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# Spectroscopic (FT-IR, FT-Raman, NMR) investigations, MEP and Magnetic Susceptibility of 2,3-d\Diphenyl-5-(thiophen-2-ylmethylidene)-2,5-dihydro-1,2,4-triazin-6(1h)-one

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Magnetic susceptibility.

**ABSTRACT**

In the present work, a combined experimental and theoretical study on ground state molecular structure, spectroscopic and nonlinear optical properties of the thiophene derivative 2,3-d\Diphenyl-5-(thiophen-2-ylmethylidene)-2,5-dihydro-1,2,4-triazin-6(1H)-one is reported. The entire quantum chemical calculations and optimized structural parameters like bond lengths and bond angles, vibrational frequencies and optimized geometry have performed at DFT/B3LYP method with cc-pVDZ and cc-pVTZ basis sets using the Gaussian 09W program package. The calculated results show that the optimized geometry parameters, the theoretical vibrational frequencies and chemical shift values show good agreement with experimental values. The FTIR and FT Raman spectra of the title compound have been recorded in the regions 4000 – 400 cm -1 and 3500 – 100 cm-1, respectively. The calculated harmonic vibrational frequencies have been compared with experimental FT-IR and FT- Raman spectra. The observed and calculated frequencies are found to be in good agreement. In addition, Mulliken atomic charges, local reactivity descriptors such as local softness (sk), Fukui function (fk), global electrophilicity and nucleophilicity of the title compound were calculated and discussed. Besides HOMO–LUMO energy gap and molecular electrostatic potential map were performed. 1H and 13C NMR isotropic chemical shifts are evaluated experimentally. Magnetic susceptibility has been determined for various range of temperature.



## 1. Introduction

Thiophene is one of the most studied heterocycles: it is easy to process, chemically stable, and its synthetic applications have been a constant matter of investigation for many years [1]. Thiophene belongs to a class of heterocyclic compounds containing a five-membered ring made up of one sulphur as heteroatom with the formula $C_4H_4S$[2]. In medicinal chemistry, thiophene derivatives have been very well known for their therapeutic applications. The normal thiophenes are stable liquids which is very similar to the benzene compounds in the character like boiling point and in smell[3]. Thiophene has a structure that is analogous to structure of pyrrole, and due to pie electron cloud, it behaves like extremely reactive benzene derivative.[4] In most cases, the $2^{nd}$ and $5^{th}$ position of thiophene are used for the polymerization[5]. The modification of the molecules for special electronic properties is operated on the $3^{rd}$ and $4^{th}$ - positions[6]. Thiophenes are part of many organic compounds[7] having vast applications in the field of electronics and optoelectronics, medicine and materials [8-10]. The remarkable pharmacological efficiency of the compounds containing a thiophene ring in their structure is known for their antidepressant, anticonvulsant, antihistaminic, anaesthetic, antipuritic, analgesic action [11]. Thiophene and its derivatives exhibit diverse biological properties such as nemoticidal[12], insecticidal[13], antibacterial, antifungal, antiviral and antioxidant activity [14].

Density functional theory (DFT) approaches, especially those using hybrid functional, have evolved to a powerful and very reliable tool, being routinely used for the determination of various molecular properties [15]. B3LYP functional has been shown to provide an excellent compromise between accuracy and computational spectra for molecules of large and medium size [16, 17]. The aim of the present study is to give a complete description of the molecular geometry and molecular vibrations of the title molecule. For that purpose, quantum chemical computations were carried out on title molecule using DFT. The calculated HOMO (Highly occupied molecular orbital's) and LUMO (Lowest Unoccupied molecular orbital's) energies show that charge transfer occurs in the title molecule. DFT calculations are characterised to give very good vibrational frequencies of organic compounds if the calculated frequencies, are scaled to indemnify correlation, for basis set deficits and for not simple harmonic [18-20].

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## 2. Experimental details

The Fourier transform infrared (FT-IR) spectrum of the sample was recorded at room temperature in the region 4000–400 $cm^{-1}$ using Perkin–Elmer spectrum RX1 spectrophotometer equipped with composition of the pellet. The signals were collected for 100 scans with a scan interval of 1$cm^{-1}$ and at optical resolution of 0.4 $cm^{-1}$. The Fourier transform Raman (FT-Raman) BRUKER-RFS 27 spectrometer was used for the Raman spectral measurements at room temperature. The spectrometer consisted of a quartz beam splitter and a high sensitive germanium diode detector cooled to the liquid nitrogen temperature. The sample was packed in a glass tube of about 5 mm diameter and excited in the 180º geometry with 1064 nm laser line at 100mW power from a diode pumped air cooled Nd:YAG laser as an excitation wavelength in the region 4000–100 $cm^{-1}$. Nuclear magnetic resonance (NMR) spectra were recorded on a Bruker 300 AVANCE spectrometer at 300 MHz for $^{1}H$ and 75 MHz for $^{13}C$ in CDCl3 solutions containing 0.03 vol.% TMS as internalstandard.

## 3. Computational details

All DFT calculations of the title compound were carried out using Gaussian 09 program package using default thresholds and parameters [21]. The ground state structural geometries were fully optimized at the B3LYP method along with the standard cc-pVDZ and cc-pVTZ basis sets.

In the DFT calculations the Lee, Yang and Parr correlation functional is used together with Becke's three parameters exchange functional B3LYP. The geometry optimization was performed at the B3LYP density functional theory with the same basis set[22, 23]. Harmonic vibrational frequencies were computed at the same level of theory. Structural analysis of the molecules has been executed to have an idea about the lowest energy structures of the category [24]. The molecular geometry has not been limited and all the calculations (vibrational wavenumbers, optimized geometric parameters and other molecular properties) have been performed using the GausssView molecular visualization program and the Gaussian 09W program package. The chemical reactivity behaviour of the compound was predicted on the basis of reactivity indices obtained by HOMO and LUMO energy Eigen values. Molecular electrostatic potential (MEP) plot has been presented to know about the different sites of electrophilic and nucleophilic attacks of the compound.

## 4. Result and discussion

### Vibrational analysis

The optimized stable geometry and the scheme of atom numbering of the compound 2,3 d\Diphenyl-5-(thiophen-2-ylmethylidene)-2,5-dihydro-1,2,4-triazin-6(1H)-one is re-presented in Fig.1. The optimized structural parameters bond length, bond angle and the dihedral angle for the more stable geometry of the title compound is determined at B3LYP with cc-pVDZ and cc-pVTZ basis sets are presented in Table 1. The impact of the substituent on the molecular parameters, mainly in the C-C bond distance of ring carbon atoms seems to be varied. The mean bond length of aromatic ring is 1.40 Å. The longer bond length (1.48 Å) of C11-C13 is due to the absence of delocalization of carbonyl lone pair of electrons towards the ring.

The observed and calculated FTIR and FT-Raman spectra of 2,3 d\Diphenyl-5-(thiophen-2-ylmethylidene)-2,5-dihydro-1,2,4-triazin-6(1*H*)-one are shown in Figs. 2 and 3 respectively. The observed FTIR and FT-Raman wavenumbers along with the theoretical IR and Raman wavenumbers along with their relative intensities and probable assignments are summarized in Table 2.

### C–S, C-N and N-N vibrations

In the case of thiophene two C-S stretching vibrations are attributed, one is fell in higher wavenumber and another one is lower wavenumber. The C-S stretching wavenumbers are observed by Kwiatowski et al.[25, 26] at 840 and 754 $cm^{-1}$ whereas Kupta et al.[27] have been predicted theoretically at 842 and 750 $cm^{-1}$ by DFT method. In our present study, the ring connected C–S bond stretching vibration is calculated 821 $cm^{-1}$. The identification of C–N vibrations is very difficult because of the interference of many bands in the area where the vibration of this bond happens. For our title molecule, the C-N stretching appears in the region 1001-1520 $cm^{-1}$ and the observed wavenumber (1002 $cm^{-1}$) is coinciding very well with calculated wavenumber (1001 $cm^{-1}$) in FT-IR. The electronegative nitrogen atom makes the carbon atom more positive and the polar -CN group has effect on the adjacent bond. C=N and N-N and each has a well-known characteristic vibrational frequency of its own parameters. N-N stretching vibration, which due to its symmetry has a very characteristic and they are difficult to observe in the infrared spectrum. Because of the change in dipole moment, the N-N bond length in the molecule also change in which has two abnormal C=N parts. These bands shift in wavenumber and intensity in a different way depending on the neighboring groups, H-bonding [28]. The substituents of title compound influence both the wavenumber and intensity. The medium band in FT-IR at 1234 $cm^{-1}$ is accredited to the N-N stretching vibration of the molecule. The theoretical calculation by B3LYP method predicts the above said vibration at 1234 $cm^{-1}$ exactly correlates with experimental findings.

