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# THEORETICAL STUDY ON THE CHARACTERIZATION OF 1,3-DIBENZOYLIMIDAZOLIDINE-2-THIONE BY QUANTUM MECHANICAL METHODS

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## ABSTRACT

In this study, the optimized molecular structures, vibrational frequencies, corresponding vibrational assignments, thermodynamic properties, atomic charges, $^{1}H$ and $^{13}C$ NMR chemical shifts, and ultra violet (UV–vis) spectra of 1,3-Dibenzoylimidazolidine-2-thione molecule have been investigated using ab initio Hartree–Fock (HF) and Density Functional Theory (B3LYP) methods at 6–31G (d,p) basis set. The bond lengths and bond angles obtained have been seen to be good agreement with the experimental data. All the calculated vibrational frequencies have been compared with each other. The correlation coefficient has been determined as 0.9991. Moreover, we have not only simulated frontier molecular orbitals (FMO) and molecular electrostatic potential (MEP) but also evaluated the transition state and energy band gap clearly. Infrared intensities and Raman activities have also been reported.

**Key Words:** 1*,3-Dibenzoylimidazolidine-2-thione, HF, B3LYP, HOMO, LUMO*

# KUANTUM MEKANIKSEL METODLARLA 1,3-DIBENZOYLIMIDAZOLIDINE-2-THIONE BILEŞIĞININ KARAKTERIZASYONUNDAKI TEORIKSEL ÇALIŞMA

## ÖZET

Bu çalışmada, temel haldeki 1,3-Dibenzoylimidazolidine-2-thione molekülünün optimize moleküler yapısı, titreşim frekansları, uygun mod tanımları, termodinamik özellikleri, atomik yükleri, $^{1}H$ and $^{13}C$ NMR kayma değerleri, ve ultraviyole spektrumu 6–31G (d,p) temel setli yoğunluk fonksiyonel teori (B3LYP) ve ab initio Hartree-Fock (HF) metotları kullanılarak incelenildi. Elde edilen bağ açıları ve bağ uzunluklarının deneysel verilerle uyumlu olduğu görüldü. Hesaplanmış olan tüm titreşim frekansları deneysel verilerle karşılaştırıldı. Uyum katsayısı 0.9991 olarak belirlendi. Ayrıca, sadece sınır moleküler orbitallerini ve moleküler elektrostatik potansiyelini göstermekle kalmadık, geçiş durumlarını ve enerji bant aralığını da açık bir şekilde değerlendirdik. İnfrared yoğunlukları ve raman aktivite tayinleri de rapor edilmiştir.

**Anahtar Kelimeler:** 1*,3-Dibenzoylimidazolidine-2-thione, HF, B3LYP, HOMO, LUMO*

## 1. INTRODUCTION

1,3-Dibenzoylimidazolidine-2-thione molecule is a heterocyclic thione, having a wide range of application as analytical reagents, metal corrosion inhibitors and pharmaceutical fields [1,2]. It is a derivative of imidazolidine–2–thione, which exhibits antimicrobial and biological activity with metal complexes [3–5], as a kind of Acylthioureas (ATUs) [6]. Acythioureas have been emphasized as a wide range of biological activity exhibitors; such as, antiviral, antibacterial, anticonvulsant, antiarrythmic, analgesic, antihyperlipidemic, local anaesthetic, antiproliferative, and have been reported in terms of antiproliferative activity against a high number of human cancer lines [7]. Besides, some fused and polysubsituted heterocyclic derivatives are highly potent and selective inhibitors of influenza virus [8]. Therefore, the SAR (Structure activity relationship) studies of ATU derivatives are in progress, prominently [9]. Scientists are also interested in theoretical studies on thione derivative molecules. It is well known from the literature, computational methods are reliable to characterize the molecule because of their efficiency and accuracy with respect to the evaluation of a number of molecular properties [10]. A suitable quantum chemical study is helpful to predict compound properties economically and to clarify some experiment phenomena insightfully [11]. Therefore, theoretical studies are both reliable and useful method to clarify the characterization of the molecule for researches. Hence, uses of computational methods increase in researches day by day. For example, Mohamed et al. [12] researched either theoretical or experimental study of benzothiazoline–2–thione and 2–mercaptobenzothiazole. In 2005 Jian et al. [13] indicated that experimental data were in good agreement with theoretical data calculated at 6–31G* basis sets of Gaussian–98 for the 2,3–Diaryl–tetrazole–5–thione title molecule**.** Similarly, density functional theory calculations were performed to study on 2,3–di(p–methylphenyl)tetrazole–5–thione [14]. Experimental data of thione derivatives were supported by quantum mechanical methods such as ab initio and density functional theory calculations [15,16]. In this study, we have pointed out the molecular structures using HF/6–31G(d,p) and B3LYP/6–31G(d,p) calculation levels and compared with the available experimental data. Comparison of theoretical and experimental data exhibits good correlation confirming the reliability of the method employed here. Vibrational frequencies have also been investigated and scaled by the factors from the literature. It has been realized that all the obtained frequencies have coincided with each other and in fact correlation coefficient has been determined as 0.9991. Moreover, the molecular electrostatic potential and frontier orbitals (HOMO and LUMO) have been visualized, thus transition states and energy band gap have been determined and interpreted. Thermodynamic properties, atomic charges, NMR and UV–vis spectra have also been mentioned for the compound. Thus, this study is both useful to take an idea and expected to serve as the way to future studies of the molecule.

## 2.COMPUTATIONAL DETAILS

The optimized molecular structures, UV–Vis spectra, atomic charges, vibrational frequencies, thermodynamic properties and translation energy |HOMO–LUMO| and molecular electrostatic potential (MEP) of the 1,3-Dibenzoylimidazolidine-2-thione molecule have been investigated using HF [17] and B3LYP [18, 19] methods at 6–31G(d,p) [20, 21] calculation level. All the computations have been performed by using Gaussian 09 program package program with molecular visualization program [22, 23] on the personal computer. Moreover, the Raman activities (Si) calculated by Gaussian 09 program have been converted to relative Raman intensities ($I_i$) with the aid of the following relation from the basic theory of Raman scattering [24, 25]

$$I_i = \frac{f(v_0 - v_i)^4 S_i}{v_i\left[1 - \exp(-hcv_i / KT)\right]} \quad (1)$$

where *h*, *c*, *k* are the universal constants and *f* is suitably chosen common normalization factor for all the intensities when $v_0$ (cm$^{-1}$) is the exciting frequency and $v_i$ is the vibrational wave number of the normal mode. The spectra results have been found to be more regular than the experimental ones due to the fact that several vibrations presenting in condensed phase lead to the strong perturbation of infrared intensities of other modes.

## 3.RESULT AND DISCUSSION

The molecular geometry, vibration frequencies including assignments, Infrared intensities and Raman activities, thermodynamic properties, frontier orbitals, atomic charges, NMR and UV–Vis spectra for the identification of 1,3-Dibenzoylimidazolidine-2-thione have been determined.

