out-of-plane bending vibration computed by B3LYP/6-31G method good agreement with literature observation.Generally, the carbon-carbon stretching vibrations in aromatic compound from the band in the region 1650-1430cm^{-1}.In the present study,the scaled frequency value at 1478cm^{-1} are assigned to carbon-carbon stretching vibration. The assignments of methyl group vibration make a significant contribution to the titled compound. The asymmetric C-H vibration for methyl group usually occurs in the region between 2975 cm^{-1} and 2920 cm^{-1}. The theoretically computed values by B3LYP/6-31G method for C-H vibrations are found at 2964,2864cm^{-1}. Thus the theoretically computed values for C-H vibrations nearly coincide with literature values.In the title compound the methyl in-plane bending modes occur in the range 1479-1411 $cm^{-1.}$ The C-H out-of plane bending vibrations occur at 888 cm^{-1} and 774 cm^{-1}.The assignments are in agreement with the literature values.The carbonyl group is present in a large number of different classes of compounds,for which a strong band observed due to the C=O stretching vibration is in the region of 1850-1550 cm^{-}1.The intensity of these bands can be increase due to conjugation or formation of hydrogen bonds.The lone pair of electrons on oxygen also determined the nature of the carbonyl group.In our present study the theoretically computed wavenumber for C=O stretching vibrations occur at 1571 cm^{-1}.The in-plane and out-of plane C=O bending mode occur at 1522 cm and 849 cm^{-1}. The identifications of C-N,C=N vibrations is a difficult task,since the mixing of several bands are possible in the region.Silver-stein et al. assigned C=N stretching absorption in the region 1382-1226 cm^{-1} for aromatic amines.The identification of wavenumber for C-N stretching in the side chains is rather difficult since there are problems in differensiating wavenumber from others. The band at 1357 cm^{-1} corresponds C-N,C=N stretching vibrations.The C-S stretching vibration is expected in the region 710-685cm-1. While DFT calculations give the C-S stretching vibration at 637cm-1 is assigned to C-S stretching vibration.The carbonyl group is important and its characteristic frequency has been extensively used to study a wide range of compounds.

Figure 2- Calculated IR spectrum of 2-[2-(ethylamino-4-methylphenylaminothiazol)-5oyl]benzothiazole

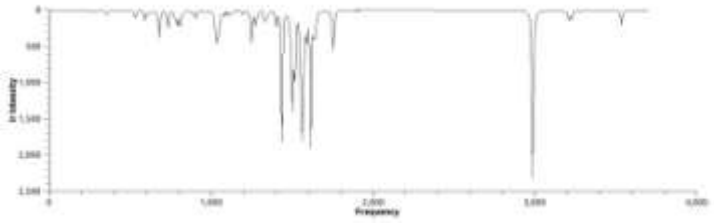


Table 2 Selected theoretical vibrational assignments along with their intensities of 2-[2-(ethylamino-4-methylphenylaminothiazol)-5oyl]benzothiazole calculated at B3LYP/6-31G level

