

## Molecular structure, Vibrational assignment, HOMO-LUMO and Mulliken analysis of 2-[4-amino-2-(4-methylphenylamino) thiazol-5-oyl]benzothiazole(AMPATOB)

Yardilya A.<sup>1\*</sup>, Abbs Fen Rejib T.F.<sup>2</sup>

<sup>1</sup>Department of Chemistry & Research Centre, Scott Christian College (Autonomous), Nagercoil - 629003, Tamilnadu, India

<sup>2</sup>Department of Chemistry & Research Centre, Nesamony Memorial Christian College, Marthandam - 629165, Tamilnadu, India

\*Corresponding author: [ayardily@gmail.com](mailto:ayardily@gmail.com)

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### Abstract

The compound 2-[4-amino-2-(4-methylphenylamino) thiazol-5-oyl]benzothiazole (AMPATOB) was prepared from 1-(4-methylphenyl)-3-(N-nitroamidino)thiourea and 2-(2-bromoacetyl)benzothiazole in the presence of triethylamine and characterised by FTIR, NMR and mass spectra. The geometry of the molecule was investigated and optimized with the help of B3LYP/ 6-31G density functional theory (DFT) method using Gaussian 09 software package. The calculated geometries such as bond lengths, bond angles, dihedral angles, atomic charges, harmonic vibrational wave numbers and intensities of vibrational bonds of the titled compound were investigated. The experimental <sup>1</sup>H NMR and IR spectrum was compared with theoretical value. The molecule consists of three ring systems, all are lying in one plane.

**Key words:** Benzothiazole, DFT, B3LYP, Thiourea, Triethylamine

### INTRODUCTION

Benzothiazole and its derivatives are the important class of organic compounds. Because of their spectroscopic properties and chemical significance, benzothiazole and its derivatives were studied extensively by spectroscopic and theoretical methods. 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. Benzothiazole analogs of dendrooine derivatives have attracted a great deal of interest due to their biological and commercial importance<sup>1</sup>. In the light of literature survey, these compounds possess benzothiazole unit having a useful pharmacophore moiety and exhibit anti-cancer<sup>2</sup>, anti-allergic<sup>3</sup>, anti-inflammatory<sup>4</sup>, anti-nematode<sup>5</sup>, anti-bacterial<sup>6</sup>, anti-fungal<sup>7</sup>, anti-tubercular<sup>8</sup>, a tropical carbonic anhydrase inhibitor<sup>9</sup> and antioxidant activities<sup>10</sup>.

The study of benzothiazoles is, therefore, of practical and theoretical importance. A density functional theory and structure-activity relationship of different benzothiazole derivatives have been calculated by using HF 6-31G(d) and B3LYP6-31G(d)11. Hakan Arslan reported the molecular structure and vibrational frequencies in the ground state have been investigated with ab initio/HF and density functional methods BLYP, B3LYP, B3PW91 and mPW1PW91 for 2-(4-methoxyphenyl)benzothiazoles derivatives implementing the standard 6-311G(d,p) set 12. Sathyanarayanamoorthi et al studied the optimized molecular geometry, vibrational frequencies, infrared activities and Raman scattering activities of the molecule in the ground state have been calculated by using ab initio HF and DFT(B3LYP) methods with 6-311++G(d,p) basis set13. Patil et al reported the DFT study on dihydroxyphenylbenzothiazole by using B3LYP/6-31G (d)14. The main objective of this paper is to present, more accurate vibrational assignments, bond lengths, bond angles, atomic charges and HOMO-LUMO of 2-[4-amino-2-(4-methylphenylamino)thiazol-5-oyl]benzothiazole (AMPATOB) using DFT/B3LYP method. A systematic study on vibrational spectra and structure of AMPATOB has been carried out.