### 3.1.Vibrational Symmetries

The title 36–atom molecule belongs to point group $C_1$ including only identity operation symmetry element, so all frequency modes ($\Gamma_{\text{vibration}}$) are produced in A species. N–atomic molecules provide 3N internal modes [26–28] because of the three Cartesian displacements. 6–mode of them is for translation and rotational modes. Thus, 102 (3N–6) vibrational modes are observed in the molecule.

### 3.2.Conformational Analysis and Molecular Geometry

A detailed potential energy surface (PES) scan in C5–C4–N30–C23 and C16–C15–N29–C32 dihedral angles has been conducted for the examination of all possible conformations of the title compound. According to the PES scan analysis, the molecular energies of these tautomeric forms have been calculated at different methods and various basis sets to find the most optimized geometry where the minimum energy is obtained to be about –1314.41985403 a.u.

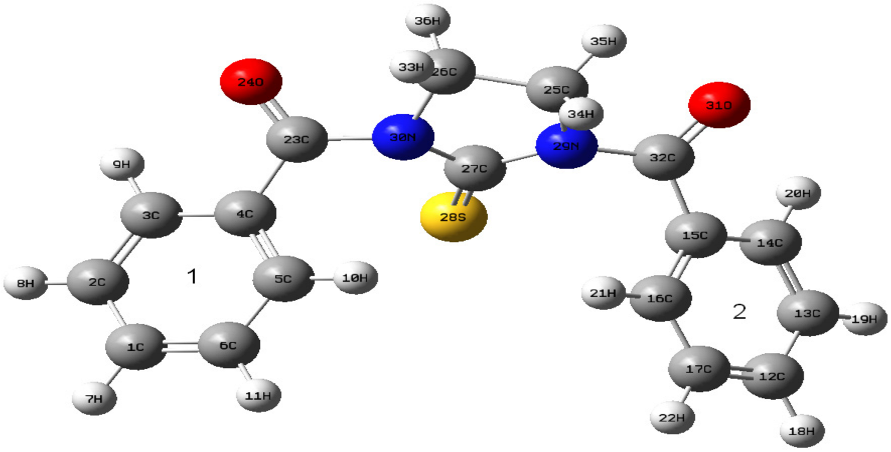


**Figure 1.** The Molecular Structure of 1,3-Dibenzoylimidazolidine-2-thione Molecule

The most optimized molecular structures including bond lengths and bond angles of 1,3-Dibenzoylimidazolidine-2-thione are shown in Fig. 1 along with labeling and symbolizing by using schema. Geometric properties of the structure have been depicted and compared with experimental parameters obtained from the X–ray structure analyses of [1] in Table 1. The experimental data have been observed to be in good agreement with the theoretic calculations for bond lengths, angles and dihedrals. The largest differences of the calculated geometries from the experimental parameters have been found to be 0.02 Å ($O_{31}$–$C_{32}$) and ($C_{27}$–$N_{29}$) at HF, 0.02 Å ($N_{29}$–$C_{32}$) and ($C_{27}$–$N_{29}$) at B3LYP for the bond lengths and $3.26^0$ ($C_{25}$–$N_{29}$–$C_{32}$) at B3LYP, $1.57^0$ ($C_{25}$–$N_{29}$–$C_{32}$) at HF for the bond angles, $4.41^0$ ($C_{27}$–$N_{29}$–$C_{32}$–$C_{25}$) at B3LYP, $31.77^0$ ($C_{27}$–$N_{29}$–$C_{32}$–$C_{25}$) at HF level of calculation for the dihedrals, respectively. As can be seen, this excellent agreement is well within the accuracy of both computational and experimental determinations.

**Table 1.** Experimental values and calculated optimized geometric parameters

| **Bond length (Å)** | **Calculated [6–31G(d, p)]** | | |
|---|---|---|---|
| | **HF** | **DFT** | **Experimental $^a$** |
| $C_{25}$–$C_{26}$ | 1.52 | 1.52 | 1.53 |
| $C_{25}$–$N_{29}$ | 1.47 | 1.47 | 1.48 |
| $N_{29}$–$C_{32}$ | 1.42 | 1.42 | 1.41 |
| $O_{31}$–$C_{32}$ | 1.19 | 1.22 | 1.21 |
| $C_{27}$–$S_{28}$ | 1.65 | 1.65 | 1.65 |
| $C_{27}$–$N_{29}$ | 1.36 | 1.40 | 1.38 |
| $C_1$–$C_2$ | 1.39 | 1.40 | |
| $C_1$–$C_6$ | 1.39 | 1.40 | |
| $C_1$–$H_7$ | 1.08 | 1.09 | |
| $C_2$–$C_3$ | 1.38 | 1.39 | |
| $C_2$–$H_8$ | 1.08 | 1.09 | |
| $C_3$–$C_4$ | 1.39 | 1.40 | |
| $C_3$–$H_9$ | 1.07 | 1.08 | |

| **Bond angles ($^0$)** | **HF** | **DFT** | **Experimental $^a$** |
|---|---|---|---|
| $S_{28}$–$C_{27}$–$N_{29}$ | 126.86 | 127.22 | 126.77 |
| $N_{29}$–$C_{27}$–$N_{30}$ | 106.50 | 105.57 | 106.48 |
| $C_{25}$–$N_{29}$–$C_{27}$ | 112.42 | 110.64 | 111.60 |
| $C_{25}$–$N_{29}$–$C_{32}$ | 118.27 | 116.58 | 119.84 |
| $C_{27}$–$N_{29}$–$C_{32}$ | 127.73 | 128.94 | 126.84 |
| $C_2$–$C_1$–$C_6$ | 120.18 | 120.10 | |
| $C_2$–$C_1$–$H_7$ | 119.93 | 119.91 | |
| $C_6$–$C_1$–$H_7$ | 119.89 | 119.99 | |
| $C_1$–$C_2$–$C_3$ | 119.92 | 120.10 | |
| $C_1$–$C_2$–$H_8$ | 120.16 | 120.13 | |
| $C_3$–$C_2$–$H_8$ | 119.92 | 119.76 | |
| $C_2$–$C_3$–$C_4$ | 120.03 | 119.96 | |
| $C_2$–$C_3$–$H_9$ | 120.72 | 120.12 | |
| $C_4$–$C_3$–$H_9$ | 119.26 | 119.91 | |
| $C_3$–$C_4$–$C_5$ | 119.89 | 119.74 | |
| $C_3$–$C_4$–$C_{23}$ | 117.78 | 122.34 | |
| $C_5$–$C_4$–$C_{23}$ | 122.11 | 117.55 | |
| $C_4$–$C_5$–$C_6$ | 120.01 | 120.12 | |
| $C_4$–$C_5$–$H_{10}$ | 120.18 | 118.87 | |
| **Bond Dihedrals($^0$)** | **HF** | **DFT** | **Experimental $^a$** |
| $C_{25}$–$N_{29}$–$C_{27}$–$N_{30}$ | –8.09 | –11.51 | –9.83 |
| $C_{25}$–$N_{29}$–$C_{27}$–$S_{28}$ | 166.68 | 168.48 | 170.19 |
| $C_{27}$–$N_{29}$–$C_{25}$–$C_{26}$ | –7.78 | 28.40 | 23.99 |

$^a$ Taken from Ref. [1]

### 3.3.Vibration Frequencies

In this study we have investigated a frequency calculation analysis to obtain the spectroscopic signature of 1,3-Dibenzoylimidazolidine-2-thione. Vibrational frequencies have been calculated by using HF/6–31G(d,p) and B3LYP/6–31G(d,p) methods. Table 2 presents the vibrational frequencies scaled by the factors [29], assignments, IR intensities and Raman activities of the title molecule, respectively. Even though there have been no frequencies for the molecule it is well known that computational programs are reliable to characterize the molecule because of their efficiency and accuracy. Thus the expectation frequencies should be close to these scaled frequencies. Moreover, the correlation coefficient ($R^2$) between the quantum mechanical methods has been determined as 0.9991.