Scaled frequency (cm^{-1})	**Intensity (km)Mol^{-1}**	**Assignments**
3469	72.8020	N22-H32 (str)
3161	43.7027	N15-H27 (str)
3144	5.2212	C21-H31,C20-H30 (str)
3108	19.4454	C6-H23,C7-H24,C8-H25,C9-H26 (str)
3098	24.8694	C6-H23,C7-H24,C8-H25,C9-H26 asym (str)
3087	12.6426	C6-H23,C7-H24,C8-H25,C9-H26 asym (str)
3077	14.1817	C17-H28,C18-H29,C20-H30 sym (str)
3073	1.9417	C6-H23,C7-H24,C8-H25,C9-H26 asym (str)
3058	28.7300	C17-H28,C18-H29,C20-H30 asym (str)
3056	29.9814	C20-H30,C21-H31,C17-H28,C18-H29 asym (str)
3018	18.8169	C38-H39-H40-H41 asym(str)
3002	33.2320	C38-H39-H40-H41, C35-H36-H37 asym(str)
2999	19.8626	C42-H43-H44-H45 asym(str)
2966	26.0823	C42-H43-H44-H45 asym(str)
2942	14.6413	C38-H39-H40-H41, C35-H36-H37 asym(str)
2930	23.2845	C38-H39-H40-H41 sym(str)
2912	65.7841	C42-H43-H44-H45 sym(str)
2910	12.8418	C35-H36-H37 sym(str)
1635	600.7341	N15-H27(ip bend), C-C(str)
1606	53.0361	N15-H27,C21-H31,C28-H30,C18-H29,C17-H28(ip bend)
1590	5.3033	C6-H23,C7-H24,C8-H25,C9-H26 (ip bend),C5-1S,N3-C2(str)
1580	392.06	N22-C33 (str), N22-H32 (ip bend)
1557	140.45	Phenyl, methyl group (ip bend),C-N (ip bend)
1551	10.9103	C6-H23,C7-H24,C8-H25,C9-H26 (ip bend)
1512	250.40	C-N(str), C35-H36-H37 (ip bend),C-S(ip bend)
1510	188.46	C-N(str), C35-H36-H37 (ip bend),C-S(ip bend)
1506	61.3432	C-N(str), C35-H36-H37 (ip bend),C-S(ip bend)
1495	637.9612	C-H (ip bend), C-S (str),C13-O14(str)
1485	122.3088	C35-H36-H37,C38-H39-H40-H41(ip bend)
1479	10.0765	C38-H39-H40-H41(ip bend)
1477	12.0666	C42-H43-H44-H45 (ip bend)
1469	7.1095	C6-H23,C7-H24,C8-H25,C9-H26 (ip bend)
1455	13.8027	C6-H23,C7-H24,C8-H25,C9-H26 (ip bend)
1432	94.9624	Ethyl,phenyl,methyl group (ip bend),C-O (str),C-N (ip bend)
1427	32.7383	N22-H32(ip bend), C-N (str), C6-H23,C7-H24,C8-H25,C9-H26 (ip bend)
1424	214.66	N22-H32(ip bend), C-O (ip bend), C-H (ip bend)
1415	579.28	C12-C13 (str), C13-O14, N15-H27, N22-H32(ip bend)
1404	5.5813	C38-H39-H40-H41(ip bend)
1402	12.6104	C42-H43-H44-H45 (ip bend)
1395	43.7686	C13-O14,N3-C2,N22-H32, S10-C12 (ip bend), C-H (ip bend)
1345	152.9015	C35-H36-H37,N22-H32(ip bend)
1332	24.3971	C20-H30,C21-H31,C17-H28,C18-H29 (ip bend)
1324	48.635	C7-H24,C8-H25,C9-H25 (ip bend),C4-C5(str)
1315	11.8160	C20-H30,C21-H31,C17-H28,C18-H29 (ip bend), C42-H43-H44-H45(ip bend)
1287	0.5921	C-N(str),C-O(ip bend), C-H (ip bend)
1279	8.562	C7-H24, C8-H25, C9-H25(ip bend)
1272	0.2422	C35-H36-H37,C38-H39-H40-H41(ip bend)
1252	69.7321	C35-H36-H37,C38-H39-H40-H41(ip bend)
1234	156.8311	C-N (str), C-N (ip bend), C-H(ip bend),C-C(str)
1217	77.5053	C-O(str), C-C(str), C-S(str), C-N (ip bend), C-N(str), C-H (ip bend)
1205	1.5148	C19-C42(str), C20-H30,C21-H31,C17-H28,C18-H29 (ip bend)
1192	2.1960	C20-H30,C21-H31,C17-H28,C18-H29 (ip bend)
1170	0.8787	C6-H23,C7-H24,C8-H25,C9-H26 (ip bend)
1152	43.6988	C38-H39-H40-H41(ip bend), N22-H32(ip bend), C-S(str)
1150	2.5949	C38-H39-H40-H41(ip bend), C35-H36-H37(ip bend)
1128	4.4351	C21-H31,C20-H30,C18-H29,C17-H28(ip bend)
1118	3.2608	C7-H24,C8-H25,C9-H25,C6-H23 (ip bend)
1088	4.6043	C-S,C-C,C-N,C-O(str),C-H,C-N, C-O,C-S(ip bend)
1054	6.6044	C42-H43-H44-H45(ip bend)
1034	1.6165	C-N,C-C, C-S (str), C-H, C-N, C-S, C-O(ip bend)
1030	6.4085	N22-H32(ip bend), C42-H43-H44-H45(ip bend)
1017	0.0910	C21-H31, C20-H30, C18-H29, C17-H28 (ip bend)
1010	6.5005	C-N,C-C, C-S , C-O (str), C-H, C-N, (ip bend)
1008	2.0475	C-N,C-C, C-S , C-O (str), C-H, C-N, (ip bend)
991	8.6008	C42-H43-H44-H45 (ip bend)
984	0.0219	C7-H24,C8-H25,C9-H25,C6-H23 (op bend)
973	30.5534	C21-H31, C20-H30, C18-H29, C17-H28 (op bend)
949	1.8586	N15-H27,C17-H28,C18-H29 9op bend)
943	10.4403	C7-H24,C8-H25,C9-H25,C6-H23 (op bend)