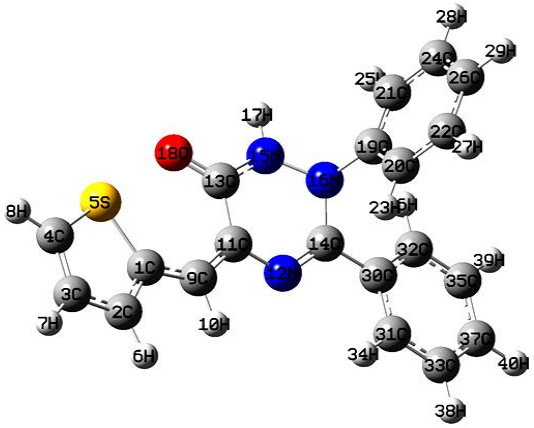


**Fig. 1 Optimized geometrical structure and atom numbering of 2, 3-d\Diphenyl-5(thiophen-2-ylmethylidene)-2, 5-dihydro-1, 2, 4-triazin-6(1*H*)-one.**

**Table 1. Optimized structural parameters of 2,3-d\Diphenyl-5-(thiophen-2-ylmethylidene)-2,5-dihydro-1,2,4-triazin-6(1*H*)-one utilizing B3LYP/cc-pVDZ and B3LYP/cc-pVTZ density functional calculation.**

| Parameter | Bond Length (A°) | | Parameter | Bond Length (A°) | | Parameter | Bond Angle (A°) | | Parameter | Bond Angle (A°) | | Parameter | Bond Angle (A°) | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | B3LYP/ cc-pVDZ | B3LYP/ cc-pVTZ | | B3LYP/ cc-pVDZ | B3LYP/ cc-pVTZ | | B3LYP/ cc-pVDZ | B3LYP/ cc-pVTZ | | B3LYP/ cc-pVDZ | B3LYP/ cc-pVTZ | | B3LYP/ cc-pVDZ | B3LYP/ cc-pVTZ |
| C1-C2 | 1.39 | 1.39 | C19-C20 | 1.40 | 1.40 | C2-C1-S5 | 109.61 | 109.70 | N12-C14-N16 | 123.62 | 122.92 | C26-C24-H28 | 120.17 | 120.17 |
| C1-S5 | 1.76 | 1.76 | C19-C21 | 1.40 | 1.40 | C2-C1-C9 | 121.31 | 121.34 | N12-C14-C30 | 120.00 | 120.36 | C22-C26-C24 | 119.78 | 119.62 |
| C1-C9 | 1.44 | 1.44 | C20-C22 | 1.40 | 1.40 | S5-C1-C9 | 129.08 | 128.95 | N16-C14-C30 | 116.37 | 116.72 | C22-C26-H29 | 120.11 | 120.21 |
| C2-C3 | 1.42 | 1.41 | C20-H23 | 1.09 | 1.09 | C1-C2-C3 | 114.32 | 114.19 | C13-N15-N16 | 125.11 | 124.00 | C24-C26-H29 | 120.10 | 120.17 |
| C2-H6 | 1.09 | 1.08 | C21-C24 | 1.40 | 1.39 | C1-C2-H6 | 121.69 | 121.80 | C13-N15-H17 | 118.27 | 117.53 | C14-C30-C31 | 119.40 | 119.54 |
| C3-C4 | 1.38 | 1.38 | C21-H25 | 1.09 | 1.09 | C3-C2-H6 | 123.99 | 124.01 | N16-N15-H17 | 116.18 | 116.31 | C14-C30-C32 | 121.64 | 121.45 |
| C3-H7 | 1.09 | 1.08 | C22-C26 | 1.40 | 1.40 | C2-C3-C4 | 111.89 | 111.84 | C14-N16-N15 | 112.11 | 113.27 | C31-C30-C32 | 118.94 | 119.00 |
| C4-S5 | 1.73 | 1.73 | C22-H27 | 1.09 | 1.09 | C2-C3-H7 | 124.20 | 124.24 | C14-N16-C19 | 117.76 | 118.87 | C30-C31-C33 | 120.46 | 120.42 |
| C4-H8 | 1.09 | 1.08 | C24-C26 | 1.40 | 1.40 | C4-C3-H7 | 123.91 | 123.92 | N15-N16-C19 | 113.27 | 113.82 | C30-C31-H34 | 118.48 | 118.74 |
| C9-H10 | 1.10 | 1.09 | C24-H28 | 1.09 | 1.09 | C3-C4-S5 | 112.79 | 112.81 | N16-C19-C20 | 121.83 | 121.70 | C33-C31-H34 | 121.06 | 120.84 |
| C9-C11 | 1.37 | 1.37 | C26-H29 | 1.09 | 1.09 | C3-C4-H8 | 127.64 | 127.61 | N16-C19-C21 | 118.17 | 118.44 | C30-C32-C35 | 120.42 | 120.42 |
| C11-N12 | 1.40 | 1.40 | C30-C31 | 1.41 | 1.41 | S5-C4-H8 | 119.57 | 119.57 | C20-C19-C21 | 120.00 | 119.86 | C30-C32-H36 | 119.53 | 119.61 |
| C11-C13 | 1.48 | 1.48 | C30-C32 | 1.41 | 1.40 | C1-S5-C4 | 91.39 | 91.45 | C19-C20-C22 | 119.75 | 119.82 | C35-C32-H36 | 120.05 | 119.97 |
| N12-C14 | 1.29 | 1.29 | C31-C33 | 1.39 | 1.39 | C1-C9-H10 | 112.17 | 112.22 | C19-C20-H23 | 119.84 | 120.02 | C31-C33-C37 | 120.25 | 120.26 |
| C13-N15 | 1.37 | 1.37 | C31-H34 | 1.09 | 1.08 | C1-C9-C11 | 135.73 | 135.28 | C22-C20-H23 | 120.40 | 120.16 | C31-C33-H38 | 119.71 | 119.69 |
| C13-O18 | 1.23 | 1.23 | C32-C35 | 1.40 | 1.40 | H10-C9-C11 | 112.07 | 112.44 | C19-C21-C24 | 120.00 | 120.05 | C37-C33-H38 | 120.04 | 120.05 |
| C14-N16 | 1.42 | 1.42 | C32-H36 | 1.09 | 1.08 | C9-C11-N12 | 116.46 | 116.87 | C19-C21-H25 | 119.40 | 119.75 | C32-C35-C37 | 120.26 | 120.23 |
| C14-C30 | 1.48 | 1.48 | C33-C37 | 1.40 | 1.40 | C9-C11-C13 | 124.88 | 125.18 | C24-C21-H25 | 120.60 | 120.20 | C32-C35-H39 | 119.65 | 119.63 |
| N15-N16 | 1.41 | 1.41 | C33-H38 | 1.09 | 1.09 | N12-C11-C13 | 118.55 | 117.69 | C20-C22-C26 | 120.34 | 120.42 | C37-C35-H39 | 120.09 | 120.14 |
| N15-H17 | 1.01 | 1.01 | C35-C37 | 1.40 | 1.40 | C11-N12-C14 | 121.11 | 120.80 | C20-C22-H27 | 119.54 | 119.41 | C33-C37-C35 | 119.67 | 119.68 |
| N16-C19 | 1.45 | 1.45 | C35-H39 | 1.09 | 1.09 | C11-C13-N15 | 113.32 | 114.07 | C26-C22-H27 | 120.12 | 120.16 | C33-C37-H40 | 120.17 | 120.16 |

**Table 2. Experimental and Calculated B3LYP/ cc-pVDZ and B3LYP/cc-pVTZ levels of vibrational frequencies ($cm^{-1}$), of 2,3-d\Diphenyl-5-(thiophen-2-ylmethylidene)-2,5-dihydro-1,2,4-triazin-6(1*H*)-one.**

