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Synthesis, structural and spectral analysis of 2-[2-(Butylamino-4-phenylaminothiazol)-5-oyl] benzothiazole by DFT study

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Abstract

The compound 2-[2-(Butylamino-4-phenylaminothiazol)-5oyl]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

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-[2,4-bis(alkylamino)thiazol-5oyl]benzothiazole using DFT/B3LYP method. A systematic study on vibrational spectra and structure of 2-[2-(Butylamino-4-phenylaminothiazol)-5-oyl]benzothiazole.

Computational details

The DFT computation of 2-[2-(Butylamino-4-phenylaminothiazol)-5oyl] benzothiazole has been performed using Gaussian' 09 program package at the Becke-3Lee-Yang-Parr(B3LYP) level with standard 6-311G 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[5].The optimized structure of 2-[2-(Butylamino-4-phenylaminothiazol)-5-oyl]benzothiazole is given in figure 1.The optimized structural parameter calculated by B3LYP level with 6-311G basis set are given in Table 1.

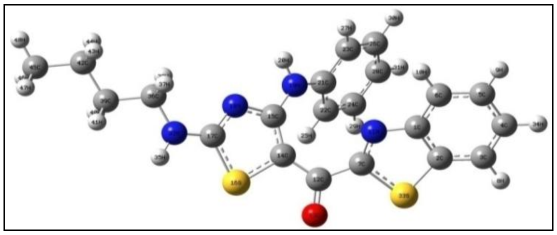


Fig 1: Optimized structure of 2-[2-(Butylamino-4-phenylaminothiazol)-5oyl]benzothiazole

Table 1: Optimized geometrical parameters of 2-[2-(Butylamino-4-phenylaminothiazol)-5oyl]benzothiazole at B3LYP with 6-311G level