917	109.3897	C35-H36-H37,C38-H39-H40,N22-H32 (op bend), C-S(str)
911	108.230	N15-H27 (op bend)
867	0.2384	N34-C11 (str), C-S (str), C-C(str),C-H (op bend)
863	16.7436	C7-H24,C8-H25,C9-H25,C6-H23 (op bend)
840	7.8063	C21-H31, C20-H30, C42-H43-H44(op bend)
830	10.6681	C-N(str), C-S(str), C-H,C-N,C-S,C-O (op bend)
814	1.0477	C17- H24,C8-H25,C9-H25,C6-H23 (op bend), C-N(op bend)
813	63.5403	C38-H39-H40-H41(op bend), C35-H36-H37(op bend)
809	50.102	C-H, C-N, C-S, C-O (op bend), C-N, C-S, C-C(str)
764	5.6612	C7-H24,C8-H25,C9-H25,C6-H23 (op bend)
750	0.7292	C-H, C-N, C-S, C-O (op bend), C-N, C-S, C-C(str)
744	12.2245	C-C(op bend), C-N (op bend), C-S(op bend)
736	21.1456	C-C(op bend), C-N (op bend), C-S(op bend)
734	0.8745	C-H, C-N, C-S, C-O (op bend), C-N, C-S, C-C(str)
708	0.7663	C7-H24,C8-H25,C9-H25,C6-H23 (op bend)
687	3.0317	C21-H31,C20-H30,C18-H29,C17-H28(op bend), C42-H43-H44-H45(op bend)
681	3.0313	C5-1S (str),C7-H24,C8-H25,C9-H25,C6-H23 (op bend)
604	40.1975	C-N (str), C-S (str), C-N(op bend), C-O (str), C-S(op bend)
643	3.4779	C-S (str), C-H, C-N, C-O,C-S (op bend)
628	66.9373	Phenyl ring vibration
619	31.9436	N22-H32(op bend), N22-C33(str)
601	3.0879	Ring vibration
592	21.9523	Ethyl group vibration
581	4.4141	Ring vibration
516	4.1842	C7-H24,C8-H25,C9-H25,C6-H23 (op bend)
516	9.9711	Ring vibration
492	7.0629	N22-H32 (op bend), C-C (str), C-H (op bend)
485	0.1412	C-S (op bend), C-S (str), C-O (op bend)
471	10.7826	Phenyl, ethyl,thiazole ring (op bend)
466	49.4251	N22-H32 (op bend)
461	7.3039	S10-C12 (str), C2-1S(op bend)
430	3.1883	C7-H24,C8-H25,C9-H25,C6-H23 (op bend)
411	0.0107	C17- H24,C8-H25,C9-H25,C6-H23 (op bend)
378	0.4325	Ethyl, thiazole ring vibration
357	13.1744	Thiazole,phenyl, methyl group vibration
354	0.9839	S10-C12 (str), C42-H43-H44-H45 (op bend)
344	5.1281	Ring vibration
313	2.2648	Ring vibration
304	0.0512	C-S(str), C-C (str), C-N (str), C-O (str)
302	0.4069	C38-H39-H40-H41(op bend), C35-H36-H37(op bend)
268	2.3475	C38-H39-H40-H41(op bend), C35-H36-H37(op bend)
253	0.5137	C38-H39-H40-H41(op bend), C35-H36-H37(op bend)
237	1.9791	Ring vibration
233	2.4004	C38-H39-H40-H41 (op bend)
192	0.7602	C-S, C-H (op bend)
192	0.6912	Ring vibration
167	0.6604	Ethyl group vibration
158	0.4496	Ring vibration
120	0.3476	Ring vibration
115	0.0775	Ring vibration