The existence of aromatic rings in a structure can easily be assigned as a result of the relation of (CH) and (C=C–C) ring vibrations. The (CH) stretching occurs above 3000 cm$^{-1}$ and is typically exhibited as a multiplicity of weak to moderate bands, compared with the aliphatic (CH) stretch [30–32]. In 1994, Roeges showed that, the (CH) stretching vibrations of the phenyl ring are expected in the region 3120–3000 cm$^{-1}$ [33]. According to Klots and Collier [34], the stretching vibration modes were reported at 3085, 3074, 3065 and 3045 cm$^{-1}$ bands for benzoxazole. The calculated values of these modes for the molecule have been obtained to be 3097–3062 and 3027–2987 cm$^{-1}$ at B3LYP/6–31G(d,p) and HF/6–31G(d,p) level of calculation, respectively. Hydrogen group frequencies ($CH_2$) have been noted to change between 2949 and 3032 cm$^{-1}$ at the B3LYP/6–31G(d,p); 2975 and 2878 at the HF/6–31G(d,p) basis set. The benzene ring possesses six–ring stretching vibrations, some of which occur near 1600, 1580, 1490 and 1440 cm$^{-1}$ for the highest wave numbers are good group vibrations. The others are active at 1315±65 and 1000cm$^{-1}$ bands [33]. In this study, the ν (ring) modes have been observed between 1197 and 1593 cm$^{-1}$ bands for DFT; 1200 and 1614 cm$^{-1}$ bands for HF level of calculation. In addition; the carbon–carbon stretching modes of the phenyl group are expected in the range from 1650 to 1200 cm$^{-1}$. The actual position of these mode are determined not so much by the nature of the substituents but by the form of substitution around the ring [35], even though heavy halogens cause the frequency to diminish undoubtedly [36]. In 1,3-Dibenzoylimidazolidine-2-thione under $C_1$ symmetry, the carbon–carbon stretching bands have been calculated to be about 941–1593 cm$^{-1}$ at the B3LYP/6–31G(d,p) and 975–1613 cm$^{-1}$ at the HF/6–31G(d,p) level of calculation. In addition, the identification of the (CN) stretching frequency in the side chains is a rather difficult task since there are problems in identifying these frequencies from other vibrations [37]. Pinchas et al. [38] assigned the (CN) stretching band at 1368 cm$^{-1}$ in benzamide. According to quantum mechanical calculations of the title molecule, (CN) strong stretching modes have been found to be 1358 cm$^{-1}$ for DFT and 1390 cm$^{-1}$ for HF level of calculation, respectively. Besides; for the (CS) stretching modes, Coates [32] observed these modes at a molecule between 710 and 685 cm$^{-1}$. Likewise; it seems that the weak bands (515 cm$^{-1}$ region) relates to (CS) stretching for this molecule at both calculation levels [39]. Furthermore, according to Badawi [40], the (CO) stretching vibrations in N–methyleneformamide were found to lie in the region 1756–1772 cm$^{-1}$. In 1,3-Dibenzoylimidazolidine-2-thione, the (CO) stretching vibration has a main contribution in this mode with B3LYP/6–31 G(d,p) and HF/6–31 G(d,p) predicted frequency of 1691 and 1771 cm$^{-1}$ (from Table 2), which indicates that the calculations are supported by the literature study. On the other hand; (CH) bending with different modes have been calculated from 23 to 1476 cm$^{-1}$ at DFT; 23 to 1493 cm$^{-1}$ at HF calculation level. Further, umbrella modes [41] have been assigned to the bands on the benzene rings at 704 and 706 cm$^{-1}$ at B3LYP/6–31 G(d,p); at 721 and 725 cm$^{-1}$ HF/6–31 G(d,p) basis sets. (CCC) group bending modes have obtained to arrange in an order from 379 to 1014 cm$^{-1}$ at B3LYP/6–31 G(d,p); 375 to 101 cm$^{-1}$ at HF/6–31 G(d,p) basis set. As for the bending modes of carbon atoms connected with the other atoms, the calculated values have been observed to change from 208 to 777 cm$^{-1}$ with B3LYP/6–31 G(d,p) and 198 to 803 cm$^{-1}$ with HF/6–31 G(d,p) calculation level, respectively.

**Table 2.** Calculated vibrational frequencies of 1,3-Dibenzoylimidazolidine-2-thione

| **Assignment** | **Calculated frequencies (cm$^{-1}$)** | | | | | |
|---|---|---|---|---|---|---|
| | **B3LYP 6–31G(d, p )** | | | **HF 6–31 G(d, p)** | | |
| | | **IR intensity (km/mol)** | **R activity (Å$^4$/amu)** | | **IR intensity (km/mol)** | **R activity (Å$^4$/amu)** |
| $^{1}\nu$(CH) | 3097 | ~0 | 367 | 3027 | 4 | 155 |
| $^{2}\nu$(CH) | 3097 | 3 | 31 | 3027 | 5 | 116 |
| $^{1}\nu$(CH)+ $^{2}\nu$(CH) | 3096 | 2 | 35 | 3021 | 17 | 147 |
| $^{2}\nu$(CH)+ $^{1}\nu$(CH) | 3096 | 22 | 2 | 3020 | 12 | 51 |
| $^{1}\nu_{asy}$(CH) | 3082 | 19 | 192 | 3009 | 34 | 119 |
| $^{2}\nu_{asy}$(CH) | 3082 | 31 | 105 | 3009 | 33 | 82 |
| $^{1}\nu_{asy}$(CH) | 3073 | 8 | 130 | 3000 | 11 | 118 |
| $^{2}\nu_{asy}$(CH) | 3073 | 11 | 123 | 2999 | 10 | 99 |
| $^{1}\nu_{asy}$(CH) | 3062 | 0 | 80 | 2987 | 0 | 50 |
| $^{2}\nu_{asy}$(CH) | 3062 | 0 | 31 | 2987 | 0 | 52 |
| $\nu_{asy}$($CH_2$) | 3032 | 13 | 104 | 2975 | 6 | 77 |
| $\nu_{asy}$($CH_2$) | 3026 | 10 | 113 | 2952 | 17 | 83 |
| $\nu$($CH_2$) | 2955 | 16 | 32 | 2900 | 25 | 101 |
| $\nu$($CH_2$) | 2949 | 23 | 167 | 2878 | 39 | 95 |
| $\nu$(CO) | 1691 | 218 | 186 | 1771 | 471 | 77 |
| $\nu$(CO) | 1691 | 241 | 60 | 1766 | 237 | 17 |
| $^{1}\nu$(ring) | 1593 | 20 | 122 | 1614 | 23 | 68 |
| $^{2}\nu$(ring) | 1593 | 22 | 83 | 1613 | 19 | 75 |
| $^{2}\nu$(ring)+ $^{1}\nu$(ring) | 1573 | 5 | 9 | 1592 | 8 | 8 |
| $^{1}\nu$(ring)+ $^{2}\nu$(ring) | 1573 | 6 | 6 | 1592 | 1 | 2 |
| $\gamma$($CH_2$) | 1476 | 1 | 7 | 1493 | 2 | 8 |
| $^{1}\nu$(ring)+ $^{2}\nu$(ring)+ $\gamma$($CH_2$) | 1475 | 3 | 1 | 1486 | 2 | 1 |
| $^{2}\nu$(ring)+ $^{1}\nu$(ring)+ $\gamma$($CH_2$) | 1472 | ~0 | 13 | 1485 | 2 | 1 |
| $\gamma$($CH_2$) | 1464 | 17 | 12 | 1476 | 20 | 16 |
| $^{1}\nu$(ring)+ $^{2}\nu$(ring) | 1432 | 7 | 8 | 1438 | 24 | 2 |
| $^{2}\nu$(ring)+ $^{1}\nu$(ring) | 1432 | 25 | 1 | 1437 | 30 | 1 |
| $\rho r$($CH_2$)+ $\nu$(CN) | 1358 | 256 | 1 | 1390 | 292 | 2 |