Parameters	Bond lengths(Å) Calculated	Parameters	Bond angles(◦) Calculated	Parameters	Dihedral angle(◦) Calculated
C1-C2	1.4158	C2-C1-C6	120.093	C6-C1-C2-C3	-0.3499
C1-C6	1.4016	C2-C1-N11	115.1965	C6-C1-C2-S33	179.0499
C1-N11	1.3975	C6-C1-N11	124.7096	N11-C1-C2-C3	179.8134
C2-C3	1.3947	C1-C2-C3	120.9802	N11-C1-C2-S33	-0.7869
C2-S33	1.8109	C1-C2-S33	110.344	C2-C1-C6-C5	0.2514
C3-C4	1.3945	C3-C2-S33	128.6726	C2-C1-C6-H10	-179.6848
C3-H8	1.0806	C2-C3-C4	118.2985	N11-C1-C6-C5	-179.9283
C4-C5	1.4083	C2-C3-H8	121.0738	N11-C1-C6-H10	-179.9283
C4-H34	1.0816	C4-C3-H8	120.6275	C2-C1-N11-C7	0.1354
C5-C6	1.3898	C3-C4-C5	121.1024	C6-C1-N11-C7	0.0317
C5-H10	1.0813	C3-C4-H34	119.3143	C1-C2-C3-C4	-179.7965
C6-H11	1.0801	C5-C4-H34	119.5833	C1-C2-C3-H8	0.2001
C7-C12	1.2956	C4-C5-C6	120.6216	S33-C2-C3-C4	-179.978
C7-S33	1.4793	C4-C5-H9	119.5211	S33-C2-C3-H8	-179.079
C12-O13	1.8554	C6-C5-H9	119.8573	C1-C2-S33-C7	0.7429
C12-C14	1.2665	C1-C6-C5	118.9029	C3-C2-S33-C7	0.9275
C14-C15	1.4326	C1-C6-H10	119.0731	C2-C3-C4-C5	-179.7316
C14-S16	1.396	C5-C6-H10	122.024	C2-C3-C4-H34	0.0389
C15-N18	1.8585	N11-C7-C12	127.9005	H8-C3-C4-C5	179.9329
C15-N19	1.3932	N11-C7-S33	115.0886	H8-C3-C4-H34	-179.738
S16-C17	1.372	C1-N11-C7	116.8074	C3-C4-C5-C6	0.1101
C17-N18	1.8296	C7-C12-O13	113.0213	C3-C4-C5-H9	-0.1326
C17-N32	1.3172	C7-C12-C14	117.2708	H34-C4-C5-C6	179.8422
N19-H20	1.3485	O13-C12-C14	121.6109	C4-C5-C6-C1	179.9737
N19-C21	1.0091	C12-C14-C15	120.9257	C4-C5-C6-H10	-0.0514
C21-C22	1.413	C12-C14-S16	137.9546	H9-C5-C6-C1	-0.0156
C21-C23	1.4027	C15-C14-S16	113.0485	H9-C5-C6-H10	179.9187
C22-C24	1.4039	C14-C15-N18	108.0485	C12-C7-N11-C1	-179.9904
C22-H20	1.3947	C14C15-N19	116.2979	S33-C7-N11-C1	-0.0561
C23-C26	1.0797	C15-C16-N20	130.8737	N11-C7-C12-O13	175.3504
C23-H27	1.3942	N18-C15-N19	112.7896	N11-C7-C12-C14	0.7466
C24-C28	1.0827	C14-S16-C17	86.4782	S33-C7-C12-O13	-158.4195
C24-H29	1.3981	S16-C17-N18	114.9915	S33-C7-C12-C14	16.5803
C26-C28	1.0817	S16-C17-N32	121.2594	N11-C7-S33-C2	16.1047
C26-H30	1.3972	N18-C17-N32	123.7076	C12-C7-S33-C2	-168.3955
C28-H31	1.0819	C15-N18-C17	112.9138	C7-C12-C14-C15	-0.99
N32-H35	1.0812	C15-N19-H20	111.8568	C7-C12-C14-S16	-176.2208
N32-C36	1.0064	C15-N19-C21	131.2734	O13-C12-C14-C15	18.289
C36-H37	1.4712	H20-N19-C21	115.7882	O13-C12-C14-S16	-155.3912
C36-H38	1.0952	N19-C21-C22	122.7441	C12-C14-C15-N18	-166.8924
C36-C39	1.0893	N19-C21-C23	117.8376	C12-C14-C15-N19	-19.4274
C39-H40	1.5322	C22-C21-C23	119.2895	S16-C14-C15-N18	-166.1854
C39-H41	1.0942	C21-C22-C24	119.8922	S16-C14-C15-N19	16.2746
C39-C42	1.0971	C21-C22-H25	120.1678	C2-C14-S16-C17	7.6733
C42-H43	1.5384	C24-C22-H25	119.8972	C15-C14-S16-C17	-169.8668
C42-H44	1.095	C21-C23-C26	120.1678	C14-C15-N18-C17	-169.0022
C45-H46	1.0948	C21-C23-H27	119.9307	N19-C15-N18-C17	-6.5321
C45-H47	1.5356	C26-C23-H27	120.3804	C14-C15-N19-H20	-4.3876
C45-H48	1.0926	C22-C24-C28	119.3941	C14-C15-N19-C21	173.5951
		C22-C24-H29	120.2213	N18-C15-N19-H20	-165.5769
		C28-C24-H29	120.8346	N18-C15-N19-C21	27.0683
		C23-C26-C228	119.1106	C14-S16-C17-N18	16.8151
		C23-C26-H30	120.0535	C14-S16-C17-N32	-150.5397
		C28-C26-H30	120.3656	S16-C17-N18-C15	4.6345
		C24-C28-C26	119.4681	N32-C17-N18-C15	-177.624
		C24-C28-H31	120.1632	S16-C17-N32-H35	-1.327
		C26-C28-H31	119.2278	S16-C17-N32-C36	-179.0061
		C17-N32-H35	120.3694	N18-C17-N32-H35	6.4241
		C17-N32-C36	120.4028	N18-C17-N32-C36	-177.715
		H35-N332-C36	118.8779	C15-N19-C21-C22	-176.0368
		C2-S33-C7	122.9818	C15-N19-C21-C23	-0.1759