### EXPERIMENTAL DETAILS

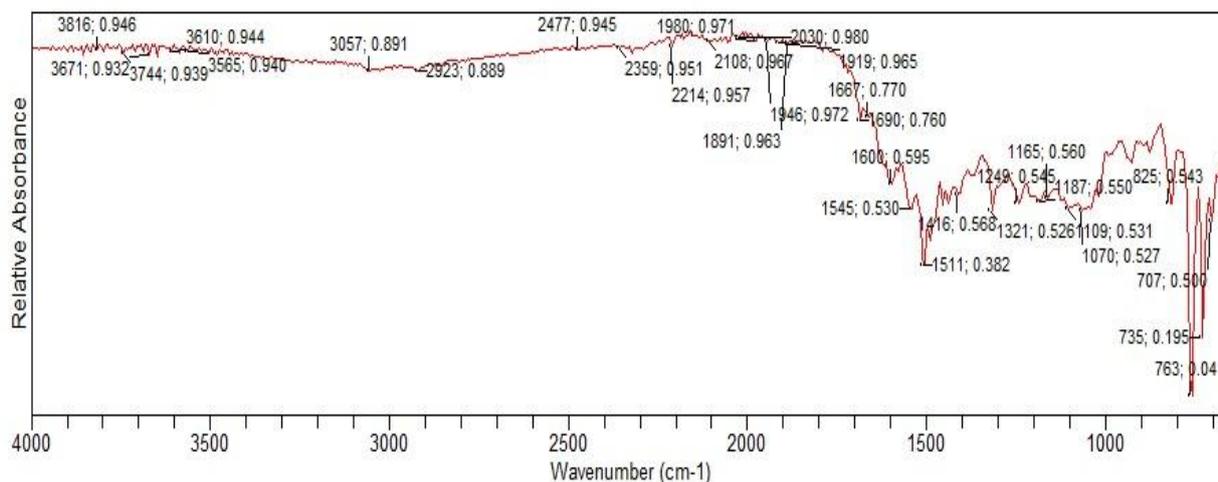
#### Preparation

A solution of 2-(2-bromoacetyl)benzothiazole (0.254 g, 1 mmol) obtained from 2-(1-hydroxyethyl)benzothiazole<sup>15,16</sup> in DMF (2 mL) was added to a solution of 1-(4-methylphenyl)-3-(N-nitroamidino)thiourea (1 mmol) in DMF (2 mL). The reaction mixture was stirred well and triethylamine (0.3mL, 2mmol) was added and warmed at 50-60°C for 15 min. It was cooled and poured into ice-cold water with constant stirring. The yellow precipitate thus obtained was filtered, washed with water and dried. The crude product was purified by crystallization by using methanol: water (2:1), and then using benzene : petroleum ether (1:1).

#### Physical measurements

The reagents and solvents used were of AR grade. All chemicals were purchased from Merck Specialities Pvt Ltd and HiMedia Laboratories Pvt Ltd. The spectra were recorded on JEOL DRX 300 NMR spectrometer (300 MHz for <sup>1</sup>H-NMR) and Agilent Cary 630 FTIR spectrometer. Melting points were uncorrected. The obtained yield was 92% and mp 277°C. Fig 1 shows experimental IR spectrum of compound.

Experimental <sup>1</sup>H NMR (DMSO-d<sub>6</sub>): 2.30(s, 3H, CH<sub>3</sub>), 7.20(d, 8.1 Hz, 2H, 2ArH), 7.50-7.68(m, 4H, H-5, H-6, 2ArH), 8.08(d, 7.8 Hz, 1H, H-4), 8.20(d, 7.8 Hz, 1H, H-7), 8.60 (br, 1H, NH), 8.75(br, 1H, NH), 10.98(s, 1H, NH).



**Figure 1: Experimental IR spectrum of AMPATOB**

### Computational details

The DFT calculations were performed on the Gaussian 09 program package without any constraint on the geometry. Geometries of AMPATOB were optimized at B3LYP/6-31G basis set. Optimized structural parameters were used in the vibrational frequency calculations at DFT level to confirm the structure as minima. Using Gauss view 5.0.9 molecular visualization program, the vibrational frequency assignments and other parameters were made. All the calculations were done for the optimized structures in gas phase.