| | | | | | | |
|---|---|---|---|---|---|---|
| ρr(CH$_2$)+ ν(CN) | 1334 | 111 | ~0 | 1381 | 157 | 3 |
| ρr(CH$_2$)+ ν(CN)+ ν(CS)+ δ(CH) | 1329 | 65 | 12 | 1369 | 344 | 6 |
| $^1$δ(CH) | 1312 | ~0 | 11 | 1308 | 28 | 1 |
| $^2$δ(CH) | 1312 | 8 | 1 | 1308 | 4 | 2 |
| ς(CH$_2$)+ ν(CN) | 1294 | 26 | ~0 | 1265 | 256 | 17 |
| ν(CN)+ ν(CC)+ δ(CH) | 1294 | 1 | ~0 | 1260 | 591 | 7 |
| ν(CS)+ ρr(CH$_2$) | 1242 | 794 | 19 | 1241 | 573 | 17 |
| ς(CH$_2$)+ $^1$Breathing(molecule) | 1239 | 124 | 33 | 1214 | 35 | 14 |
| δ(CH)+ $^1$ν(ring) | 1201 | 2 | 75 | 1201 | 3 | 3 |
| δ(CH)+ $^2$ν(ring) | 1197 | 710 | 9 | 1200 | 5 | 2 |
| ς(CH$_2$)+ δ(CH)+ ν(CC) | 1176 | 10 | 25 | 1193 | 72 | 7 |
| δ(CH)+ ν(CC)+ ς(CH$_2$)+ ν(CN) | 1159 | ~0 | 9 | 1157 | 4 | 5 |
| δ(CH)+ δ(CH)+ ν(CC) | 1157 | 137 | 0 | 1154 | 41 | 3 |
| ρr(CH$_2$)+ δ(CH)+ ν(CC)+ ν(CN) | 1143 | 2 | 14 | 1149 | 23 | 32 |
| ρr(CH$_2$)+ δ(CH)+ ν(CC)+ ν(CN) | 1143 | ~0 | 6 | 1117 | 36 | 6 |
| δ(CH)+ ρr(CH$_2$)+ ν(CC) | 1142 | 14 | 20 | 1094 | 17 | 13 |
| δ(CH)+ ν(CC)+ ν(CN) | 1103 | 111 | 5 | 1092 | 10 | 6 |
| ρr(CH$_2$)+ ν(CH=CH) | 1082 | 8 | 4 | 1089 | 69 | 5 |
| ν(CH=CH) | 1069 | ~0 | ~0 | 1055 | 1 | 1 |
| ν(CH=CH) | 1069 | 24 | 0 | 1055 | 1 | 0 |
| ν(CS)+ ν(CH=CH)+ ν(CN)+ δ(CH) | 1019 | 1 | 1 | 1018 | 8 | 5 |
| δ(CH)+ ν(CN)+ δ(CCC) | 1014 | 6 | 8 | 1011 | ~0 | 1 |
| δ(CH)+ ν(CN)+ ν(CS)+ δ(CCC) | 1013 | 1 | 26 | 1010 | 1 | 3 |
| δ(CH)+ ν(CC) + ν(CN) | 979 | 1 | 70 | 1007 | 1 | 4 |
| δ(CH)+ ν(CN)+ ν(CS)+ ν(CC) | 979 | 3 | 14 | 1006 | 2 | 12 |
| δ(CH)+ δ(CCC) | 974 | ~0 | 4 | 990 | 1 | 1 |
| δ(CH)+ δ(CCC) | 968 | 16 | ~0 | 989 | 1 | 0 |
| ν(CC)+ ν(CS)+ δ(CH) | 965 | ~0 | 0 | 977 | 7 | 19 |
| δ(CCC)+ ν(CN) | 964 | 5 | ~0 | 975 | 5 | 34 |
| δ(CCC)+ ν(CN)+ ν(CC) | 941 | 1 | 3 | 975 | 5 | 20 |
| ν(CN)+ δ(CCC) | 941 | 1 | ~0 | 972 | 13 | 3 |
| δ(CH)+ δ(CCC)+ ν(CN)+ ν(CS) | 910 | 2 | 5 | 949 | 3 | 2 |
| δ(CH)+ δ(CCC)+ ν(CN) | 909 | ~0 | ~0 | 945 | 2 | 1 |
| δ(CCC)+ ν(CC)+ ν(CS)+ν(CN) | 888 | ~0 | 5 | 885 | 26 | 3 |
| ρr(CH$_2$)+ ν(CN) | 860 | 127 | 2 | 856 | 87 | 3 |
| δ(CH)+ δ(CCC) | 826 | 2 | 5 | 854 | 2 | 4 |
| δ(CH)+ δ(CCC)+ ν(CN) | 826 | 2 | 6 | 852 | 0 | 2 |
| δ(CH)+ δ(CCC)+ ν(CN) | 785 | 1 | 1 | 809 | 1 | 0 |
| δ(CH)+ δ(CCC)+ δ(C-CO-N) | 777 | 23 | 4 | 803 | 32 | 1 |
| ς(CH$_2$)+ δ(CCC)+ ν(CN) | 753 | 14 | 3 | 762 | 22 | 3 |
| $^1$U(ring)+ ρr(CH$_2$) | 706 | 13 | 5 | 725 | 80 | 2 |
| $^1$U(ring)+ ρr(CH$_2$) | 704 | 85 | ~0 | 721 | 70 | 2 |
| $^2$w(ring)+ $^1$w(ring)+ δ(C-CO-N) | 680 | 14 | 12 | 685 | 23 | 5 |
| $^1$w(ring)+ $^2$w(ring)+ ρr(CH$_2$) | 676 | 28 | 0 | 681 | 28 | 0 |
| δ(CCC)+ δ(NCN)+ ρr(CH$_2$) | 657 | 2 | 12 | 664 | 17 | 7 |
| δ(CCC)+ ρr(CH$_2$)+ δ(C-CO-N) | 646 | 92 | 1 | 647 | 60 | 1 |
| δ(NCN)+ δ(CCC)+ ρr(CH$_2$) | 621 | 13 | 4 | 640 | 22 | 3 |
| ρr (CH$_2$)+ δ(C-CO-N)+ δ(CCC) | 609 | 14 | 2 | 630 | 15 | 1 |
| δ(CCC) | 606 | 0 | 7 | 604 | 0 | 8 |
| δ(CCC)+ ρr(CH$_2$) | 603 | 2 | 3 | 602 | ~0 | 4 |
| $^2$w(ring)+ $^1$w(ring)+ δ(C-CO-N) | 552 | 15 | 5 | 543 | 8 | 4 |
| ν(CS)+ ν(CN)+ $^2$w(ring) | 515 | 10 | 17 | 515 | 34 | 10 |
| $^2$w(ring)+ $^1$w(ring) | 490 | 3 | 1 | 492 | ~0 | 2 |