		N32-C36-H37	118.0159	H20-N19-C21-C22	19.8626
		N32-C36-H38	86.3376	H20-N19-C21-C23	-164.2981
		N32-C36-C39	109.9129	N19-C21-C22-C24	-147.0962
		H37-C36-H38	107.45	N19-C21-C22-H25	28.743
		H37-C36-C39	110.9098	C23-C21-C22-C24	176.425
		H38-C36-C39	107.0582	C23-C21-C22-H25	-2.8178
		C36-C39-H40	110.3651	N19-C21-C23-C26	0.6437
		C36-C39-H41	111.0299	N19-C21-C23-H27	-178.5991
		C36-C39-C42	109.0869	C22-C21-C23-C26	-176.0988
		H40-C39-H41	109.59	C22-C21-C23-H27	4.6487
		H40-C39-C42	112.5434	C21-C22-C24-C28	-0.1111
		H41-C39-C42	106.7881	C21-C22-C24-H29	-179.3636
		C39-C42-C43	109.6931	H25-C22-C24-C28	0.5796
		C39-C42-H44	108.9741	H25-C22-C24-H29	179.8269
		C39-C42-C45	120.4658 109.3013	C21-C23-C26-C28	178.665
		H43-C42-H44	109.1342	C21-C23-C26-H30	-0.9285
		H43-C42-C45	112.9063	H27-C23-C26-C28	-0.4964
		H44-C42-C45	1063088	H27-C23-C26-H30	-179.8526
		C42-C45-H46	109.4977	C22-C24-C28-C26	178.7498
		C42-C45-H47	111.1574	C22-C24-C28-H31	-0.6063
		C42-C45-H48	111.1719	H29-C24-C28-C26	-0.0259
		H46-C45-H47	111.1758	H29-C24-C28-H31	179.9263
		H46-C45-H48	107.7198	C23-C26-C28-C24	179.5638
		H47-C45-H48		C23-C26-C28-H31	-0.484
				H30-C26-C28-C24	0.5637
				H30-C26-C28-H31	-179.3884
				C17-N32-C36-H37	179.9154
				C17-N32-C36-C39	-0.0368
				H35-N32-C36-H37	-83.5476
				H35-N32-C36-H38	32.6148
				H35-N32-C36-C39	154.1339
				N32-C36-C39-H40	92.347
				N32-C36-C39-H41	-151.4906
				N32-C36-C39-C12	-29.9715
				H37-C36-C39-H40	-58.8495
				H37-C36-C39-H41	57.7377
				H37-C36-C39-C42	179.1638
				H38-C36-C39-H40	179.0955
				H38-C36-C39-H41	-64.3173
				H38-C36-C39-C42	57.1088
				C36-C39-C42-H43	60.5443
				C36-C39-C42-H44	177.1315
				C36-C39-C42-C45	-61.4421
				H40-C39-C42-H43	-57.748
				H40-C39-C42-H44	58.1294
				H40-C39-C42-C45	-179.8562
				H41-C39-C42-C43	-179.3908
				H41-C39-C42-H44	-63.5134
				H41-C39-C42-C45	58.501
				C39-C42-C45-H46	64.0283
				C39-C42-C45-H47	179.9057
				C39-C42-C45-H48	-58.0799
				H43-C42-C45-H46	-59.9316
				H43-C42-C45-H47	60.0605
				H43-C42-C45-H48	-179.9416
				H44-C42-C45-H46	178.0591
				H44-C42-C45-H47	-61.9488
				H44-C42-C45-H48	58.0491

Results and discussion

Molecular geometry

The optimized structure of 2-[2-(Butylamino-4-phenylaminothiazol)-5oyl]benzothiazole is given in figure 1.The optimized structural parameter calculated by B3LYP level with 6-311G basis set are given in Table1.The self-consistent field(SCF) energy of 2-[2-(Butylamino-4-phenylaminothiazol)-5oyl]benzothiazole at B3LYP level with the basis set 6-311G is found to be -1902.8297 a.u; with dipole moment 5.8946 Debye.The bond lengths of C1-C2,C2-C3,C3-C4,C4-C5,C5-C6 and C6-C1 shows double bond character(aromatic bond). similarly, the bond lengths of C21-

C22,C22-C24,C24-C28,C28-C26,C26-C23 and C23-C221 shows double bond characters (aromatic bond).The bond angle (C2-S33-C7) is very less (86.337°**)** than the bond angle (N11-C7-C12)127.900° which is due to the fact that electronegativity of nitrogen is greater than sulphur. The dihedral angles shows that the molecule consists of two planes, indole ring lies in one plane but the thiazole and phenyl rings are lying in another plane.