## RESULTS AND DISCUSSION

### Molecular geometry

AMPATOB was subjected to geometry optimizations in the ground state. The optimized structural parameter of it was calculated by DFT/B3LYP 6-31G basis set is listed in Table 1 in accordance with the atom numbering scheme given in Fig 2. The self-consistent field(SCF) energy of AMPATOB at B3LYP level with the basis set 6-31G is found to be -1775.6144 a.u. with dipole moment 4.6186 Debye. The bond lengths of C1-C2, C2-C3, C3-C4, C4-C5, C5-C6, C1-C6, C12-N34, C12-C13 and C21-N20 show double bond character(aromatic bond). Bond length of C7-C15 possesses single bond character. Similarly, the bond lengths of C22-C23, C24-C22, C23-C25, C27-C24, C25-C29 and C29-C-27 show double bond characters.

### Mulliken atomic charges

Atomic charges are very much dependent on how the atoms are defined. It plays an important role in the application of quantum chemical calculations to molecular systems. The Mulliken atomic charges calculated by B3LYP level with 6-31G basis set are given in Table 2. From the Table 2, C6 has more negative charge (-0.066e) and C13 has more positive charge (0.537e). All hydrogen carries positive charge.

**Table 1- Optimized geometrical parameters of AMPATOB**

Bond length (Å°)					
C1-C2	1.413	C21-14S	1.836	C27-H31	1.081
C2-C3	1.391	14S-C12	1.839	C24-H28	1.085
C3-C4	1.394	C21-N32	1.357	C36-H37	1.117
C4-C5	1.406	N32-C22	1.413	C36-H38	1.117
C5-C6	1.389	C22-C23	1.403	C36-H39	1.070
C6-C1	1.399	C23-C25	1.394	N17-H18	1.013
C1-N34	1.404	C25-C29	1.386	N17-H19	1.036
N34-C7	1.298	C29-C27	1.387	N32-H33	1.017
C7-S35	1.839	C27-C24	1.391	C36-H39	1.070
S35-C2	1.808	C24-C22	1.406	N20-C21	1.308
C7-C15	1.486	C29-C36	1.540	C25-H30	1.082



C15-O16	1.263	C3-H8	1.082	C13-N20	1.395
C15-C12	1.415	C4-H9	1.083	C23-H26	1.078
C12-C13	1.403	C5-H10	1.083		
C13-N17	1.336	C6-H11	1.082		

Bond angle (°)					
C1-C2-C3	121.02	C13-N20-C21	110.10	C5-C6-H11	121.54
C2-C3-C4	118.38	N20-C21-14S	115.20	C1-C6-H11	119.59
C3-C4-C5	120.98	C21-14S-C12	89.30	C13-N17-H18	117.84
C4-C5-C6	120.63	N20-C21-N32	123.10	C13-N17-H19	118.66
C5-C6-C1	118.90	C21-N32-C22	124.58	C21-N32-H33	116.14
C6-C1-C2	120.06	N32-C22-C23	124.58	H33-N32-C22	115.13
C1-C2-S35	110.51	N32-C22-C24	117.40	C22-C24-H28	119.95
C2-S35-C7	86.62	C22-C23-C25	120.49	C27-C24-H28	119.30
S35-C7-N34	115.20	C24-C22-C23	120.40	C24-C27-H31	120.72
C7-N34-C1	113.03	C23-C25-C29	120.40	H31-C27-C29	120.50
N34-C1-C2	114.63	C25-C29-C36	119.11	C29-C25-H30	120.21
C3-C2-S35	128.46	C36-C29-C27	119.11	H30-C25-C23	120.30
S35-C7-C15	112.83	C25-C29-C27	121.77	C25-C23-H26	121.49
N34-C7-C15	131.96	C29-C27-C24	118.77	H26-C23-C22	118.50
C7-C15-O16	116.45	C27-C24-C22	120.74	H37-C36-C29	108.99
O16-C15-C12	122.20	C2-C3-H8	120.92	H38-C36-C29	108.19
C7-C15-C12	121.35	H8-C3-C4	120.69	H39-C36-C29	110.71
C15-C12-C13	137.43	C3-C4-H9	119.46	H18-N17-H19	123.49
C15-C12-S14	112.88	C5-C4-H9	119.55	H37-C36-H39	110.72
C12-C13-N17	126.95	C4-C5-H10	119.56	H38-C36-H39	110.73
N17-C13-N20	117.01	C6-C5-H10	119.79		