| S.No. | Observed frequency ($cm^{-1}$) | | Calculated frequency ($cm^{-1}$) | | | | Vibrational assignment/ (%) |
|---|---|---|---|---|---|---|---|
| | FT-IR | FT-Raman | Unscaled | | Scaled | | |
| | | | B3LYP/ cc-pVDZ | B3LYP/ cc-pVTZ | B3LYP/ cc-pVDZ | B3LYP/ cc-pVTZ | |
| 1. | 3250 | | 3496 | 3603 | 3255 | 3251 | νNH(96) |
| 2. | | 3099 | 3243 | 3240 | 3094 | 3098 | νCH(98) |
| 3. | 3078 | | 3242 | 3218 | 3075 | 3076 | νCH(98) |
| 4. | | 3063 | 3222 | 3216 | 3060 | 3065 | νCH(98) |
| 5. | 3031 | | 3220 | 3215 | 3033 | 3034 | νCH(97) |
| 6. | | | 3211 | 3207 | 3021 | 3024 | νCH(98) |
| 7. | 3009 | | 3205 | 3201 | 3010 | 3010 | νCH(96) |
| 8. | 3002 | | 3202 | 3200 | 3004 | 3003 | νCH(96) |
| 9. | | | 3199 | 3197 | 2991 | 2992 | νCH(98) |
| 10. | 2984 | | 3187 | 3191 | 2985 | 2983 | νCH(98) |
| 11. | | | 3186 | 3184 | 2962 | 2960 | νCH(96) |
| 12. | 2937 | | 3178 | 3182 | 2936 | 2937 | νCH(95) |
| 13. | | | 3174 | 3175 | 2879 | 2882 | νCH(95) |
| 14. | 2859 | | 3165 | 3174 | 2860 | 2860 | νCH(98) |
| 15. | 2835 | | 3156 | 3154 | 2835 | 2836 | νCH(98) |
| 16. | | 1689 | 1776 | 1753 | 1688 | 1690 | νCO(88) |
| 17. | 1671 | | 1678 | 1668 | 1670 | 1671 | νCC(80), δCH(19) |
| 18. | | 1627 | 1656 | 1654 | 1627 | 1626 | νCC(80), δCH(18) |
| 19. | 1609 | | 1651 | 1647 | 1610 | 1609 | νCC(81), δCH(17) |
| 20. | | 1598 | 1650 | 1637 | 1594 | 1598 | νCC(69), δCN(12), δCH(10), δNH(10) |
| 21. | 1578 | 1580 | 1626 | 1631 | 1576 | 1579 | νCC(69), δCH(12) |
| 22. | | 1522 | 1561 | 1617 | 1520 | 1523 | νCN(67), νCC(16), δNH(10) |
| 23. | | | 1546 | 1544 | 1515 | 1516 | νCC(68), δCH(18), δNH(11) |
| 24. | | | 1542 | 1520 | 1509 | 1510 | δNH(88) |
| 25. | | 1501 | 1524 | 1518 | 1500 | 1501 | νCC(86), δCH(18) |
| 26. | 1484 | | 1519 | 1479 | 1483 | 1485 | δCH(76), νCC(18) |
| 27. | | 1441 | 1478 | 1475 | 1440 | 1441 | δCH(71), νCC(16) |
| 28. | 1421 | | 1471 | 1470 | 1420 | 1422 | δCH(69), δNH(11), νCC(10) |
| 29. | | 1413 | 1465 | 1435 | 1414 | 1412 | νCC(66), δCH(17) |
| 30. | | | 1415 | 1409 | 1388 | 1384 | νNN(66), νCN(19), δNH(10) |
| 31. | 1375 | | 1410 | 1365 | 1376 | 1376 | δCH(79) |
| 32. | 1348 | 1346 | 1365 | 1362 | 1345 | 1347 | νCC(68), δCH(18) |
| 33. | 1328 | | 1363 | 1356 | 1326 | 1328 | νCC(67), δCH(19) |
| 34. | | 1321 | 1350 | 1351 | 1320 | 1321 | δCH(69) |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| 35. | 1296 | | 1331 | 1326 | 1295 | 1297 | δCH(73) |
| 36. | 1284 | | 1327 | 1322 | 1280 | 1282 | δCH(73) |
| 37. | 1234 | | 1310 | 1300 | 1231 | 1234 | νCC(66), νCN(12), νNN(10) |
| 38. | | 1225 | 1273 | 1263 | 1220 | 1225 | νCC(65), δCH(18) |
| 39. | 1173 | | 1253 | 1248 | 1170 | 1173 | δCH(66) |
| 40. | | | 1247 | 1228 | 1152 | 1155 | δCH(66), νCC(12) |
| 41. | | | 1195 | 1210 | 1148 | 1149 | δCH(65), νCC(10) |
| 42. | | 1144 | 1189 | 1187 | 1142 | 1144 | νCC(65), νCC(11) |
| 43. | 1115 | | 1189 | 1185 | 1113 | 1117 | νCC(67), νCC(11) |
| 44. | | 1109 | 1171 | 1171 | 1110 | 1110 | δCH(67), νCC(12) |
| 45. | | | 1169 | 1170 | 1091 | 1093 | δCH(66), νCC(10) |
| 46. | | 1082 | 1143 | 1148 | 1083 | 1082 | νCN(65), νCC(11) |
| 47. | 1062 | | 1108 | 1100 | 1063 | 1062 | δCH(60), νCC(16) |
| 48. | | 1056 | 1101 | 1098 | 1055 | 1056 | δCH(63), νCC(16) |
| 49. | 1039 | 1039 | 1088 | 1086 | 1039 | 1036 | δCH(66), νCC(12) |
| 50. | | | 1073 | 1073 | 1020 | 1022 | δCH(65) |
| 51. | 1002 | 1001 | 1062 | 1057 | 1001 | 1002 | νCN(60), δCO(17), νCC(11) |
| 52. | | | 1050 | 1049 | 994 | 995 | δring(70) |
| 53. | | | 1048 | 1037 | 989 | 989 | δring(71) |
| 54. | | | 1022 | 1017 | 985 | 983 | γCH(88) |
| 55. | | | 1014 | 1015 | 979 | 976 | δring(71) |
| 56. | | | 1009 | 1014 | 963 | 960 | δring(70), δCH(12) |
| 57. | 957 | | 1008 | 1012 | 957 | 955 | γCH(69), γCC(16) |
| 58. | | | 998 | 998 | 942 | 940 | γCH(66), γCC(15) |
| 59. | | | 973 | 986 | 931 | 932 | γCH(66), γCC(15) |
| 60. | | | 966 | 970 | 919 | 920 | γCH(65), γCC(17) |
| 61. | | 912 | 949 | 954 | 910 | 911 | γCH(65), γring(18) |
| 62. | 906 | | 926 | 940 | 905 | 907 | νCC(66), δring(18) |
| 63. | 890 | | 923 | 937 | 895 | 890 | γCH(66) |
| 64. | | | 903 | 918 | 881 | 880 | γCH(65) |
| 65. | 828 | | 873 | 867 | 829 | 830 | γCH(65) |
| 66. | | | 863 | 864 | 821 | 823 | νCS(67), δCH(12) |
| 67. | | 818 | 856 | 853 | 815 | 817 | γNH(60) |
| 68. | | | 839 | 836 | 808 | 810 | γCH(67) |
| 69. | | | 834 | 831 | 801 | 804 | γCH(68) |
| 70. | | | 819 | 806 | 797 | 799 | δring(69), δNH(12) |
| 71. | | | 802 | 791 | 788 | 788 | γCH(61), γCC(11) |
| 72. | 781 | | 794 | 776 | 780 | 781 | γCO(62), γCC(13), γCN(10) |
| 73. | | | 778 | 754 | 761 | 760 | γCH(66) |
| 74. | | 741 | 770 | 748 | 745 | 742 | γCH(54), δring(18) |
| 75. | 734 | | 744 | 731 | 735 | 734 | δring(55) |
| 76. | | | 724 | 719 | 720 | 718 | γCH(55) |
| 77. | | | 713 | 713 | 706 | 705 | γCH(61) |
| 78. | | | 712 | 712 | 693 | 695 | γCH(60) |

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| 79. | | 687 | 707 | 706 | 685 | 683 | γCH(61) |
| 80. | 656 | | 701 | 683 | 655 | 653 | γCN(58), γring(12) |
| 81. | | | 682 | 643 | 637 | 636 | δring(51), δNH(15) |
| 82. | | 625 | 649 | 630 | 624 | 625 | δNH(61) |
| 83. | | | 630 | 627 | 617 | 618 | δring(55) |
| 84. | | | 627 | 614 | 608 | 609 | δring(58) |
| 85. | | 599 | 615 | 596 | 600 | 598 | δring(55) |
| 86. | 593 | | 595 | 581 | 590 | 592 | γNN(58) |
| 87. | 562 | | 593 | 566 | 560 | 562 | γring(58) |
| 88. | | | 562 | 522 | 533 | 530 | γring(55) |
| 89. | | | 524 | 515 | 504 | 504 | γCC(61), γring(11) |
| 90. | | | 507 | 510 | 489 | 490 | γCH(60), γring(12) |
| 91. | | | 494 | 466 | 461 | 462 | γring(61), γNH(50) |
| 92. | | | 447 | 449 | 413 | 410 | δCC(61) |
| 93. | | | 422 | 429 | 407 | 405 | γCC(60), γring(12) |
| 94. | | | 416 | 420 | 400 | 402 | γring(61) |
| 95. | | | 414 | 418 | 386 | 385 | γring(60) |
| 96. | | | 361 | 363 | 341 | 340 | γring(58), γCC(12) |
| 97. | | | 353 | 353 | 322 | 321 | γCC(51) |
| 98. | | | 329 | 340 | 301 | 300 | γCN(53) |
| 99. | | 283 | 286 | 295 | 283 | 282 | δCO(52) |
| 100. | | | 258 | 275 | 240 | 242 | δCC(50) |
| 101. | | | 242 | 250 | 223 | 220 | γNH(55), γCO(13) |
| 102. | | | 220 | 214 | 202 | 201 | γCC(76), γring(10) |
| 103. | | | 207 | 209 | 189 | 189 | γCC(61) |
| 104. | | | 185 | 175 | 167 | 165 | γNH(62) |
| 105. | | | 152 | 148 | 139 | 140 | γCC(62) |
| 106. | | 127 | 140 | 136 | 125 | 130 | γCN(60) |
| 107. | | 89 | 97 | 93 | 88 | 88 | γCO(60) |
| 108. | | | 79 | 73 | 77 | 75 | γCC(58) |
| 109. | | | 71 | 58 | 70 | 71 | γCN(58) |
| 110. | | | 43 | 46 | 42 | 40 | γCC(51) |
| 111. | | | 38 | 41 | 38 | 36 | γring(53) |
| 112. | | | 35 | 24 | 33 | 31 | γring(52) |
| 113. | | | 25 | 17 | 24 | 24 | γring(52) |
| 114. | | | 19 | 15 | 20 | 20 | γring(48) |

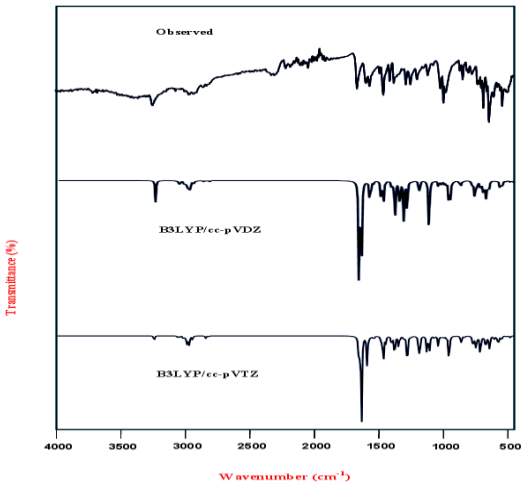


**Fig. 2 Observed and simulated infrared spectra of 2, 3-d\Diphenyl-5-(thiophen-2-ylmethylidene)-2, 5-dihydro-1, 2, 4-triazin-6(1*H*)-one.**

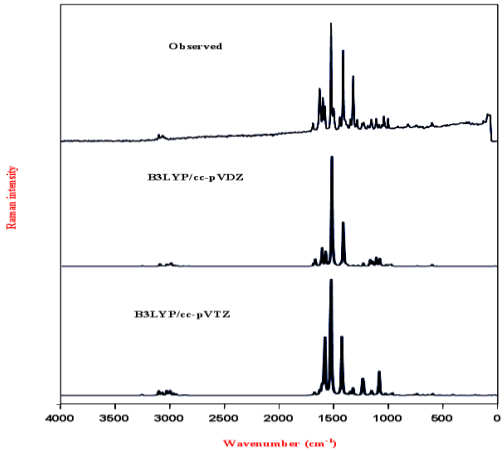


**Fig. 3 Observed and simulated Raman spectra of 2, 3-d\Diphenyl-5-(thiophen-2-ylmethylidene)-2, 5-dihydro-1, 2, 4-triazin-6(1*H*)-one.**

**C = O vibrations**

The carbonyl stretching frequency is very sensitive to the factors that disturb the nature of the carbonyl group and its precise frequency is characteristic of the type of the carbonyl compound being studied. This region is considered as a very important region by organic chemists. The carbonyl stretching vibrations in ketones are expected in the region 1715-1680 $cm^{-1}$[29]. The carbon oxygen double bond is formed by $\pi - \pi$ between carbon and oxygen, and the lone pair of electron on oxygen also determines the nature of the carbonyl group. For our present study, the band caused by C=O stretching vibration is observed in the region 1689 $cm^{-1}$ in FT-Raman is very much correlated with calculated wavenumber 1688 $cm^{-1}$. If the spectrum contains a strong absorption band between 1900-1600 $cm^{-1}$, the carbonyl group (C=O) will be presented in a compound. The position of the peak or the band not only tells the presence of a particular group but also reveals a good deal about the environments affecting the group.[30]

**C-C and C–H vibrations**

The aromatic ring vibrational modes of the title molecule have been verified based on the vibrational spectra of previously published vibrations of the benzene molecule are helpful in the identification of the phenyl ring modes [31]. The ring stretching vibrations are very prominent, as the double bond is in conjugation with the ring, in the vibrational spectra of benzene and its derivatives[32]. The ring carbon-carbon stretching vibrations occur in the region 1650-1450 $cm^{-1}$. In the title compound, the wavenumbers observed in the FT-IR spectrum at 1609, 1578, 1348, 1328 $cm^{-1}$ have been assigned to C-C stretching vibrations. The theoretically computed values at 1610, 1576, 1515, 1414, 1345, 1326 $cm^{-1}$ show the excellent agreement with the experimental data. The characteristic region for the identification of C-H stretching vibration, the heteroaromatic structure illustrated in the region 3100–3000 $cm^{-1}$. The calculated wavenumbers of the C-H symmetric stretching vibrations using B3LYP/cc-pVDZ in title molecule at 3094, 3075, 3060, 3033, 3021, 3010 and 3004 $cm^{-1}$are in good agreement with the experimental data. The C–H in-plane bending and C–H out-of-plane bending vibrations are normally found in the range 1300–1000 and 1000–750 $cm^{-1}$, respectively in aromatic compounds and are very useful for characterization purposes[33, 34]. The C-H in-plane bending vibrations are observed at 1484, 1421, 1375, 1296, 1156 $cm^{-1}$ in FT-IR and the calculated wavenumbers are 1483, 1420, 1376, 1295, 1155 $cm^{-1}$ that are well correlated with the experimental wavenumber. The C-H out-of-plane bending vibrations are calculated at 957, 910, 829, 685 $cm^{-1}$. The experimental values are assigned at 957, 912, 828, 687 $cm^{-1}$ which show excellent agreement with calculated ones.