Vibrational assignments

In order to obtain the spectroscopic signature of the title compound, we performed a frequency calculation analysis[6].Vibrational frequency were calculated by using B3LYP/6-311G, method. 2-[2-(Butylamino-4-phenylaminothiazol)-5oyl] benzothiazole molecules consists of 48 atom therefore it got 138 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 6-311G 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 [7] 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 [8] absorb at 1615-1580 cm^{-1}.The N-H in-plane bending vibration computed by B3LYP/6-311G 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 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 [9] 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 [10] in the region 999-750cm^{-1}.In the present work, the C-H out-of-plane bending vibration computed by B3LYP/6-311G method good agreement with literature observation.Generally, the carbon-carbon stretching vibrations in aromatic compound from the band in the [11] 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/6-311G 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 [12] 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 [13] 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.

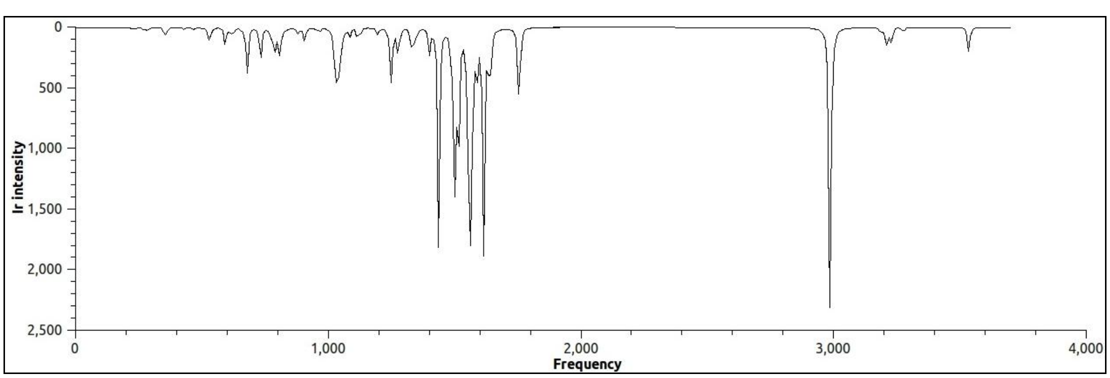


Fig 4: Calculated IR spectrum of 2-[2-(Butylamino-4-phenylaminothiazol)-5oyl]benzothiazole

Table 2: Selected theoretical vibrational assignments along with their intensities of 2-[2-(Butylamino-4-phenylaminothiazol)-5oyl]benzothiazole