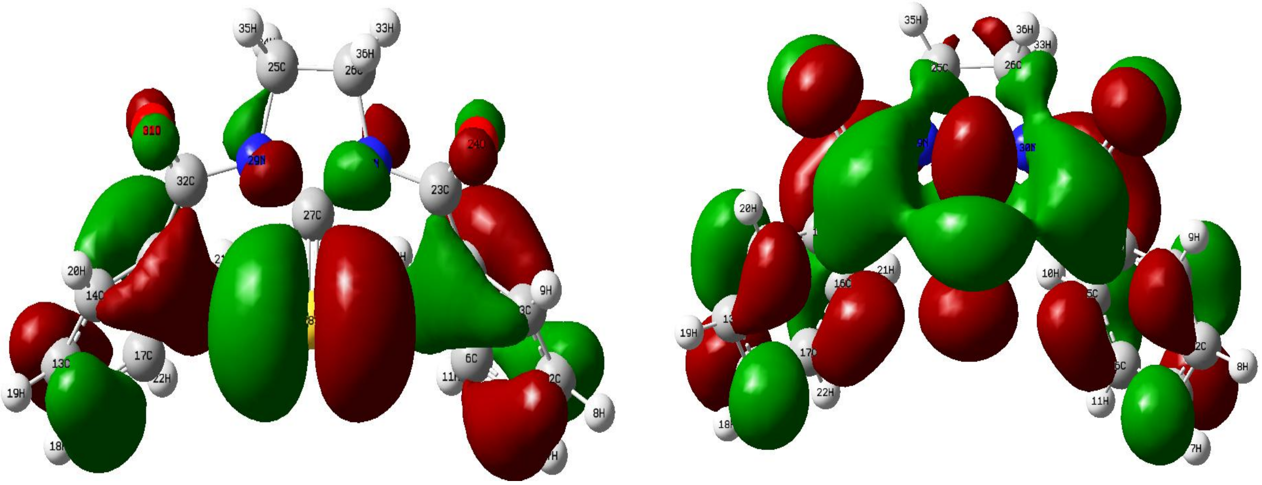
| | | | | | | |
|---|---|---|---|---|---|---|
| $^1$w(ring)+ $^2$w(ring) | 419 | 3 | 2 | 430 | 4 | 1 |
| $^1$w(ring)+ $^2$w(ring)+ ρr(CH$_2$)+ δ(CCO) | 402 | 17 | 1 | 408 | 13 | ~0 |
| $^2$w(ring)+ $^1$w(ring) | 400 | 0 | 1 | 406 | 0 | ~0 |
| $^1$w(ring)+ $^2$w(ring) | 399 | ~0 | 5 | 406 | 1 | 1 |
| δ(CCC)+ δ(CCO) | 379 | ~0 | 2 | 375 | 3 | 3 |
| ρr(CH$_2$)+ $^1$w(ring)+ $^2$w(ring) | 351 | 1 | 0 | 355 | 1 | 0 |
| w(molecule) | 299 | 3 | 2 | 303 | ~0 | 1 |
| $^1$τ(ring)+ $^2$τ(ring)+ ρr(CH$_2$)+ δ(CNC) | 282 | 6 | 1 | 249 | 5 | 1 |
| $^1$τ(ring)+ $^2$τ(ring)+ δ(CNC) | 239 | 1 | ~0 | 243 | 2 | 2 |
| ρr(CH$_2$)+ δ(CNC)+ $^2$τ(ring) | 234 | 0 | 4 | 234 | 11 | 1 |
| $^1$w(ring)+ $^2$w(ring)+ δ(NCS) | 208 | 10 | 3 | 198 | 9 | 4 |
| $^1$w(ring)+ $^2$w(ring)+ ρr(CH$_2$) | 197 | 3 | 2 | 180 | 2 | 11 |
| ρr(CH$_2$)+ $^2$τ(ring) | 172 | 1 | 21 | 141 | ~0 | 2 |
| ρr(CH$_2$)+ $^1$τ(ring) | 142 | 0 | 3 | 134 | 0 | 2 |
| ρr(CH$_2$)+ $^1$w(ring)+ $^2$w(ring) | 113 | 1 | 2 | 108 | 2 | 1 |
| w(molecule) | 106 | 3 | 2 | 91 | 2 | 4 |
| ρr(CH$_2$)+ $^1$τ(ring)+ $^2$τ(ring) | 76 | ~0 | 4 | 80 | 2 | 3 |
| w(molecule) | 60 | 5 | 8 | 59 | 8 | 8 |
| $^1$w(ring)+ $^2$w(ring) | 49 | 7 | 1 | 46 | 2 | 1 |
| $^1$w(ring)+ $^2$w(ring) | 39 | ~0 | 11 | 37 | 2 | 9 |
| w(molecule) | 27 | 1 | 9 | 24 | 1 | 2 |
| w(molecule) | 23 | 1 | 2 | 23 | 1 | 1 |

**Abbreviations Used:** ν: stretching; δ: bending; ρr: rocking; τ: torsion; w: wagging; asy: asymmetric; γ: scissoring; ς: twisting, U: umbrella
$^1$: ring–1, $^2$: ring–2
The frequencies have also been depicted in Table 2 with IR intensity values. As can be seen, infrared intensity calculations at HF basis set have been found to be slightly larger than B3LYP ones and the maximum IR intensity (794 km/mol) has been found to be 1242 cm$^{-1}$ at B3LYP/6–31G(d,p) level of calculation whereas the maximum IR intensity (591 km/mol) has been found to be 1260 cm$^{-1}$ at HF/6–31G(d,p) calculation level.