**N-H Vibrations**

In N-H stretching mode, the strong band of N-H stretching extends from 3400 to 3100 $cm^{-1}$, with the centre of the band at 3370 $cm^{-1}$[35-37]. The calculated wavenumber of the above mode is at 3255 $cm^{-1}$ for the B3LYP/cc-pVDZ method. The strong band in the FT-IR spectrum at 3250 $cm^{-1}$ also supports the formation of a strong N-H…N hydrogen bond. The lowering of the N-H stretching wavenumber can be attributed to the red shifting due to intermolecular N-H---N interaction. The red shifting is further enhanced by the reduction in the N-H bond order values, occurring due to donor-acceptor interaction. The first overtone of the N-H bending mode falling on the N-H stretching band positions produces two bands of comparable intensities, equally displaced on either side of this wavenumber resulting from Fermi resonance with one or more N-H stretching.

**Frontier Molecular Orbitals**

Highly occupied molecular orbital (HOMO) and Lowest unoccupied molecular orbital (LUMO) are the main orbital that take part in chemical stability. Molecular orbital's can provide insight into the nature of reactivity and some of the structural and physical properties. The HOMO represents the ability to donate an electron, while LUMO as an electron acceptor represents the ability to obtain an electron. The one electron excitation from HOMO and LUMO mainly described the electronic transition absorption correspond to the transition from ground to first excited state [38]. The energy gap between HOMO and LUMO has been used to prove the bioactivity from intramolecular charge transfer [39]. The energy gap measures the kinetic energy stability of the molecules. Considering the chemical hardness, large HOMO-LUMO gap means a hard molecule and small HOMO-LUMO gap means a soft molecule and also can relate the stability of the molecule to hardness, which means that increase of the HOMO-LUMO energy gap decreases reactivity of the compound that leads to increase in the stability of the molecule [40]. The frontier molecules orbital, HOMO and LUMO and frontier molecular energy gap helping the reactivity and kinetic stability of molecules are essential parameters in the electronic studies[41, 42]. From the Fig. 4, the energy values of HOMO ($E_{HOMO}$) and LUMO ($E_{LUMO}$) are -5.28736 and -1.98749 eV respectively. In the studied compound the HOMO-LUMO energy gap ($\Delta E$) is 3.29987 eV that reflects the chemical reactivity of the

molecule. Using HOMO and LUMO orbital energies, the ionization energy and electron affinity can be expressed as: I = $-E_{HOMO}$ = 5.28736 eV. A = $-E_{LUMO}$ = 1.98749 eV. The hardness (η) and chemical potential (μ) are given the following formula η = (I-A)/2 and μ = -(I+A)/2, where I and A are the first ionization potential and electron affinity of the chemical species. For the title compound, $E_{HOMO}$ = -5.28736 eV, $E_{LUMO}$ = -1.98749 eV, Energy gap = HOMO-LUMO = 3.29987 eV, Ionization potential (I) = 5.28736 eV, Electron affinity (A) = 1.98749 eV, Chemical hardness (η) = 1.64993 eV, Electronegativity (χ) = -3.637425 eV, Softness (*s*) = 0.606086 $eV^{-1}$, Chemical potential (μ) = 3.637425 eV, Electrophilicity index (ω) = 4.00952.

**Fukui Functions**

Fukui function is an indigenous reactivity identifier that predicts the ideal regions where a molecular fragment will change its density when the number of electrons is changed and it specified the tendency of the electronic density to deform at a given position upon accepting or donating electrons [43-45].

Also, it is probable to define the atomic Fukui functions on the $j^{th}$ atom site

$$f_j^+ = q_j(N+1) - q_j(N)$$
$$f_j^- = q_j(N) - q_j(N-1)$$
$$f_j^0 = \tfrac{1}{2}[q_j(N+1) - q_j(N-1)]$$

For an electrophilic $f_j^-$ (r), nucleophilic or free radical attack $f_j^+$ (r), on the reference molecule, respectively. In these equation, $q_j$ is the atomic charge (evaluated from Mulliken population analysis, electrostatic derived charge, etc.) at the $j^{th}$ atomic site is the neutral (N), anionic (N+1) or cationic (N-1) chemical species. Chattaraj et al. [46] proposed the idea of generalized philicity and it contains almost all information about the known different global and local reactivity and selectivity descriptor, in addition to the information regarding electrophilic/nucleophilic power of a given atomic site in a molecule. Morell et al. [47] have proposed a dual descriptor (Δf(r)), which is defined as the difference between the nucleophilic and electrophilic Fukui function and in given by,

$\Delta f(r) = [\, f^+(r) - f^-(r) \,]$

If $\Delta f(r) > 0$, then the site is favoured for a nucleophilic attack,

$\Delta f(r) < 0$, then the site may be favoured for an electrophilic attack.

Under this situation, the reactivity descriptor Δf(r) provide useful information on both stabilising and destabilising interactions between a nucleophile and an electrophile and helps in identifying the electrophilic/nucleophilic behaviour of a specific site within a molecule. It provides positive value for site prone for nucleophilic attack and a negative value prone for electrophilic attack and these values reported in Table. 3 according to the condition for dual descriptor, nucleophilic sit for in our title molecule is C2, C3, H8, C9, C11, N13 (positive value i.e. $\Delta f(r)>0$). Similarly, the electrophilic site is C1, C4, S5, H6, H7, H10, C12, C14, N15, O16, N17, H18, C19, H20, C21, C22, H23, C24, H25, C26, H27, H28, H29, C30, C31, C32, C33, H34, C35, H36, C37, H38, H39, H40 (Negative i.e. $\Delta f(r)<0$). The behaviour of molecules as electrophiles/nucleophiles during reaction depends on the local behaviour of molecules.

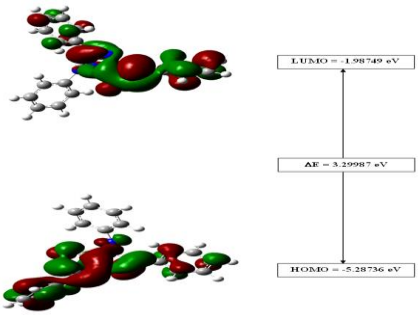


**Fig. 4. HOMO- LUMO plot of 2, 3-d\Diphenyl-5-(thiophen-2-ylmethylidene)-2, 5- dihydro- 1, 2, 4-triazin-6(1*H*)-one.**

**NBO analysis**

Natural bond orbital analysis gives a measurable method for studying intra and intermolecular bonding and interaction among bonds, and also gives a appropriate basis for examining charge transfer or conjugative interactions in molecular systems. NBO method gives useful information about interactions in both filled and virtual orbital spaces which could enhance the analysis of intra and intermolecular interactions [48]. Estimating their energy importance by second order perturbation theory and considering all possible interactions between filled donor and empty acceptor NBOs. The second order Fock matrix was carried out to evaluate the donor-acceptor interactions in the NBO analysis. The change in electron density (ED) in the (σ*, π*) antibonding orbitals and E(2) energies have been calculated by natural bond orbital (NBO) analysis using DFT method to give clear evidence of stabilization originating from various molecular interactions. Delocalization of electron density between occupied Lewis type (bond or lone pair) NBO orbitals and formally unoccupied (antibonding or Rydberg) non-Lewis NBO orbitals correspond to a stabling donor acceptor interaction. Accumulation of natural charges and electron population of atoms in core, valance, Rydberg orbitals of 2,3-d\Diphenyl-5-(thiophen-2-ylmethylidene)-2,5-dihydro-1,2,4-triazin-6(1*H*)-one is calculated and shown in Table. 4

The stabilization energy E(2) is estimated as

$$E(2) = \Delta E_{ij} = q_i \frac{F(i,j)^2}{\varepsilon_j - \varepsilon_i}$$

where *i* is the donor and *j* is the acceptor associated with E(2).

Some electron donor orbital, acceptor orbital and the interacting stabilization energy resulting from the second order micro-disturbance theory are reported where qi is the donor orbital occupancy, εi and εj are diagonal elements and F(i,j) is the off diagonal NBO second-order Fock matrix element reported [49, 50]. The larger E(2) value, the more intensive is the interaction among electron donors and acceptors, i.e. the high donating tendency from electron donors to electron acceptors and the greater the extent on formation of the whole system. NBO analysis was performed on the molecule at the DFT/B3LYP/cc-pVTZ level in order to elucidate the intra molecular rehybridization and delocalization of electron density within the molecule [51]. In this study, the intramolecular hyperconjugative (interaction of the electrons in a sigma bond) interaction of $\sigma(C_1\text{-}C_2)$ distributed to $\sigma^*(C_3\text{-}H_8)$ resulting the stabilization energy of 3.16 kcal/mole are shown in Table. 5. This improved further conjugation with the $\pi^*(C_1 - C_2)$ antibonding orbital with a stabilization energy of 65.21 kcal/mole. In the title compound, the $\pi(C_{14}) \rightarrow \pi^*(C_{30} - C_{31})$, $\pi^*(C_{11} - N_{13})$ and $\pi(C_3) \rightarrow \pi^*(C_4 - C_9)$ show stabilization energies of 40.11 kcal/mole, 57.22 kcal/mole and 74.3 kcal/mole respectively.