calculated at B3LYP/6-311G level

Scaled frequency (cm^{-1})	Intensity (km)Mol^{-1}	Assignments
3484	84.495	N32-H35 str(sym)
3448	40.825	N19-H20 str(sym)
3081	15.554	C6-H10,C5-H9,C4-H34,C3-H8 str(sym)
3078	3.9744	C22-H25,C24-H29,C28,H31,C26-H30 str(sym)
3072	29.611	C3-H8,C4-H34,C5-H9,C6-H10str (asym)
3068	31.9468	C22-H25,C26-H30,C28-H31,C24-H29,C23-H27str(asym)
3058	14.226	C3-H8,C4-H34,C5-H9,C6-H10str(asym)
3053	27.994	C22-H25,C23-H27,C26-H30,C28,H31,C24,H29str(asym)
3045	2.1032	C3-H8,C4-H34,C5-H9,C6-H10str(asym)
3044	1.1769	C22-H25,C23-H27,C26-H30,C28-H31,C24-C29str(asym)
3033	8.337	C23-H27,C26-H30,C28-H31,C24-H29str(asym)
2967	33.124	C36-H38-H37,C39-H41-H40,C42-H43-H44,C45-H47-H45,str(asym)
2964	48.511	C45-H46-H47-H48,C42-H43-H44str(asym)
2957	59.010	C45-H46-H47,C42-H43-H44,C45-H48,C36-H38-H37str(asym)
2923	34.078	C39-H41-H40,C36-H37-H38,C42-H43-H44,C45-H47-H46str(asym)
2901	9.0670	C42-H43-H44,C39-H40-H41,C36-H37-H38str(asym)
2890	42.336	C45-H46-H47,C45-H48(sym)str
2881	52.858	C42-H43-H44,C45-H48,C36-H37-H38asym(str)
2877	24.991	C36-H37-H38,C39-H41-H40,C42-H43-H44asym(str)
2866	18.530	C39-H40-H41,C36-H37-H38,C42-H43-H44sym(str)
1580	31.088	C23-H27,C26-H30,C24-H29,C22-H25(ip bend)C-C(str),N18-C17(str)
1574	2.2617	N19-H20,C-H(ip bend),C-C(str),C17-N18(str)
1571	6.3170	N19-H20,C-H(ip bend),C-C(str),C-S(str),C-O(str)
1545	286.13	N32-H35,N19-H20,C-H(ip bend),N18-C17(str),C-C(str)
1532	9.6337	C3-H8,C4-H34,C5-H9,C6-H10,C-S(ip bend),C-C(str)
1523	635.20	N32-H35,N19-H20,C36-H37,H38(ip bend),C-N(str)
1500	310.98	N32-H35,C-H(ip bend),C12-O139str),C-N(str)
1490	312.01	N19-H20,N32-H35,C-H(ip bend),C-O(str),C-N(str)
1489	293.99	C7-N11,C15-N19(str),C-S,C-O,C-H(ip bend)
1486	306.68	N19-H20,N32-H35,C-H(ip bend),C12-O13(str),C-N(str)
1484	206.25	N32-H35,C23-H27,C26-H30,C24-H29,C22-H25(ip bend)C-O(str),C-N(str),C-C(str)
1480	14.323	C45-H46-H47-H48(ip bend)N32-H35(ip bend)
1478	9.2974	N32-H35,C-H(ip bend),C-C(str),C17-N18,C7-N11,C12-O13(str)
1475	21.145	C36-H37-H37-H38,C39-H40-H41,C42-H43-H44,C45-H46-H47-H48(ip bend)
1470	9.7838	C39-H40-H41,C42-H43-H44,C45-H46-H47-H48(ip bend)
1458	362.04	C12-O13,C-C,C-N(str)C-S,C-H(ip bend)
1442	12.732	C5-H9,C4-H34,C3-H8,C6-H10(ip bend),C-O(str)
1432	165.99	C23-C27,C26-H30,C28-H31,C24-H29,C22-H25,N19-H20(ip bend)
1415	10.558	C6-H10,C5-H9,C4-H34,C3-H8,C2-S33(ip bend),C-N(str)
1395	1.800	C45-H46-H47-H48(ip bend)
1357	6.513	C36-H37-H38,C39-H40-H41,C42-H43-H44(ip bend),C-N(str)
1346	160.08	C36-H37-H38,C39-H40-H41,C42-H43-H44,C45-H47(ip bend),C-N,C-O(ip bend)
1341	329.242	C-N(str),C36-H37-H38,N32-H35(ip bend)
1330	22.758	C23-H27,C26-H30,C28-H31,C24-H29,C22-H25(ip bend),C12-O13(ip bend)
1300	1.5570	C42-H43-H44,C39-H40-H41,C45-H47-H46-H48(ip bend)
1299	71.396	C7-N11,C12-O13(str),C-H(ip bend),C-N(ip bend)
1287	22.059	C42-H43-H44,C39-H40-H41,C45-H47-H46-H48(ip bend)
1284	12.021	C-C(str),C-O,C-N,C-S,C-H(ip bend)
1278	12.012	C42-H43-H44,C39-H40-H41,C45-H47-H46-H48(ip bend)
1268	7.3188	C6-H10,C5-H9,C4-H34,C3-H8,C2-S33,C1-N11(ip bend)
1249	36.250	C23-H27,C26-H30,C28-H31,C24-H29,C22-H25,C-N(ip bend)
1245	53.314	C42-H43-H44,C39-H40-H41,C45-H47-H46-H48,C-N(ip bend)
1232	35.048	C-H,C-N,C-O(ip bend)
1204	14.360	C23-H27,C26-H30,C28-H31,C22-H25,C24-H29(ip bend)
1176	10.851	C17-S16,C17-N18,C7-N11,(str),N-H,C-H(ip bend)
1167	144.84	C23-H27,C26-H30,C28-N31,C22-H25,C24-H29(ip bend)
1162	3.982	C6-H10,C5-H9,C4-H34,C3-H8,C2-S33(ip bend)
1159	0.094	C36-H37-H38,C39-H40-H41,C42-H43-H44,C45-H46-H47-H48(ip bend)
1150	12.704	C6-H10,C5-H9,C4-H34,C3-H8,C-N(ip bend),C12-O13,C2-S33(str)
1109	10.174	C6-H10,C5-H9,C4-H34,C3-HH8(ip bend),C-C,C-S(str)
1104	2.022	C23-H27,C26-H30,C28-H31,C24-H29,C22-H25,C-N(ip bend),C-C,C-O(str)
1084	3.535	C6-H10,C5-H9,C4-H34,C3-H8,C36-H37-H38,C39-H40-H41,C42-C42-H43-H44 (ip bend)
1067	16.309	C14-S16,C2-S339str),C-N,C-H(ip bend)