Dihedral angle (°)					
C1-C2-C3-H8	-180.00	C12-C13-N17-H18	180.00	H26-C23-C25-C29	-180.00
C2-C3-C4-H9	-180.00	H19-N17-C13-N20	-180.00	C23-C25-C29-C36	180.00
C3-C4-C5-H10	-180.00	N17-C13-N20-C21	180.00	C36-C29-C27-C24	-180.00
C4-C5-C6-H11	180.00	C13-N20-C21-N32	180.00	C25-C29-C36-H39	-148.93
C5-C6-C1-N34	-180.00	N20-C21-N32-H33	179.99	C25-C29-C36-H37	89.57
C1-N34-C7-C15	-180.00	H33-N32-C22-C23	180.00	C27-C29-C36-H38	152.57
C6-C1-C2-S35	-180.00	S14-C21-N32-C22	179.99	C27-C29-C36-H37	-90.43
C2-S35-C7-C15	180.00	N17-C13-C12-S14	-180.00	C25-C29-C27-H31	-180.00
N34-C7-C15-O16	180.00	N32-C22-C23-C25	-180.00	H31-C27-C24-C22	-180.00
C7-C15-C12-S14	180.00	N32-C22-C24-C27	180.00	C29-C27-C24-H28	180.00
S35-C7-C15-C12	-180.00	C22-C23-C25-H30	180.00	H28-C24-C22-C23	180.00
O16-C15-C12-C13	180.00	H30-C25-C29-C27	180.00		
C15-C12-C13-N20	-180.00	H26-C23-C22-C24	180.00		

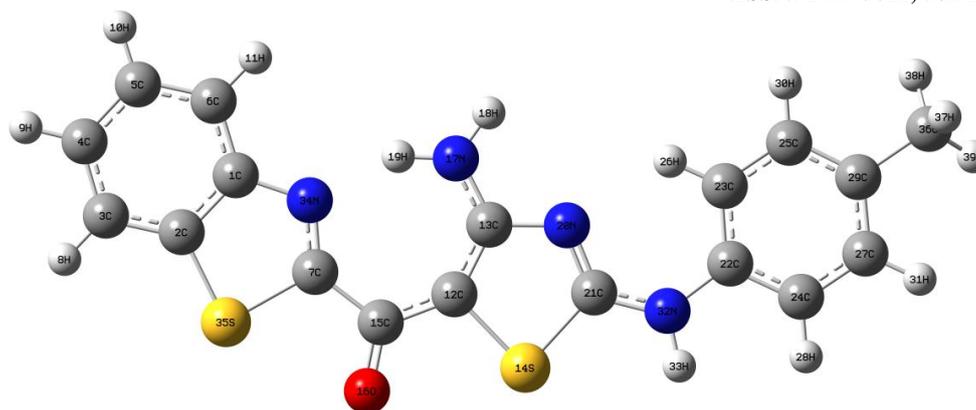


Figure 2: Optimized molecular structure of AMPATOB

### HOMO-LUMO

Optimized geometry of AMPATOB at DFT/B3LYP/6-31G level as shown in Fig. 2. It shows that the frontier molecular orbital of AMPATOB is mainly composed of p atomic orbital, so electronic transition corresponds to above electronic spectra are due to  $n-\pi^*$  and  $\pi-\pi^*$  electronic transitions. Figure 3&4 shows the HOMO-LUMO of APATOB. Analysis of wave function indicates that the electron absorption corresponds to the transition from the ground to the first excited state and is explained by one electron excitation from the highest occupied molecular orbital (HOMO) to the lowest unoccupied molecular orbital (LUMO). The LUMO, i.e., of  $\pi$  nature of A, B and C ring of the compounds is delocalized over the entire C-C and C-O bond. The LUMO as an electron acceptor represents the ability to obtain an electron and HOMO represents the ability to donate an electron.