**Table 3. Values of Fukui function considering Mulliken charges of 2,3-d\Diphenyl-5-(thiophen-2-ylmethylidene)-2,5-dihydro-1,2,4-triazin-6(1*H*)-one.**

| Mulliken Atomic Charges (a.u) | | | | Fukui's Function (a.u) | | | | Atomic Softness | | | Electrophilicity Indices | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| **Atom** | **Neutral (N)** | **Cation (N-1)** | **Anion (N+1)** | $f_k^+$ | $f_k^-$ | $f_k^\circ$ | **Δf(r)** | $s_k^+$ | $s_k^-$ | $s_k^\circ$ | $\omega_k^+$ | $\omega_k^-$ | $\omega_k^\circ$ |
| C1 | -0.173753 | -0.459 | -0.624 | -0.4502 | 0.28525 | -0.0825 | -0.7355 | -0.173 | 0.110 | -0.032 | -1.472 | 0.933 | -0.2698 |
| C2 | -0.127572 | 0.156 | 0.026 | 0.15357 | -0.2836 | -0.065 | 0.43714 | 0.059 | -0.109 | -0.025 | 0.502 | -0.927 | -0.2126 |
| C3 | -0.149615 | -0.015 | -0.136 | 0.01362 | -0.1346 | -0.0605 | 0.14823 | 0.005 | -0.052 | -0.023 | 0.045 | -0.440 | -0.1978 |
| C4 | 0.047176 | -0.103 | -0.173 | -0.2202 | 0.15018 | -0.035 | -0.3704 | -0.085 | 0.058 | -0.013 | -0.720 | 0.491 | -0.1145 |
| S5 | 0.169374 | 0.214 | 0.028 | -0.1414 | -0.0446 | -0.093 | -0.0967 | -0.054 | -0.017 | -0.036 | -0.462 | -0.146 | -0.3041 |
| H6 | 0.134155 | 0.212 | 0.027 | -0.1072 | -0.0778 | -0.0925 | -0.0293 | -0.041 | -0.030 | -0.036 | -0.350 | -0.255 | -0.3025 |
| H7 | 0.124401 | -0.499 | -0.666 | -0.7904 | 0.6234 | -0.0835 | -1.4138 | -0.304 | 0.240 | -0.032 | -2.585 | 2.039 | -0.273 |
| H8 | 0.121516 | 0.352 | 0.246 | 0.12448 | -0.2305 | -0.053 | 0.35497 | 0.048 | -0.089 | -0.020 | 0.407 | -0.754 | -0.1733 |
| C9 | -0.117912 | 0.362 | 0.235 | 0.35291 | -0.4799 | -0.0635 | 0.83282 | 0.136 | -0.185 | -0.024 | 1.154 | -1.569 | -0.2076 |
| H10 | 0.13615 | 0.159 | -0.196 | -0.3322 | -0.0229 | -0.1775 | -0.3093 | -0.128 | -0.009 | -0.068 | -1.086 | -0.075 | -0.5804 |
| C11 | -0.011716 | 0.831 | 0.737 | 0.74872 | -0.8427 | -0.047 | 1.59143 | 0.288 | -0.325 | -0.018 | 2.448 | -2.756 | -0.1537 |
| C12 | 0.127944 | -0.019 | -0.037 | -0.1649 | 0.14694 | -0.009 | -0.3119 | -0.064 | 0.057 | -0.003 | -0.539 | 0.481 | -0.0294 |
| N13 | -0.245287 | 0.555 | 0.492 | 0.73729 | -0.8003 | -0.0315 | 1.53757 | 0.284 | -0.308 | -0.012 | 2.411 | -2.617 | -0.103 |
| C14 | 0.093139 | -0.236 | -0.301 | -0.3941 | 0.32914 | -0.0325 | -0.7233 | -0.152 | 0.127 | -0.013 | -1.289 | 1.076 | -0.1063 |
| N15 | -0.005492 | -0.257 | -0.315 | -0.3095 | 0.25151 | -0.029 | -0.561 | -0.119 | 0.097 | -0.011 | -1.012 | 0.822 | -0.0948 |
| O16 | -0.248589 | -0.254 | -0.314 | -0.0654 | 0.00541 | -0.03 | -0.0708 | -0.025 | 0.002 | -0.012 | -0.214 | 0.018 | -0.0981 |
| N17 | -0.242846 | -0.267 | -0.323 | -0.0802 | 0.02415 | -0.028 | -0.1043 | -0.031 | 0.009 | -0.011 | -0.262 | 0.079 | -0.0916 |
| H18 | 0.153837 | -0.276 | -0.3295 | -0.4833 | 0.42984 | -0.0268 | -0.9132 | -0.186 | 0.166 | -0.010 | -1.581 | 1.406 | -0.0875 |
| C19 | 0.179381 | -0.285 | -0.336 | -0.5154 | 0.46438 | -0.0255 | -0.9798 | -0.198 | 0.179 | -0.010 | -1.685 | 1.519 | -0.0834 |
| H20 | 0.204925 | -0.294 | -0.3425 | -0.5474 | 0.49893 | -0.0243 | -1.0464 | -0.211 | 0.192 | -0.009 | -1.790 | 1.631 | -0.0793 |
| C21 | -0.13545 | -0.303 | -0.349 | -0.2136 | 0.16755 | -0.023 | -0.3811 | -0.082 | 0.065 | -0.009 | -0.698 | 0.548 | -0.0752 |
| C22 | -0.098462 | -0.312 | -0.3555 | -0.257 | 0.21354 | -0.0218 | -0.4706 | -0.099 | 0.082 | -0.008 | -0.841 | 0.698 | -0.0711 |
| H23 | 0.099709 | -0.321 | -0.362 | -0.4617 | 0.42071 | -0.0205 | -0.8824 | -0.178 | 0.162 | -0.008 | -1.510 | 1.376 | -0.067 |
| C24 | -0.097705 | -0.33 | -0.3685 | -0.2708 | 0.2323 | -0.0193 | -0.5031 | -0.104 | 0.089 | -0.007 | -0.885 | 0.760 | -0.0629 |
| H25 | 0.114526 | -0.339 | -0.375 | -0.4895 | 0.45353 | -0.018 | -0.9431 | -0.189 | 0.175 | -0.007 | -1.601 | 1.483 | -0.0589 |
| C26 | -0.108431 | -0.348 | -0.3815 | -0.2731 | 0.23957 | -0.0168 | -0.5126 | -0.105 | 0.092 | -0.006 | -0.893 | 0.783 | -0.0548 |
| H27 | 0.103508 | -0.357 | -0.388 | -0.4915 | 0.46051 | -0.0155 | -0.952 | -0.189 | 0.177 | -0.006 | -1.607 | 1.506 | -0.0507 |
| H28 | 0.104788 | -0.366 | -0.3945 | -0.4993 | 0.47079 | -0.0143 | -0.9701 | -0.192 | 0.181 | -0.005 | -1.633 | 1.539 | -0.0466 |
| H29 | 0.103752 | -0.375 | -0.401 | -0.5048 | 0.47875 | -0.013 | -0.9835 | -0.194 | 0.184 | -0.005 | -1.651 | 1.566 | -0.0425 |
| C30 | 0.070184 | -0.384 | -0.4075 | -0.4777 | 0.45418 | -0.0118 | -0.9319 | -0.184 | 0.175 | -0.005 | -1.562 | 1.485 | -0.0384 |
| C31 | -0.134765 | -0.393 | -0.414 | -0.2792 | 0.25824 | -0.0105 | -0.5375 | -0.108 | 0.099 | -0.004 | -0.913 | 0.844 | -0.0343 |
| C32 | -0.093252 | -0.402 | -0.4205 | -0.3272 | 0.30875 | -0.0092 | -0.636 | -0.126 | 0.119 | -0.004 | -1.070 | 1.010 | -0.0302 |
| C33 | -0.109552 | -0.411 | -0.427 | -0.3174 | 0.30145 | -0.008 | -0.6189 | -0.122 | 0.116 | -0.003 | -1.038 | 0.986 | -0.0262 |
| H34 | 0.094887 | -0.42 | -0.4335 | -0.5284 | 0.51489 | -0.0068 | -1.0433 | -0.203 | 0.198 | -0.003 | -1.728 | 1.684 | -0.0221 |
| C35 | -0.100586 | -0.429 | -0.44 | -0.3394 | 0.32841 | -0.0055 | -0.6678 | -0.131 | 0.126 | -0.002 | -1.110 | 1.074 | -0.018 |
| H36 | 0.114661 | -0.438 | -0.4465 | -0.5612 | 0.55266 | -0.0043 | -1.1138 | -0.216 | 0.213 | -0.002 | -1.835 | 1.807 | -0.0139 |
| C37 | -0.109888 | -0.447 | -0.453 | -0.3431 | 0.33711 | -0.003 | -0.6802 | -0.132 | 0.130 | -0.001 | -1.122 | 1.102 | -0.0098 |
| H38 | 0.105512 | -0.456 | -0.4595 | -0.565 | 0.56151 | -0.0018 | -1.1265 | -0.218 | 0.216 | -0.001 | -1.848 | 1.836 | -0.0057 |
| H39 | 0.107663 | -0.465 | -0.466 | -0.5737 | 0.57266 | -0.0005 | -1.1463 | -0.221 | 0.221 | 0.000 | -1.876 | 1.873 | -0.0016 |
| H40 | 0.106442 | -0.474 | -0.4725 | -0.5789 | 0.58044 | 0.00075 | -1.1594 | -0.223 | 0.224 | 0.000 | -1.893 | 1.898 | 0.00245 |