1034	0.799	C36-H36-H37-N32-H35(ip bend),C36-N32(str)
1031	20.318	C23-H27,C26-H30,C28-H31,C24-H29,C22-H25(ip bend)
1016	3.221	C6-H10,C5-H9,C4-H34,C3-H8(ip bend),C-C(str)
1011	3.511	C23-H27,C26-H30,C28-H31,C24-H29,C22-H25(ip bend),C-C(str)
998	7.462	C23-H27,C26-H30,C28-H31,C24-H29,C22-H25(ip bend),butyl group,C-N(ip bend)
987	1.499	C-6-H10,C5-H9,C4-H34,C3-H8(ip bend)
982	1.5263	C23-H27,C26-H30,C28-H31,C24-H29,C22-H25(ip bend)
981	0.8451	C-N,C-C,C-S(str),C-H,C-N(ip bend)
978	0.040	C5-H9,C6-H10,C4-H34,C3-H8(op bend)
959	0.158	C36-H37-H38,C39-H40-H41,C42-H43-H44,C45-H46-H47-H48(op bend)
951	67.550	C23-H27,C26-H30,C28-H31,C24-H29,C22-H25(op bend)
943	1.749	C-H,N32-H35(op bend)
941	2.907	C6-H10,C5-H9,C4-H34,C3-H8(op bend)
903	10.876	C23-H27,C26-H30,C28-H31,C24-H29,C22-H25,C-N(op bend)
883	7.264	C23-H27,C26-H30,C28-H31,C24-H29,C22-H25(op bend)
855	1.480	C23-H27,C26-H30,C28-H31,C24-H29,C22-H25(op bend)
850	27.343	C36-H37-H38,C39-H40-H41,C42-H43-H44,C45-H46-H47-H48(op bend)
842	4.595	C-H,C-N(op bend),C-S,C-0(str)
827	2.504	C6-H10,C5-H9,C4-H34,C3-H8,C12-O13(op bend)
801	0.1608	C23-H27,C26-H30,C28-H31,C24-H24,C22-H25(op bend)
780	2.2244	C12-O13,C14-S16(str),C-H(op bend)
761	62.624	C36-H37-H38,C39-H40-H41,C42-H43-H44,C45-H46-H47-H48(op bend)
755	76.387	C12-O13,C-H(op bend),C-S(str)
746	31.932	C6-H10,C5-H9,C4-H34,C3-H8,C12-O13(op bend)
730	3.932	C-0,C-H,C-N(op bend),C-N,C-C(str)
721	31.834	C23-H27,C26-H30,C28-H31,C24-H29,C22-H29(op bend)
719	29.170	C6-H10,C5-H9,C4-H34,C3-H8,(op bend)C-S,C-C(str)
706	36.935	N19-H20,N32-H35(op bend),C-H(op bend)
688	26.928	N19-H20,N32-H35,C-H(op bend),C-S(str)
676	3.041	C-N,C-H(op bend).C7-N11,C-C,C7-S33(str)
646	12.782	C23-H27,C26-H30,C28-H31,C24-H29,C22-H25(op bebend),C-N(str)
628	10.148	C7-S33,C14-S16-C17(str),C12-O13,C-N,C-H(op bend)
623	24.517	N19-H20,C17-S16,C-H,C-N(op bend),N18-C17(str)
619	8.770	N18-C17(str),C-H,C-N(op bend)
584	74.258	C-H(op bend),C-N,C-S(op bend)N18-C17(str)
579	7.933	N19-H20,C14-S16(op bend)
576	1.855	N19-H20,C23-H27,C26-H30,C28-H31,C24-H29,C22-H25(op bend)
563	4.843	C-H,C-O,C-S,C-N(op bend)
539	32.650	C-H,C-O,C-S,C-N(op bend)
494	15.265	C2-S33,C-H(op bend)
488	54.294	Ring vibration
483	61.629	C17-S16(str)
479	0.986	C6-H10,C5-H9,C4-H34,C3-H8,C2-S33(op bend)
471	40.471	C23-H27,C26-H30,C28-H31,C24-H29,C22-H28(op bend)
447	8.350	ring vibration
429	9.348	ring vibration
409	0.325	C-N,C-H,C-O,C-S(op bend)
404	4.121	N19-H20,C12-O13,C14-S16(op bend)
367	4.414	ring vibration
336	9.947	ring vibration
315	16.065	ring vibration
304	1.619	ring vibration
296	3.695	ring vibration
273	4.423	ring vibration
248	5.501	ring vibration
237	3.461	phenyl ring vibration
235	4.997	ring vibration
208	4.434	ring vibration