### 3.4.HOMO and LUMO Analyses

Highest Occupied Molecular Orbital (HOMO) and Lowest Unoccupied Molecular Orbital (LUMO) are important parameters for quantum chemistry. We can determine the way the molecule interacts with other species; hence, they are called the frontier orbitals. HOMO, which can be thought the outermost orbital containing electrons, tends to give these electrons such as an electron donor. On the other hand; LUMO can be thought the innermost orbital containing free places to accept electrons [42]. Owing to the interaction between HOMO and LUMO orbital of a structure, transition state transition of π–π* type is observed with regard to the molecular orbital theory [43]. Therefore, while the energy of the HOMO is directly related to the ionization potential, LUMO energy is directly related to the electron affinity. Energy difference between HOMO and LUMO orbital is called as energy gap that is an important stability for structures [44] and given in Table 3. In addition, 3D plots of highest occupied molecular orbitals (HOMO) and lowest unoccupied molecular orbitals (LUMO) are shown in Fig. 2.

**Figure 2.** 3D plots of a) the HOMO and b) LUMO of 1,3- Dibenzoylimidazolidine-2-thione molecule (obtained from HF method)



The energy band gap │(ΔE)│ (the value of the energy separation between HOMO and LUMO) of the title molecule has been found to be about 0.14 (a.u.) with regard to B3LYP/6–31G(d,p) calculation while it has been noted to be about 0.39 (a.u.) at HF/6–311G(d,p) level of calculation. The highest occupied molecular orbitals are localized mainly on the molecule but slightly on cyclopentane ring and hydrogen atoms of benzene rings. Similarly, the lowest unoccupied molecular orbitals are localized mainly on the molecule (denser than HOMO) except for hydrogen atoms. Moreover, Lowest MO Eigen value is –88.84 and –91.89(a.u.) at B3LYP/6–31G(d,p) and HF/6–311G(d,p) basis sets, respectively. Highest MO Eigen value is also found to be 4.84 (a.u.) at B3LYP/6–31G(d,p) and 5.29 (a.u.) at HF/6–31G(d,p) calculation level.

**Table 3.** Some of the calculated energy values of 1,3-Dibenzoylimidazolidine-2-thione in its ground state with singlet symmetry at DFT and HF methods

| **Quantity** | **Value** | |
|---|---|---|
| | **DFT** | **HF** |
| **Lowest MO Eigen value (a.u.)** | –88.84 | –91.89 |
| **Highest MO Eigen value (a.u.)** | 4.84 | 5.29 |
| **The virial (–V/T)** | 2.0077 | 2.0011 |
| **HOMO (a.u.)** | –0.21 | –0.32 |
| **LUMO (a.u.)** | –0.07 | 0.07 |
| **HOMO–LUMO gap, │ΔE│ (a.u.)** | 0.14 | 0.39 |
| **HOMO–1 (a.u.)** | –0.24 | –0.33 |
| **HOMO–2 (a.u.)** | –0.26 | –0.34 |
| **LUMO+1 (a.u.)** | –0.05 | 0.10 |
| **LUMO+2 (a.u.)** | –0.02 | 0.13 |

### 3.5.Atomic Charges

Atomic charges of 1,3-Dibenzoylimidazolidine-2-thione, which have been calculated by Mulliken method [45, 46] at the HF/6–31G(d,p) and B3LYP/6–31G(d,p) levels of calculation, have been shown in Table 4. The magnitudes of the carbon atomic charges have been found to be either positive or negative at the basis sets. These magnitudes have been obtained to change between – 0.16 and 0.79. $C_{23}$ and $C_{32}$ connected with oxygen and nitrogenous atoms have the maximum charge value (0.52 at B3LYP/6–31G(d,p) and 0.79 at the HF/6–31G(d,p) levels of calculation). The magnitudes of charges calculated on N atoms at HF basis set have been found to be more negative than DFT calculations. These calculations have been obtained to be – 0.53 ($N_{29}$), – 0.53 ($N_{30}$) at the B3LYP/6–31G(d,p), and – 0.79 ($N_{29}$), – 0.77 ($N_{30}$) at the HF/6–31G(d,p) levels of calculation. For $S_{28}$ atom, the magnitude of charge has been noted to be –0.20 and –0.24 at B3LYP/6–31G(d,p) and HF/6–31G(d,p) basis sets, respectively. Furthermore, while the magnitudes of charges of O atoms have been determined to be –0.46 at DFT calculation level, they have been calculated to be – 0.54 ($O_{24}$) and – 0.53 ($O_{31}$) at HF calculation level. In addition, the magnitudes of the hydrogen atomic charges have been noticed to arrange in an order from 0.09 to 0.19. The charge on $H_{35}$ connected with $C_{25}$ has the maximum magnitude (0.14 at B3LYP/6–31G(d,p) and 0.19 at the HF/6–31G(d,p) levels of calculation). The results show that:
*All the hydrogen atoms in molecule lost electrons.
*All the oxygen atoms in molecule accepted electrons.
*Charge migration to heavy atoms can be related to molecular interactions.
*HF/6–31G(d,p) basis set calculations have more negative magnitudes than the others.
*Computations of B3LYP and HF calculation levels are in good agreement with each other.

**Table 4.** Atomic charges for optimized geometry of 1,3-Dibenzoylimidazolidine-2-thione

| Atom No | B3LYP/6–31G(d,p) | HF/6–31G(d,p) |
|---|---|---|
| $C_1$ | –0.07 | –0.13 |
| $C_2$ | –0.09 | –0.16 |
| $C_3$ | –0.07 | –0.10 |
| $C_4$ | –0.08 | –0.10 |
| $C_5$ | –0.09 | –0.10 |
| $C_6$ | –0.10 | –0.16 |
| $H_7$ | 0.09 | 0.16 |
| $H_8$ | 0.09 | 0.16 |
| $H_9$ | 0.10 | 0.19 |
| $H_{10}$ | 0.11 | 0.16 |
| $H_{11}$ | 0.09 | 0.15 |
| $C_{12}$ | –0.07 | –0.13 |
| $C_{13}$ | –0.10 | –0.16 |
| $C_{14}$ | –0.09 | –0.10 |
| $C_{15}$ | –0.08 | –0.10 |
| $C_{16}$ | –0.07 | –0.09 |
| $C_{17}$ | –0.09 | –0.16 |
| $H_{18}$ | 0.09 | 0.16 |
| $H_{19}$ | 0.09 | 0.16 |
| $H_{20}$ | 0.11 | 0.19 |
| $H_{21}$ | 0.10 | 0.16 |
| $H_{22}$ | 0.09 | 0.16 |

| | | |
|---|---|---|
| $C_{23}$ | 0.52 | 0.79 |
| $O_{24}$ | –0.46 | –0.54 |
| $C_{25}$ | –0.05 | –0.01 |
| $C_{26}$ | –0.04 | –0.02 |
| $C_{27}$ | 0.34 | 0.49 |
| $S_{28}$ | –0.20 | –0.24 |
| $N_{29}$ | –0.53 | –0.79 |
| $N_{30}$ | –0.53 | –0.77 |
| $O_{31}$ | –0.46 | –0.53 |
| $C_{32}$ | 0.52 | 0.79 |
| $H_{33}$ | 0.14 | 0.16 |
| $H_{34}$ | 0.14 | 0.15 |
| $H_{35}$ | 0.14 | 0.19 |
| $H_{36}$ | 0.14 | 0.18 |