**Table 4. Accumulation of natural charges and electron population of atoms in core, valance, Rydberg orbitals of 2,3-d\Diphenyl-5-(thiophen-2-ylmethylidene)-2,5-dihydro-1,2,4-triazin-6(1*H*)-one.**

| Atoms[a] | Charge (e) | Natural population (e) | | | Total (e) | Atoms[b] | Charge (e) | Natural population (e) | | | Total (e) |
|---|---|---|---|---|---|---|---|---|---|---|---|
| | | Core | Valence | Rydberg | | | | Core | Valence | Rydberg | |
| S5 | 0.49999 | 9.99871 | 5.45335 | 0.04795 | 15.50001 | C1 | -0.39006 | 1.99926 | 4.36810 | 0.02270 | 6.39006 |
| H6 | 0.23045 | 0.00000 | 0.76759 | 0.00195 | 0.76955 | C2 | -0.23613 | 1.99926 | 4.21823 | 0.01864 | 6.23613 |
| H7 | 0.21840 | 0.00000 | 0.77965 | 0.00196 | 0.78160 | C3 | -0.20934 | 1.99912 | 4.19191 | 0.01831 | 6.20934 |
| H8 | 0.22017 | 0.00000 | 0.77786 | 0.00197 | 0.77983 | C4 | -0.25350 | 1.99914 | 4.22751 | 0.02685 | 6.25350 |
| H10 | 0.20350 | 0.00000 | 0.79302 | 0.00348 | 0.79650 | C9 | -0.07243 | 1.99922 | 4.05306 | 0.02016 | 6.07243 |
| C11 | 0.00280 | 1.99917 | 3.96569 | 0.03234 | 5.99720 | N13 | -0.46381 | 1.99948 | 5.43675 | 0.02758 | 7.46381 |
| C12 | 0.56043 | 1.99911 | 3.40423 | 0.03623 | 5.43957 | N15 | -0.25465 | 1.99930 | 5.23108 | 0.02427 | 7.25465 |
| C14 | 0.38931 | 1.99925 | 3.58717 | 0.02427 | 5.61069 | O16 | -0.53903 | 1.99973 | 6.50715 | 0.03215 | 8.53903 |
| H18 | 0.38130 | 0.00000 | 0.61432 | 0.00438 | 0.61870 | N17 | -0.47408 | 1.99941 | 5.45012 | 0.02455 | 7.47408 |
| C19 | 0.13518 | 1.99895 | 3.84424 | 0.02163 | 5.86482 | C20 | -0.19713 | 1.99910 | 4.17941 | 0.01861 | 6.19713 |
| H23 | 0.21227 | 0.00000 | 0.78502 | 0.00271 | 0.78773 | C21 | -0.21177 | 1.99910 | 4.19552 | 0.01715 | 6.21177 |
| H25 | 0.21149 | 0.00000 | 0.78624 | 0.00227 | 0.78851 | C22 | -0.19197 | 1.99924 | 4.17519 | 0.01754 | 6.19197 |
| H27 | 0.20541 | 0.00000 | 0.79257 | 0.00203 | 0.79459 | C24 | -0.19397 | 1.99924 | 4.17712 | 0.01760 | 6.19397 |
| H28 | 0.20493 | 0.00000 | 0.79304 | 0.00203 | 0.79507 | C26 | -0.20205 | 1.99924 | 4.18471 | 0.01809 | 6.20205 |
| H29 | 0.20396 | 0.00000 | 0.79410 | 0.00194 | 0.79604 | C30 | -0.09173 | 1.99899 | 4.07100 | 0.02175 | 6.09173 |
| H34 | 0.20562 | 0.00000 | 0.79166 | 0.00273 | 0.79438 | C31 | -0.19769 | 1.99914 | 4.18125 | 0.01730 | 6.19769 |
| H36 | 0.23188 | 0.00000 | 0.76560 | 0.00251 | 0.76812 | C32 | -0.16595 | 1.99915 | 4.14906 | 0.01775 | 6.16595 |
| H38 | 0.20487 | 0.00000 | 0.79312 | 0.00200 | 0.79513 | C33 | -0.19508 | 1.99924 | 4.17832 | 0.01752 | 6.19508 |
| H39 | 0.20608 | 0.00000 | 0.79190 | 0.00202 | 0.79392 | C35 | -0.19584 | 1.99924 | 4.17861 | 0.01799 | 6.19584 |
| H40 | 0.20386 | 0.00000 | 0.79414 | 0.00200 | 0.79614 | C37 | -0.19569 | 1.99924 | 4.17782 | 0.01863 | 6.19569 |

[a]Atoms containing positive charges
[b]Atoms containing negative charges

**Table 5. Significant second-order interaction energy (E (2), kcal/mol) between donor and acceptor orbitals of2,3-d\Diphenyl-5-(thiophen-2-ylmethylidene)-2,5-dihydro-1,2,4-triazin-6(1*H*)-one calculated at B3LYP/cc-pVTZ level of theory.**

| Donor (i) | Acceptor (j) | E(2)[a] kcal/mol | $(\varepsilon_i - \varepsilon_j)$[b] a.u | $F_{ij}$[c] a.u | Donor (i) | Acceptor (j) | E(2)[a] kcal/mol | $(\varepsilon_i - \varepsilon_j)$[b] a.u | $F_{ij}$[c] a.u | Donor (i) | Acceptor (j) | E(2)[a] kcal/mol | $(\varepsilon_i - \varepsilon_j)$[b] a.u | $F_{ij}$[c] a.u |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| σ(C1-C2) | σ*(C3-H8) | 3.16 | 1.14 | 0.054 | σ(C19-C20) | σ*(C21-C24) | 20.69 | 0.28 | 0.068 | σ(C32-H36) | σ*(C30-C31) | 5.41 | 1.03 | 0.067 |
| σ(C1-S5) | σ*(C2-H7) | 4.31 | 1.1 | 0.062 | σ(C19-C20) | σ*(C22-C26) | 19.86 | 0.28 | 0.067 | σ(C32-H36) | σ*(C35-C37) | 4.6 | 1.04 | 0.062 |
| σ(C1-S5) | σ*(C4-C9) | 5.4 | 1.1 | 0.069 | σ(C20-C22) | σ*(N17-C19) | 4.93 | 1.05 | 0.064 | σ(C33-C37) | σ*(C30-C31) | 20.4 | 0.28 | 0.068 |
| σ(C1-H6) | σ*(C2-C3) | 3.09 | 1.04 | 0.051 | σ(C20-H23) | σ*(C19-C21) | 4.95 | 1.05 | 0.064 | σ(C33-C37) | σ*(C32-C35) | 18.88 | 0.28 | 0.066 |
| σ(C2-C3) | σ*(C1-H6) | 3.92 | 1.08 | 0.058 | σ(C20-H23) | σ*(C22-C26) | 4.23 | 1.05 | 0.06 | σ(C33-H38) | σ*(C30-C31) | 5.03 | 1.04 | 0.065 |
| σ(C2-C3) | σ*(C4-C9) | 5.87 | 1.08 | 0.071 | σ(C21-C24) | σ*(N17-C19) | 4.79 | 1.05 | 0.064 | σ(C33-H38) | σ*(C35-C37) | 4.54 | 1.05 | 0.062 |
| σ(C2-H7) | σ*(C1-S5) | 3.83 | 0.77 | 0.049 | σ(C21-C24) | σ*(C19-C20) | 20.87 | 0.28 | 0.069 | σ(C35-H39) | σ*(C30-C32) | 4.93 | 1.05 | 0.064 |
| σ(C3-C4) | σ*(C2-H7) | 3.28 | 1.13 | 0.055 | σ(C21-C24) | σ*(C22-C26) | 20.41 | 0.28 | 0.068 | σ(C35-H39) | σ*(C33-C37) | 4.6 | 1.05 | 0.062 |
| σ(C3-H8) | σ*(C4-S5) | 4.87 | 0.77 | 0.055 | σ(C21-H25) | σ*(C19-C20) | 4.85 | 1.06 | 0.064 | σ(C37-H40) | σ*(C31-C33) | 4.6 | 1.05 | 0.062 |
| σ(C4-S5) | σ*(C1-H6) | 3.58 | 1.1 | 0.056 | σ(C21-H25) | σ*(C24-C26) | 4.19 | 1.06 | 0.06 | σ(C37-H40) | σ*(C32-C35) | 4.53 | 1.06 | 0.062 |
| σ(C4-S5) | σ*(C3-H8) | 3.99 | 1.1 | 0.059 | σ(C22-C26) | σ*(C19-C20) | 20.76 | 0.28 | 0.068 | π(C3) | π*(C1-C2) | 65.21 | 0.12 | 0.096 |
| σ(C4-C9) | σ*(C11-C12) | 3.7 | 0.77 | 0.051 | σ(C22-C26) | σ*(C21-C24) | 20.6 | 0.28 | 0.068 | π(C3) | π*(C4-C9) | 74.3 | 0.11 | 0.095 |
| σ(C4-C9) | σ*(C11-N13) | 3.29 | 0.74 | 0.049 | σ(C22-H27) | σ*(C19-C20) | 4.7 | 1.05 | 0.063 | π(S5) | π*(C1-C2) | 27.19 | 0.25 | 0.075 |
| σ(C9-H10) | σ*(C4-S5) | 5.35 | 0.77 | 0.057 | σ(C22-H27) | σ*(C24-C26) | 4.59 | 1.05 | 0.062 | π(S5) | π*(C4-C9) | 27.39 | 0.24 | 0.072 |
| σ(C9-H10) | σ*(C11-N13) | 3.24 | 0.54 | 0.043 | σ(C24-H28) | σ*(C19-C21) | 4.69 | 1.05 | 0.063 | π(N13) | π*(C11-C12) | 6.4 | 0.89 | 0.068 |
| σ(C9-C11) | σ*(C3-C4) | 3.31 | 1.19 | 0.056 | σ(C24-H28) | σ*(C22-C26) | 4.57 | 1.05 | 0.062 | π(N13) | π*(C14-N15) | 8.56 | 0.74 | 0.071 |
| σ(C11-C12) | σ*(C12-O16) | 3.69 | 1.45 | 0.066 | σ(C26-H29) | σ*(C20-C22) | 4.54 | 1.05 | 0.062 | π(C14) | π*(C11-N13) | 57.22 | 0.13 | 0.089 |
| σ(C11-C12) | σ*(N15-N17) | 5.34 | 0.98 | 0.065 | σ(C26-H29) | σ*(C21-C24) | 4.57 | 1.05 | 0.062 | π(C14) | π*(C30-C31) | 40.11 | 0.15 | 0.084 |
| σ(C11-N13) | σ*(C14-C30) | 5.44 | 1.16 | 0.071 | σ(C30-C31) | σ*(C32-C35) | 18.87 | 0.29 | 0.067 | π(N15) | π*(C12-O16) | 43.98 | 0.32 | 0.107 |
| σ(C11-N13) | σ*(C9-H10) | 3.13 | 0.71 | 0.044 | σ(C30-C31) | σ*(C33-C37) | 19.73 | 0.28 | 0.067 | π(N15) | π*(N17-H18) | 5.43 | 0.68 | 0.06 |
| σ(C11-N13) | σ*(C12-O16) | 18.77 | 0.34 | 0.074 | σ(C31-C33) | σ*(C14-C30) | 4.41 | 1.09 | 0.062 | π(O16) | π*(C11-C12) | 25.84 | 0.76 | 0.128 |
| σ(C12-N15) | σ*(C14-C30) | 4.01 | 1.16 | 0.061 | σ(C31-H34) | σ*(C30-C32) | 4.74 | 1.06 | 0.063 | π(O16) | π*(C12-N15) | 41.66 | 0.63 | 0.147 |
| σ(C12-O16) | σ*(C11-N13) | 5.36 | 0.39 | 0.047 | σ(C31-H34) | σ*(C33-C37) | 4.16 | 1.06 | 0.059 | π(N17) | π*(C12-N15) | 6.83 | 0.65 | 0.059 |
| σ(N13-C14) | σ*(C9-C11) | 5.54 | 1.23 | 0.074 | σ(C32-C35) | σ*(C14-C30) | 4.04 | 1.09 | 0.059 | π(N17) | π*(C14-N15) | 5.28 | 0.62 | 0.052 |
| σ(N13-C14) | σ*(N15-N17) | 4.69 | 1.09 | 0.064 | σ(C32-C35) | σ*(C30-C31) | 20.25 | 0.27 | 0.068 | π(N17) | π*(C19-C20) | 5.43 | 0.81 | 0.061 |
| σ(C14-N15) | σ*(C12-O16) | 3.53 | 1.56 | 0.066 | σ(C32-C35) | σ*(C33-C37) | 21.23 | 0.28 | 0.068 | π(N17) | π*(C19-C20) | 5.08 | 0.29 | 0.036 |
| | | | | | | | | | | π(N17) | π*(C19-C21) | 5.36 | 0.8 | 0.06 |