Table 2: Mullikan atomic charges for AMPATOB

Atom	Charge	Atom	Charge
C1	0.226	C21	0.189
C2	-0.302	C22	0.324
C3	-0.173	C23	-0.107
C4	-0.099	C24	-0.177
C5	-0.155	C25	-0.162
C6	-0.066	H26	0.176
C7	-0.094	C27	-0.14
H8	0.152	H28	0.122
H9	0.136	C29	0.092
H10	0.136	H30	0.129
H11	0.141	H31	0.131
C12	-0.380	N32	0.763
C13	0.537	H33	0.342
S14	0.437	N34	-0.506
C15	0.364	S35	0.512
O16	-0.466	C36	-0.410
N17	-0.765	H37	0.153
H18	0.328	H38	0.141
H19	0.380	H39	0.147
N20	-0.469		

Table 3: Selected experimental and theoretical vibrational assignments along with their intensities of AMPATOB

Abbreviations: *asym.*- asymmetric, *sym.*- symmetric, *vibn.*- vibration, *str.*- stretching, *bend.(ip)*- in-plane bending, *bend.(op)*- out-of-plane bendng, *wag*- wagging, *rock*- raking, *scis*- scissoring, *def.*- deformation.

Experimental IR (cm <sup>-1</sup> )	Calculated IR frequency (cm <sup>-1</sup> )	Intensity(km)mol <sup>-1</sup>	Assignment
3565	3475	97.00	H-N-H str (asym) (H18-N17-H19)
	3405	64.20 21.78	N33-H str (asym) C36-H str(asym)
	3219		
	3153	17.08	C23-H, C25-H, C27-H & C29-H Str (asym)
	3119	12.48	C3-H, C4-H, C5-H & C6-H str (sym)



Experimental IR (cm <sup>-1</sup> )	Calculated IR frequency (cm <sup>-1</sup> )	Intensity(km)mol <sup>-1</sup>	Assignment
	3109	19.87	C23-H, C25-H, C29-H, C27-H & C24-H str (sym)
	3102	3.23	C3-H, C4-H, C5-H & C6-H str (sym)
	3093	17.32	C23-H, C25-H, C29-H, C27-H & C24-H str (sym)
3057	3073	9.50	C27-H & C24-H str (asym)
2923	2867	1081.45	H-N-H str (asym) (H18-N17-H19)
	2101	5.67	C2-S36-C7 str (asym) skeletal vib. of fused benzothiazole Ph ring & NH <sub>2</sub> group
1667	1989 1660	12.26 355.8	C2-S36-C7 str (asym) skeletal vib. of fused benzothiazole Ph ring & NH <sub>2</sub> group C15=O str., H18-N17-H19 def.,(scissoring), N33-H def., str.of benzothiazole C-H, C-N & C=C of phenyl ring
1545	1585	36.07	N33-H34Ar & H18-N17-H19 def. (ip), C21=N20-C13 str. (asym) of thiazole & skeletal vib. of fused benzothiazole Ph ring
	1580	49.67	N33-H34Ar & H18-N17-H19 def. (ip), C21=N20-C13 str. (asym) of thiazole & skeletal vib. of fused benzothiazole Ph ring
	1562	478.77	C15=O str (asym), N20=C21-N33 str (sym), C15- C12=C13 def. (ip), H19-N17-H18 def. (ip), & skeletal vib. of NHAr ring..
	1518	7.95	C=O, N20=C21-N33 str (sym), benzothiazole Ph ring all C-H ip bend, C-C, C=C str (sym) of benzothiazole Ph ring and skeletal vib. of NHAr ring
1511	1515	165.41	H18-N17-H19 def. (scissoring), C=O, C=N, C-N & C-S36 str (sym) of benzothiazole, NHAr & thiazole ring and all C-H, N-H ip bending
	1496	20.46	H18-N17-H19 and all C-H, N-H ip bending, C=O, C=N, C-N & C-S36 str (sym) of benzothiazole, NHAr & thiazole ring (except C2-C3)
	1494	715.14	H18-N17-H19 and all C-H, N-H ip bending, C=O, C=N, C-N & C-S str (sym) of benzothiazole, NHAr & thiazole ring
	1446	156.93	C21=N33, C15=O & NHAr of Ph C-C, C=C str (sym) and NH <sub>2</sub> , NHAr of all C-H ip bend.
	1440	26.47	Fused benzothiazole Ph ring all C-H, & NH <sub>2</sub> ip bend., C=O, C-S36, C=N, C-C & C=C str (sym) of fused benzothiazole Ph ring
1416	1406	849.56	C15=O, C15-C12, C12=C3, C13-N & C21-N20 str (asym) and all C-H & N-H ip bend.
1321	1354	27.69	C=C, C-C, N-H & C-H of NHAr ip bend, C=O str (sym) & skeletal vibn. of fused benzothiazole Ph ring
	1295	11.92	Fused benzothiazole Ph ring all C-H, & NH <sub>2</sub> ip bend., C=O, C-S36, C=N, C-N, C-C & C=C str (sym) of fused benzothiazole Ph ring
	1286	94.22	H18-N17-H19 and all C-H, N-H ip bending, C-C, C=C C=O, C=N, C-N & C-S36 str (asym) of NHAr & thiazole ring and C-C & C=C str (sym) of fused benzothiazole Ph ring
1249	1235	75.53	H18-N17-H19 and all C-H, N-H ip bending, C-C, C=C,C=O, C=N, C-N & C-S36 str (asym) of NHAr & thiazole ring and C-C & C=C str (sym) of fused benzothiazole Ph ring
	1233	14.42	H18-N17-H19 and all C-H, N-H ip bending, C-C, C=C, C=N, & C-N str (asym) of fused benzothiazole Ph ring and C=O,C-S36, C-C & C=C str (sym) of NHAr & thiazole ring