### 3.6.Thermodynamic Properties

Several thermodynamic parameters have been calculated by using HF and B3LYP with 6–31G (d,p) basis set and have been given in Table 5. Scale factors have been recommended [29] for an accurate prediction in determining the zero–point vibration energies. The total energies and the change in the total entropy and enthalpy of the molecule at room temperature at different theoretical methods have been presented. Table 5 demonstrates several thermodynamic parameters of the molecule without results of experimental. Calculations of HF/6–31G(d,p) basis set for energy parameters and rotational constants are closer to B3LYP/6–31G(d,p) ones while HF data are slightly smaller than DFT data for the entropy and enthalpy values. In addition, the dipole moment that is an important tool for the electronic property of a molecule results from non-uniform distribution of charges on the various atoms in the molecule and is mainly used to study the intermolecular interactions involving the van der Waal type dipole–dipole forces, etc., because larger the dipole moment, stronger will be the intermolecular interactions [47]. The dipole moment of the title compound is found to be 0.23 and 0.01 Debye at B3LYP/6–31G(d,p) and HF/6–31G(d,p) level of theory (Table 5). Based on these results, calculation of DFT method is found to be more polar (non-uniform distribution of charges) than that of HF.

**Table 5.** Theoretically computed energies (a.u.), zero–point vibrational energies (kcal mol$^{-1}$), rotational constants (GHz), entropies and heat capacities (cal mol$^{-1}$ K$^{-1}$) and dipole moment (Debye)

| Parameters | B3LYP/6–31G(d,p) | HF/6–31G(d,p) |
|---|---|---|
| **Total energy** | –1314.42 | –1308.10 |
| **Zero–point energy** | 171.42 | 171.37 |
| **Rotational constant** | 0.51 | 0.46 |
| | 0.15 | 0.18 |
| | 0.13 | 0.14 |
| **Entropy (S)** | | |
| **Total** | 144.16 | 140.78 |
| **Translational** | 43.09 | 43.09 |

| | | |
|---|---|---|
| **Rotational** | 34.70 | 34.61 |
| **Vibrational** | 66.37 | 63.08 |
| **Heat Capacity ($C_v$)** | | |
| **Total** | 70.24 | 65.02 |
| **Translational** | 2.98 | 2.98 |
| **Rotational** | 2.98 | 2.98 |
| **Vibrational** | 64.28 | 59.06 |
| **Dipole Moment** | 0.23 | 0.01 |

### 3.7.UV–Vis Spectra Analyses

Ultra violet spectra analyses of 1,3-Dibenzoylimidazolidine-2-thione have been investigated by various theoretical results. Absorption maxima ($\lambda_{max}$) of the molecule have been calculated by the ZINDO [48] and TD [49] methods. The calculated visible absorption maxima of λ, which are a function of the electron availability, have been reported in Table 6. Calculations of molecular orbital geometry show that the visible absorption maxima of this molecule correspond to the electron transition between frontier orbitals such as translation from HOMO to LUMO. As can be seen from the Table 6, the calculated absorption maxima values have been found to be 2453, 1115 and 833 nm at ZINDO calculation level. Moreover, $\lambda_{max}$ have been found to arrange in an order from 740 to 2213 nm at TD–B3LYP/6–31G(d,p) whereas they have been observed to change from 399 to 1312 nm (the smallest values in the all levels) at TD–HF/6–31G(d,p) calculation level. As seen, calculations of ZINDO and TD–B3LYP/6–31G(d,p) are close to each other. Furthermore, oscillator strength values have also been depicted in the same table. Not only are these values close to each other for ZINDO and TD–HF/6–31G(d,p) calculations but also observe the similar trend (firstly decrease then increase) at all levels of calculation.

**Table 6.** Theoretical electronic absorption spectra values of 1,3-Dibenzoylimidazolidine-2-thione

| **Calculated, λcal (nm)** | | | | | |
|---|---|---|---|---|---|
| **Zindo** | | **TD–B3LYP/6–31G(d,p)** | | **TD–HF/6–31G(d,p)** | |
| **Wavelength (nm)** | **Oscillator Strength** | **Wavelength (nm)** | **Oscillator Strength** | **Wavelength (nm)** | **Oscillator Strength** |
| 2453 | 0.0402 | 2213 | 0.0091 | 1312 | 0.0373 |
| 1115 | 0.0118 | 884 | 0.0082 | 535 | 0.0217 |
| 833 | 0.0562 | 740 | 0.0107 | 399 | 0.0892 |

### 3.8.NMR Spectra Analyses

Whereas no electron correlation effects are taken into account in HF methods, DFT methods treat the electronic energy as a function of the electron density of all electrons simultaneously and thus include electron correlation effect [50–52]. In this study, GIAO $^{13}$C and $^{1}$H NMR chemical shifts of 1,3-Dibenzoylimidazolidine-2-thione have been calculated and depicted in Table 7. These calculations have been obtained at HF/6–31G(d,p) and B3LYP/6–31G(d,p) levels for the optimized geometry. $^{1}$H chemical shift values have been found to be about 3.36–47.37 and 2.64–46.66 parts per million (ppm) at HF/6–31G(d,p)//HF/6–31G(d) and HF/6–31G(d,p)//B3LYP/6–311+G(2d,p) calculation level whereas these values have been observed in 2.95–51.85 and 2.23–51.13 ppm at B3LYP/6–31G(d,p)//HF/6–31G(d) and B3LYP/6–31G(d,p)//B3LYP/6–311+G(2d,p) calculation levels, respectively. Further, the minimum chemical shifts of hydrogen atoms bond connected with $C_{25}$ and $C_{26}$ atoms have been found to arrange in an order from 2.23–5.25 ppm whereas the maximum chemical shifts have been obtained for $H_{21}$ and $H_9$ atoms (the nearest neighbors to sulfur atom). On the other hand, $^{13}C$ chemical shifts with regard to TMS have been calculated at the same basis sets and given in the same table. $^{13}C$ chemical shift values have been found to be about 5.12–204.65 and -12.39–187.13 ppm at HF/6–31G(d,p)//HF/6–31G(d) and HF/6–31G(d,p)//B3LYP/6–311+G(2d,p) basis set while these values have been obtained to be about 21.54–199.54 and 4.02–182.02 ppm at B3LYP/6–31G(d,p)//HF/6–31G(d) and B3LYP/6–31G(d,p)//B3LYP/6–311+G(2d,p) basis sets, respectively. $C_{25}$ has the minimum chemical shift of C atoms changing from –12.39 to 21.54 ppm. As can be seen from Table 7, generally the large chemical shift values for hydrogen atoms have been found at B3LYP/6–31G(d,p)//HF/6–31G(d) level of calculation whereas the small ones have been obtained at B3LYP6–31G(d,p)//B3LYP/6–311+G(2d,p) calculation level.