**Molecular electrostatic potential (MEP)**

Molecular electrostatic potential provides a visual method to understand the relative polarity of the molecule. MEP is in valuable tool in predicting and analysing the molecular interactions such as Drug – receptor and enzyme – substrate interactions. MEP is very helpful for the qualitative elucidation of electrophilic and nucleophilic reactions for the study of biological discovery process and hydrogen bonding interactions [52]. An electron density iso-surface mapped with electrostatic potential surface depicts the size, shape, charge density and site of chemical reactivity of the molecule.

From the MEP picture, oxygen has higher electronegativity value than nitrogen and sulphur. Oxygen atom would consequently possess higher electric density around it, than nitrogen and sulphur atoms. Thus, the spherical region that corresponds to an oxygen atom would have a red position on it. However, the light-yellow region spread on the MEP surface due to potential halfway between the two extreme regions and this confirms the existence of an intermolecular interaction.

To predict the reactive sites of electrophilic and nucleophilic attack for the investigated molecule, the MEP at the B3LYP/cc-pVDZ optimized geometry was calculated and shown in Fig. 5a. The MEP is related to the electronic density and is very useful descriptor for determining sites for electrophilic attack and nucleophilic reactions as well as hydrogen-bonding interactions[53-56]. The negative (red and yellow) regions of MEP were related to electrophilic reactivity and the positive (blue) regions to nucleophilic reactivity as shown in Fig. 5b. These are two possible sites of electrophilic attack. The negative regions are mainly localized on the carbonyl oxygen atoms and also a negative electrostatic potential region is observed around the N atom. The Fig. 5b confirms the existence of an intermolecular N-H----N interaction between the protonated (addition of a proton (H+) to an atom or molecule) and unprotonated N, O and S atoms. The molecular electrostatic potential map shows that the positive potential sites are around the hydrogen atoms and negative potential sites are on electronegative atoms. These sites give information about the region from where the compound can have noncovalent interactions.

**Non-Linear optical activity**

Highly NLO active molecular materials are attracting wide interest because of their potential applications in opto electronic devices of telecommunications, information storage, optical switching signal processing[57, 58] and THz wave generation[59]. THz region which lies between microwaves and infrared region of the electromagnetic spectrum, offers diverse applications such as wireless communications, inspection of drugs, spectroscopy and imaging[60]. Due to measures in the field of technology, there is an increasing interest in designing new organic materials with desired nonlinear optical properties.

The dipole moment (μ), the statistic polarizability ($\alpha_0$) and first static hyperpolarizability ($\beta_{tot}$) are related directly to the non-linear optical (NLO) activity of molecular structures. NLO activities of molecules have also reverse relationship with their biological activities.

The calculated values of the polarizabilities and the hyper polarizabilities from Gaussian 09 output were converted from atomic units into electrostatic units [61]. The total dipole moment (μ) = $(\mu_x^2 + \mu_x^2 + \mu_x^2)^{1/2}$

The calculation of static polarizability ($\alpha_{ave}$)

$<\alpha> = 1/3\ (\alpha_{xx} + \alpha_{yy} + \alpha_{zz})$

and first static hyper polarizability ($\beta_{tot}$) from Gaussian output,[62]

$\beta_{tot} = [(\beta_{xxx} + \beta_{xyy} + \beta_{xzz})^2 + (\beta_{yyy} + \beta_{yzz} + \beta_{yxx})^2 + (\beta_{zzz} + \beta_{zxx} + \beta_{zyy})^2]^{1/2}$

The calculated ($\beta_{tot}$) &<α> and ground state dipole moment were computed to be $7.739 \times 10^{-30}$ esu and -137.64183 esu.

According to the Table. 6, B3LYP/cc-pVTZ results are listed as the electronic dipole moment $\mu_i$ = (i= x,y,z) polarizability $\alpha_0$ and the first hyperpolarizability $\beta_0$ for the title compound. The calculated dipole moment is equal to 1.3054 D. For direction x,y and z, these values are equal to 0.1569 D, 0.7740 D and -1.0394 D, respectively. The calculated polarizability value $\alpha_0$ is equal to -137.64183 esu. The hyperpolarizability β dominated by the longitudinal components of $\beta_{xxx}$, $\beta_{yyy}$, $\beta_{xyy}$, $\beta_{xxy}$, and $\beta_{yyz}$. The large values of particular components of polarizability and hyperpolarizability indicate substantial delocalization of charges in these directions. Most of the research papers have indicated that the frontier molecular orbitals (FMO's) have

**Table 6. The *Ab initio* B3LYP/cc-pVTZ (5D, 7F) calculated electric dipole moments (Debye), Dipole moments compound, polarizability (in a.u), β components and $\beta_{tot}$ ($10^{-30}$ esu) value of 2,3-d\Diphenyl-5-(thiophen-2-ylmethylidene)-2,5-dihydro-1,2,4-triazin-6(1*H*)-one.**

| Parameters | B3LYP/ cc-pVTZ | Parameters | B3LYP/ cc-pVTZ |
|---|---|---|---|
| $\mu_x$ | 0.1569 | $\beta_{xxx}$ | 140.7219 |
| $\mu_y$ | 0.7740 | $\beta_{yyy}$ | 24.0891 |
| $\mu_z$ | -1.0394 | $\beta_{zzz}$ | -8.3086 |
| μ | 1.3054 | $\beta_{xyy}$ | -59.6642 |
| $\alpha_{xx}$ | -123.1406 | $\beta_{xxy}$ | -23.4127 |
| $\alpha_{yy}$ | -147.7063 | $\beta_{xxz}$ | -9.3903 |
| $\alpha_{zz}$ | -142.0786 | $\beta_{xzz}$ | 18.7507 |
| $\alpha_{xy}$ | -2.2233 | $\beta_{yzz}$ | -22.3321 |
| $\alpha_{xz}$ | 0.7697 | $\beta_{YYZ}$ | 0.0588 |
| $\alpha_{yz}$ | -1.8150 | $\beta_{XYZ}$ | 1.8801 |
| Δα(esu) | -137.64183 | βtot(esu) | $7.739 \times 10^{-30}$ |

significant effect on material NLO properties [63-67].

**Mulliken atomic charge**

The computation of the reactive atomic charges plays an important role in the application of quantum mechanical calculations for the molecular system. The Mulliken atomic charges of the title molecule were tabulated in Table 7 and shown in Fig. 6. The Mulliken atomic charges were calculated by the DFT/B3LYP method with cc-pVTZ basis set. This calculation depicts the charges of every atom in the title molecule. The magnitudes of the carbon atoms connected to hydrogen atoms were found to be generally negative value and also the carbon atoms connected to oxygen and nitrogen atoms were calculated to be negative value as expected.

**Magnetic susceptibility**

Atoms, molecules, free radicals or ions which contain one or more unpaired electron will possess permanent magnetic dipole moment that arises from the residual spin and angular moment of the unpaired electrons. All substances having permanent magnetic moment display paramagnetic behaviour in nature. When a paramagnetic substance is placed in a magnetic field, they will align themselves in the direction of the field and thus produces positive magnetic susceptibility, which depends on the temperature; since thermal agitation will oppose the alignment of the magnetic dipoles. The effectiveness of

diminishes increases with increase in temperature. The magnetic susceptibility ($\chi_m$) of the molecules for various temperatures are predicted with knowledge of unpaired electron [68] and presented in Table 8. The graphical representation of ($1/\chi_m$) with T (temperature) is shown in Fig. 7. The effective magnetic moment is found to be a constant, which is $3.514\times10^{-5}$(BM) and Curie constant is obtained from the magnetic moment ($\mu_m$) and is found to be 0.00083.