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

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. 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-methylphenylaminothiazol)-5oyl]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 (-0.8279eV) and C (11) has more positive charge (0.5246eV).The mulliken atomic charge of all hydrogen and sulpur carries positive charge.

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

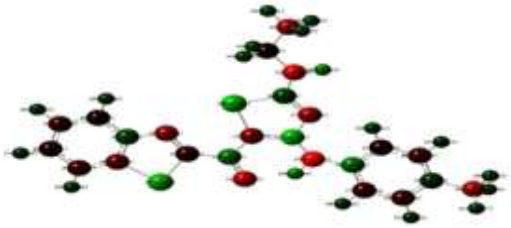


Table 51 Mulliken atomic charges

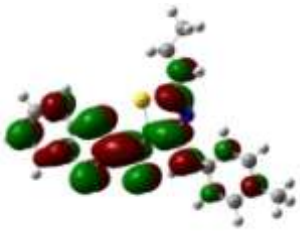
Atom	Mulliken atomic charges	Atom	Mulliken atomic charges
S1	0.48742	H24	0.1316
C2	-0.1287	H25	0.1317
N3	-0.4177	H26	0.1479
C5	0.1946	H27	0.3842
C6	-0.2892	H28	0.1411
C7	0.0631	H29	0.1272
C8	-0.1500	H30	0.1603
C9	-0.1734	H31	0.3426
S10	0.5162	H32	0.3426
C11	0.5246	C33	0.1778
C12	-0.3390	N34	-0.4564
C13	0.3128	C35	-0.0824
O14	-0.5346	H36	0.1747
N15	-0.8279	H37	0.1747
C16	0.3324	C38	-0.445
C17	-0.1850	H39	0.1552
C18	-0.1465	H40	0.1606
C19	0.0917	H41	0.1552
C20	-0.1644	C42	-0.4714
C21	-0.1017	H43	0.1510
N22	-0.6491	H44	0.1510
H23	0.1463	H45	0.1397

HOMO-LUMO energy gaps

The relative energy of the molecular orbitals have been calculated and a graphical representation of the highest occupied molecular orbital (HOMO) and the lowest un occupied molecular orbital (LUMO) of 2-[2-(ethylamino-4-methylphenylaminothiazol)-5oyl]benzothiazole are given in **figure 4**. LUMO is an electron acceptor that represents the ability to obtain an electron and HOMO represents the ability to donate an electron. The HOMO-LUMO energy gap of 2-[2-(ethylamino-4-methylphenylaminothiazol)-5oyl]benzothiazole have been calculated at the B3LYP/6-31G level are shown in **Table 4**.

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

HOMO



LUMO

Table 4 HOMO-LUMO energy value calculated by B3LYP/6-31G level

Paremeters (a.u)	B3LYP/6-31G
HOMO	**-0.07851**
LUMO	**-0.18946**
HOMO-LUMO	**0.11095**

IV. Conclusion

The structure of 2-[2-(ethylamino-4-methylphenylaminothiazol)-5oyl]benzothiazole was optimized by the DFT methods using the basis sets 6-311G.Using the optimized geometry,the vibrational frequencies,have been found to agree well with the literature reported values.The energy of highest occupied molecular orbital (HOMO) and lowest un occupied molecular orbital (LUMO) is also made.

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