Abbreviations: sym-symmetric, asym-asymmetric, str-stretching, p 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-(Butylamino-

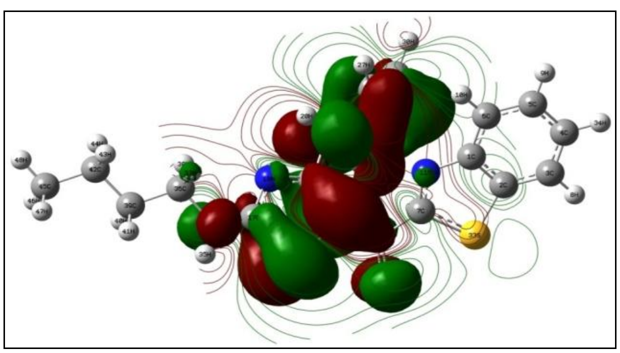
4-phenylaminothiazol)-5oyl] benzothiazole has been calculated using B3LYP/6-311G basis set. The corresponding characteristics of the atomic charge populations of the constituent atoms are presented in Table 3. It was found that N (19) has more negative charge(-0.8435eV) and C(15) has more positive charge(0.6950eV).The mulliken atomic charge of all hydrogen and sulpur carries positive charge.

Table 3: Mulliken atomic charges

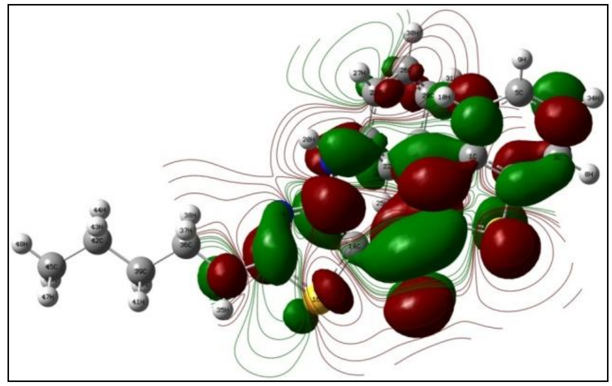
Atom	Mulliken atomic charges	Atom	Mulliken Atomic Charges
C	0.1775	H	0.1998
C	-0.3727	C	-0.1615
C	-0.1250	H	0.1603
C	-0.1564	C	-0.1338
C	-0.1560	H	0.1551
C	-0.0186	H	0.1493
C	-0.2115	H	0.1522
H	0.17058	N	-0.5233
H	0.15625	S	0.4075
H	0.16930	H	0.1526
N	-0.3443	H	0.3122
C	0.4422	C	-0.2003
O	-0.3915	H	0.1885
C	-0.5504	H	0.2164
C	0.6950	C	-0.3658
S	0.3376	H	0.1924
C	0.1101	H	0.1743
N	-0.4043	C	-0.3571
N	-0.8435	H	0.1788
H	0.3405	H	0.1811
C	0.3471	C	-0.5183
C	-0.1156	H	0.1789
C	-0.1905	H	0.1773
C	-0.1631	H	0.1806

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-[2,4-bis(alkylamino)thiazol-5oyl]benzothiazole are given in figure 2. 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-(Butylamino-4-phenylaminothiazol)-5oyl]benzothiazole have been calculated at the B3LYP/6-311G level are shown in Table 4.



HOMO



LUMO

Fig 3: HOMO-LUMO of of 2-[2-(Butylamino-4-phenylaminothiazol)-5oyl]benzothiazole

Table 4: Homo-Lumo Energy Value Calculated By B3lyp/6-311g Level

Paremeters (a.u)	B3LYP/6-311G
HOMO	-0.2043
LUMO	-0.0885
HOMO-LUMO	0.1158

Conclusion

The structure of 2-[2-(Butylamino-4-phenylaminothiazol)-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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