Experimental IR (cm <sup>-1</sup> )	Calculated IR frequency (cm <sup>-1</sup> )	Intensity(km) <sup>mol</sup> <sup>-1</sup>	Assignment
	1202	8.27	H18-N17-H19 and all C-H, N-H ip bending, C-C, C=C, C=N & C-N str (sym) of fused benzothiazole Ph ring, NHAr & thiazole ring
1187	1190	0.94	All C-H & N-H of NHAr ip bend. and C-C, C=C, C=N & C-N str (sym) of NHAr & thiazole ring
	1168	27.75	All C-H & N-H of fused benzothiazole Ph ring, NHAr & thiazole ring ip bend. and C-C, C=C, C=N & C-N str (asym) of NHAr & thiazole ring
	1159	3.19	Fused benzothiazole Ph ring all C H, & NH2 ip bend., C=O, C-S36, C=N, C-N, C-C & C=C str (sym) of fused benzothiazole Ph ring
	1117	4.99	H18-N17-H19 and all C-H, N-H ip bending and C-C, C=C C=O, C=N, C-N & C-S36 str (sym) of NHAr, fused benzothiazole Ph ring & thiazole ring
	1100	9.39	H18-N17-H19 rock. and all C-H, N-H ip bend. C-C, C=C C=O, C=N, C-N, C-S14 & C-S36 str (sym) of NHAr, fused benzothiazole Ph ring & thiazole ring.
1070	1089	26.74	Rock. of NHAr all C-H and C-C, C=C C=O, C=N & C-N str (sym) of NHAr
	1031	133.32	Rock. of NHAr all C-H & NH2group. C-S36, C-S14, C-C, C=C, C=O, C=N & C-N str (sym) of NHAr, fused benzothiazole Ph ring & thiazole ring.
	1023	9.08	C23-H, C25-H, C29-H & C27-H bend. (op)
	1008	0.77	C3-H, C4-H, C5-H, C6-H & N17-H19 bend. (op).
	999	3.92	Bend. (ip) of fused benzothiazole Ph ring & all C-H and skeletal vib. of NHAr & thiazole ring. C-C, C=N & C=C str (sym) of fused benzothiazole Ph ring
	979	0.86	C23-H, C25-H, C29-H, C24-H & C27-H bend. (op)
	974	132.64	C3-H, C4-H, C5-H, C6-H & N17-H19 bend. (op).
	961	28.57	C1=C2 & C12-S14 str (asym), thiazole, & benzothiazole ring bend (ip) and skeletal vibn. of NHAr
	896	15.65	C22, C23-H, C25-H, C29-H, C24-H, C27-H & N33-H bend. (op)
	876	5.62	C3-H, C4-H, C5-H, C6-H, C1, C2, N35, C7, C15, C12, C13 & N17-H19 bend. (op).
	856	26.68	C1=C2 & C12-S14 str (asym), thiazole, & benzothiazole ring bend (ip) and skeletal vib. of NHAr
825	842	1.15	C23-H, C25-H, C29-H, C24-H, C27-H & N33-H bend. (op)
	819	44.45	C1=C2 & C12-S14 str (asym), thiazole, & benzothiazole ring bend (ip) and skeletal vib. of NHAr
	793	9.02	Thiazole, NHAr and benzothiazole bend. (ip)
	779	70.82	C23-H, C25-H, C29-H, C24-H, C27-H, C21, C22 & N33-H bend. (op)
763	762	3.75	C3-H, C4-H, C5-H, C6-H, C1, C2, N35, C7, C15, C12, C13, N20, C21, C23-H, C25-H, C29-H, C24-H, C27-H, N33-H & H18-N17-H19 bend. (op).
735	747	73.07	C3-H, C4-H, C5-H, C6-H, C2, C13 & H18-N17-H19 def. (op).
	709	47.26	C22, C23-H, C25-H, C29-H, C24-H, C27-H & N33-H bend. (op)
	649	25.34	C23-H, C25-H, C29-H, C24-H, C27-H, C21, N20, C13, H18-N17-H19 & N33-H bend. (op)
	631	2.95	All C=C, C-C, C=N, C-N, C-S & C=O bend. (ip)