**Nuclear magnetic resonance (NMR)**

The NMR phenomenon is based on the fact that nuclei of atoms have magnetic properties that can be utilized to give chemical information. It is a research technique that exploits the magnetic properties of certain atomic nuclei. It determines physical and chemical properties of atoms or molecules. If the number of neutrons and the number of protons are both even, the nucleus has no spin. If the number of neutrons plus the number of protons is odd, then the nucleus has a half-integer spin (i.e. 1/2, 3/2, 5/2). If the number of neutrons and the number of protons are both odd, then the nucleus has an integer spin (i.e. 1, 2, and 3). The hydrogen atoms are mostly localized on periphery of the molecules and their chemical shifts would be more susceptible to intermolecular interactions as compared to that for other heavier atoms. Unsaturated carbons give signals in overlapped areas of the spectrum with chemical shift values from 100 to 200 ppm[69]. $^{13}$C NMR spectra exhibit signals somewhat downfield of 170 ppm depending on the structure. Such signals are typically weak due to the absence of nuclear Overhauser effects. The external magnetic field experienced by the carbon nuclei is affected by the electronegativity of the atoms attached to them. The carbonyl carbon atom C13 in the title molecule show very downfield effect and the corresponding observed chemical shift is 168.82 ppm. The more electronegative character of the oxygen atoms renders a positive charge to the carbon and thus C1 chemical shift is observed in the more downfield shift at 159.44ppm. The chemical shift values of other carbon atoms of the title compound are observed at 147.03, 136.82 and 134.07 ppm. The $^{1}$H chemical shifts of the title molecule are obtained by complete analysis of their NMR spectra and interpreted critically in an attempt to quantify the possible different effects acting on the shielding constant and in turn to the chemical shift of protons. $^{1}$H NMR spectra of the title compound indicates, the hydrogen atoms are attached with the aromatic carbons in which the peak values at 9.01, 8.19, 7.83, 7.21 and 6.72 ppm. The experimental $^{1}$H and $^{13}$C NMR chemical shifts are represented in the Fig. 8.

**5. Conclusion**

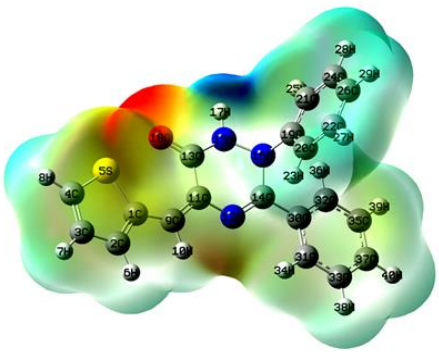

**Fig. 5a. Molecular Electrostatic Potential map of 2, 3-d\Diphenyl-5-(thiophen-2-ylmethylidene)-2, 5-dihydro-1, 2, 4-triazin-6(1*H*)-one.**

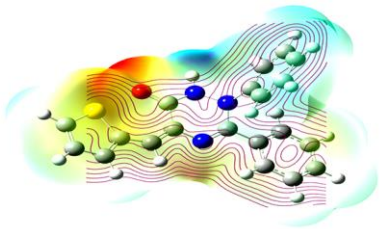

**Fig. 5b. Molecular Electrostatic Potential contour map of 2, 3-d\Diphenyl-5-(thiophen- 2- ylmethylidene)-2, 5-dihydro-1, 2, 4-triazin-6(1*H*)-one.**

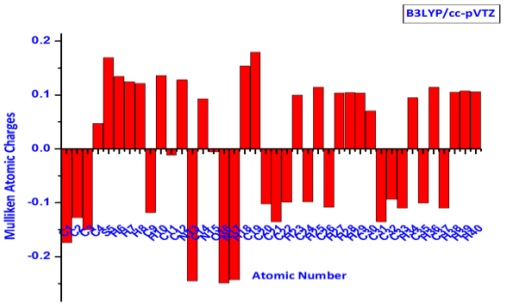


**Fig. 6. Mulliken Atomic Charges of 2, 3-d\Diphenyl-5-(thiophen-2-ylmethylidene)-2, 5- dihydro - 1, 2, 4-triazin-6(1*H*)-one.**

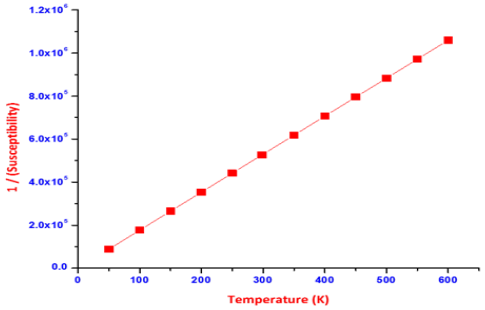


**Fig. 7. Magnetic Susceptibility of 2, 3-d\Diphenyl-5-(thiophen-2-ylmethylidene) -2, 5-dihydro - 1, 2, 4-triazin-6(1*H*)-one.**

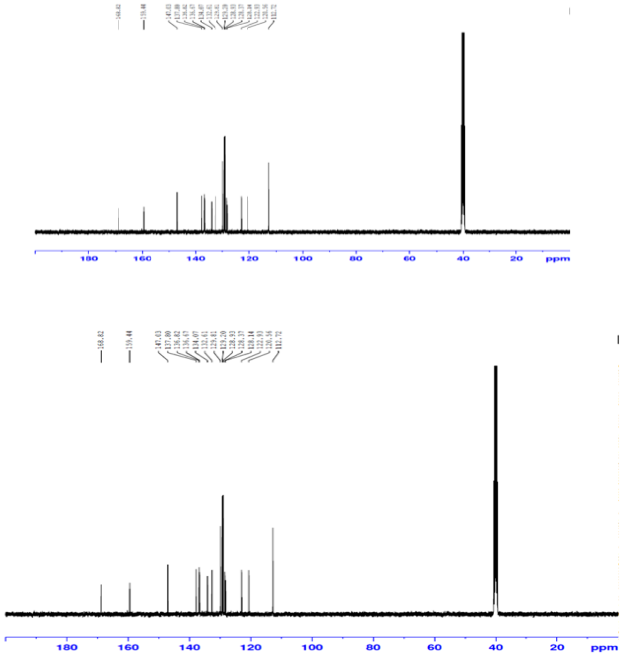


**Fig. 8. $^{13}$C and $^{1}$H NMR spectra of 2, 3-d\Diphenyl-5(thiophen-2-ylmethylidene)-2, 5- dihydro- 1, 2, 4-triazin-6(1*H*)-one.**

**Table 7. Mulliken population analysis of 2,3-d\Diphenyl-5-(thiophen-2-ylmethylidene)-2,5-dihydro-1,2,4-triazin 6(1*H*)-oneperformed at B3LYP/cc-pVTZ.**

| zzAtoms | Atomic Charges B3LYP/cc-pVTZ | | Atoms | Atomic Charges B3LYP/cc-pVTZ |
|---|---|---|---|---|
| C1 | -0.173753 | | C21 | -0.13545 |
| C2 | -0.127572 | | C22 | -0.098462 |
| C3 | -0.149615 | | H23 | 0.099709 |
| C4 | 0.047176 | | C24 | -0.097705 |
| S5 | 0.169374 | | H25 | 0.114526 |
| H6 | 0.134155 | | C26 | -0.108431 |
| H7 | 0.124401 | | H27 | 0.103508 |
| H8 | 0.121516 | | H28 | 0.104788 |
| C9 | -0.117912 | | H29 | 0.103752 |
| H10 | 0.13615 | | C30 | 0.070184 |
| C11 | -0.011716 | | C31 | -0.134765 |
| C12 | 0.127944 | | C32 | -0.093252 |
| N13 | -0.245287 | | C33 | -0.109552 |
| C14 | 0.093139 | | H34 | 0.094887 |
| N15 | -0.005492 | | C35 | -0.100586 |
| O16 | -0.248589 | | H36 | 0.114661 |
| N17 | -0.242846 | | C37 | -0.109888 |
| H18 | 0.153837 | | H38 | 0.105512 |
| C19 | 0.179381 | | H39 | 0.107663 |
| C20 | -0.101832 | | H40 | 0.106442 |

**Table 8. Magnetic susceptibility of 2,3-d\Diphenyl-5-(thiophen-2-ylmethylidene)-2,5-dihydro-1,2,4-triazin-6(1*H*)-one at various temperatures.**

| S. No | Temperature (K) | Susceptibility ($\chi_m$) mole per $m^3$ | 1/ Susceptibility $1/\chi$ |
|---|---|---|---|
| 1 | 50 | 0.000011322 | 88323.61774 |
| 2 | 100 | 0.000005661 | 176647.2355 |
| 3 | 150 | 0.000003774 | 264970.8532 |
| 4 | 200 | 2.8305E-06 | 353294.4709 |
| 5 | 250 | 2.2644E-06 | 441618.0887 |
| 6 | 298.15 | 1.89871E-06 | 526673.7326 |
| 7 | 350 | 1.61743E-06 | 618265.3241 |
| 8 | 400 | 1.41525E-06 | 706588.9419 |
| 9 | 450 | 0.000001258 | 794912.5596 |
| 10 | 500 | 1.1322E-06 | 883236.1774 |
| 11 | 550 | 1.02927E-06 | 971559.7951 |
| 12 | 600 | 9.435E-07 | 1059883.413 |

2,3-d\Diphenyl-5-(thiophen-2-ylmethylidene)-2,5-dihydro-1,2,4-triazin-6(1*H*)-one has been characterized the spectroscopic techniques such as FT-IR, FT-Raman and $^1$H NMR experimentally and using the recent development of computational tool such as DFT method allow the structural analysis of the title compound conducted by B3LYP/cc-pVDZ and B3LYP/cc-pVTZ methods theoretically. The vibrational frequencies of the title compound have been precisely assigned, examined and the theoretical results were compared with the experimental results. The very good coherence has been observed between scaled wavenumbers and experimental wavenumbers. The theoretical support has been addressed by DFT calculations. NBO analysis gives the information about intermolecular and intramolecular charge transfer within the molecule. HOMO-LUMO studies reveal the intra molecular charge transfer through conjugated system. The molecular stability increased by the interaction of the electrons in a sigma bond with antibonding sigma orbital and charge delocalization has evaluated. The molecular electrostatic potential map shows the positive potential sites are around the hydrogen atoms and the negative potential sites are on electronegative atoms. $^1$H and $^{13}$C NMR chemical shifts are experimentally analyzed. Above said sites give details about the region where the compound can have intermolecular interactions. This work will be very useful for the design and synthesis new materials.

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