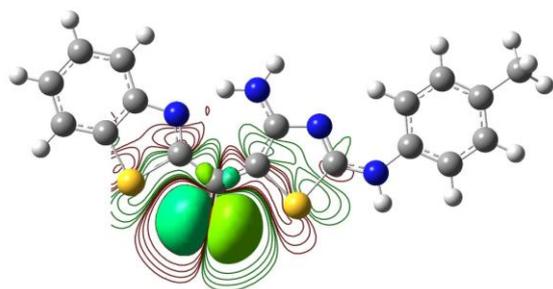


Figure 3: HOMO of AMPATOB

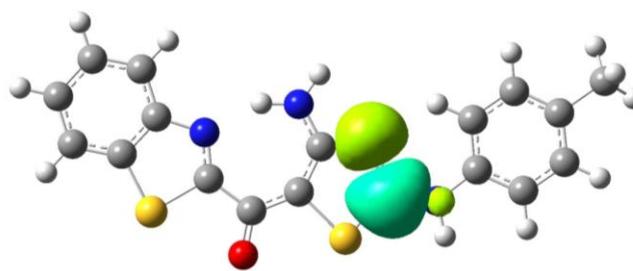


Figure 4: LUMO of AMPATOB

### Vibrational assignments

The spectral assignments of the titled compound has been made on the recorded FT-IR (solid phase) and theoretically predicted wave numbers by DFT/B3LYP/6-31G method. The scaling factor of 0.96 is used for getting theoretical vibrational frequencies. 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 experimental observation. The selected calculated vibrational frequencies are numbered from largest to smallest fundamental wave number. The calculated and experimental wave numbers and intensities of the normal mode of vibrations and corresponding vibrational assignments for selected fundamental modes of vibrations of AMPATOB are given in Table. The calculated band at  $3475\text{ cm}^{-1}$  is due to asymmetric N-H stretching of  $\text{NH}_2$  group and experimentally it is assigned at  $3565\text{ cm}^{-1}$ . The calculated band at  $3073\text{ cm}^{-1}$  is due to asymmetric C-H stretching of phenyl group and experimentally it is assigned at  $3057\text{ cm}^{-1}$ . The C=O stretching is experimentally observed around  $1667\text{ cm}^{-1}$  which is in close agreement with the calculated frequency  $1660\text{ cm}^{-1}$ . The bands in the range  $1585\text{-}1100\text{ cm}^{-1}$  are assigned for C-H in-plane bending vibrations which are in close agreement with the experimental. The bands in the range  $1023\text{-}649\text{ cm}^{-1}$  are assigned for C-H out-of-plane bending vibrations which are in close agreement with the experimental value.

### CONCLUSIONS

AMPATOB has been synthesized and characterized by FTIR and  $^1\text{H}$  NMR spectroscopy. Vibrational assignments are also examined theoretically. The data obtained during the course of present investigation shows a good agreement between the experimental and computed data obtained by using the DFT method with 6-31G basis set. The LUMO-HOMO energy gap reveals the activity of AMPATOB.

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