**Table 7.** 13C and 1H isotropic chemical shifts (with respect to TMS, all values in ppm) for 1,3-Dibenzoylimidazolidine-2-thione

| | **Calculated Chemical Shift (ppm)** | | | |
|---|---|---|---|---|
| **Atom** | **HF/6–31G(d,p)// HF/6–31G(d)** | **HF/6–31G(d,p)// B3LYP/6–311+G(2d,p)** | **B3LYP/6–31G(d,p)// HF/6–31G(d)** | **B3LYP/6–31G(d,p)// B3LYP/6–311+G(2d,p)** |
| $H_{33}$ | 3.36 | 2.64 | 2.95 | 2.23 |
| $H_{34}$ | 3.44 | 2.73 | 3.29 | 2.58 |
| $H_{35}$ | 3.45 | 2.74 | 3.47 | 2.75 |
| $H_{36}$ | 5.25 | 4.53 | 4.06 | 3.35 |
| $H_{22}$ | 6.24 | 5.52 | 4.29 | 3.57 |
| $H_{19}$ | 6.84 | 6.12 | 5.64 | 4.92 |
| $H_{18}$ | 7.84 | 7.13 | 5.78 | 5.06 |
| $H_{11}$ | 8.23 | 7.54 | 6.06 | 5.34 |
| $H_8$ | 8.27 | 7.56 | 8.09 | 7.37 |
| $H_7$ | 8.39 | 7.67 | 8.37 | 7.65 |
| $H_{20}$ | 8.80 | 8.08 | 8.41 | 7.69 |
| $H_{10}$ | 9.14 | 8.43 | 8.90 | 8.19 |
| $H_{21}$ | 21.54 | 20.80 | 44.64 | 43.93 |
| $H_9$ | 47.37 | 46.66 | 51.85 | 51.13 |
| $C_{26}$ | 5.12 | -12.39 | 21.54 | 4.02 |
| $C_{25}$ | 32.19 | 14.67 | 61.80 | 44.28 |
| $C_{16}$ | 46.09 | 28.57 | 104.67 | 87.15 |
| $C_{17}$ | 97.97 | 80.45 | 109.13 | 91.61 |
| $C_{27}$ | 105.83 | 88.31 | 110.35 | 92.83 |
| $C_{15}$ | 115.53 | 90.01 | 118.06 | 100.54 |
| $C_{13}$ | 121.90 | 104.38 | 118.25 | 100.73 |
| $C_2$ | 123.54 | 106.02 | 121.35 | 103.83 |
| $C_6$ | 127.80 | 110.82 | 132.83 | 115.31 |
| $C_5$ | 132.59 | 115.07 | 133.94 | 116.42 |
| $C_1$ | 132.94 | 115.42 | 134.59 | 117.07 |
| $C_{14}$ | 133.26 | 115.74 | 142.28 | 124.76 |
| $C_{12}$ | 137.85 | 120.33 | 148.56 | 131.04 |
| $C_4$ | 139.46 | 121.95 | 149.87 | 132.35 |
| $C_3$ | 171.74 | 154.22 | 182.73 | 165.21 |
| $C_{32}$ | 190.48 | 172.96 | 189.34 | 171.82 |
| $C_{23}$ | 204.65 | 187.13 | 199.54 | 182.02 |

### 3.9.Molecular Electrostatic Potential

At any given point r(x, y, z) in the vicinity of a molecule, the molecular electrostatic potential, V(r) is defined in terms of the interaction energy between the electrical charge generated from the molecule electrons and nuclei and a positive test charge (a proton) located at r [53]. The molecular electrostatic potential (MEP) is related to the electronic density and a very useful descriptor for determining sites for electrophilic attack and nucleophilic reactions as well as hydrogen–bonding interactions [54–56]. In Fig. 3, whereas electrophilic reactivity has been presented by negative (red) regions, nucleophilic reactivity has been shown by the positive (blue) regions of MEP. As seen from the figure, the red region has been localized on the vicinity of oxygen atoms. On the other hand, although the blue region has not been seen clearly the nucleophilic reactivity of the molecule has been localized on the hydrogen atoms (especially benzene rings). In this respect, the compound is useful to both bond metallically and interact intermolecularly. This result has also been supported by the evidences of charge analyses part.

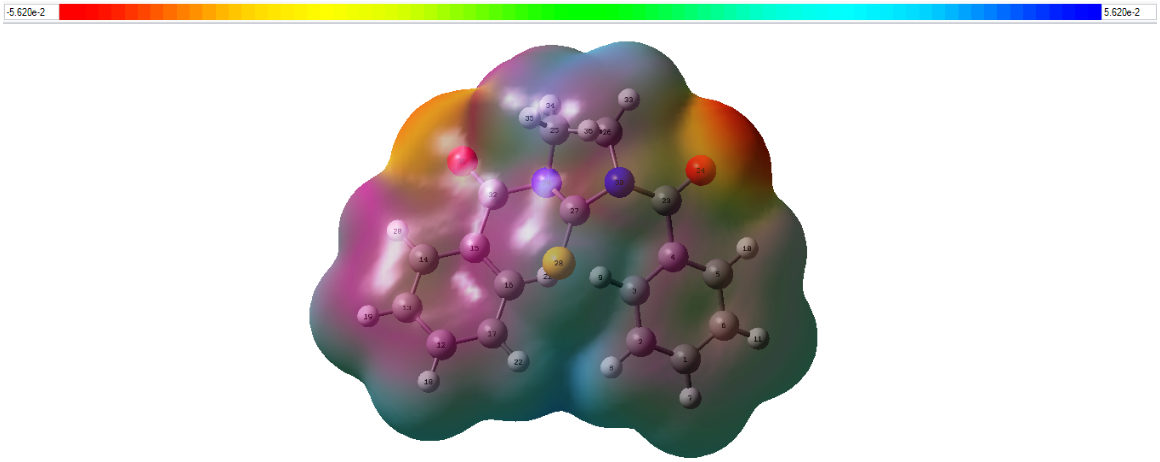


**Figure 3.** 3D plots of the molecular electrostatic potential map of p-biphenyloxycarbonylphenyl acrylate obtained from DFT method (Red color shows the negative regions while blue color presents the positive regions of MEP).

## 4.CONCLUSION

In this study, the characterization of 1,3-Dibenzoylimidazolidine-2-thione has been carried out by the quantum mechanical methods for the first time. Bond lengths, angles and dihedrals have, in this respect, been calculated by using B3LYP/6–31G(d,p) and HF/6–31G(d,p) methods and compared with experimental values. All compared data have been shown to have a good agreement with each other, confirming that the computational programs are reliable to characterize the molecule and helpful to predict compound properties economically and to clarify some experiment phenomena insightfully. Moreover, vibration frequencies including assignments, Infrared intensities and Raman activities have been calculated and theoretical vibrational spectra obtained have been interpreted by means of normal coordinate analysis based on scaled density functional force field. It has been observed that all the scaled frequencies are in good agreement with each other and in fact the correlation coefficient between them has been determined as 0.9991. At the same time, Mulliken atomic charges, thermodynamic properties, UV–vis and NMR spectra have been investigated by means of the methods. The results obtained indicate that not only is the charge migration to heavy atoms related to molecular interactions for the compound but also the hydrogen atoms lost electrons while all the oxygen atoms in molecule accepted electrons. Furthermore, after the frontier molecular orbitals and molecular electrostatic potential have been simulated, the dipole moment, transition state and energy band gap values have been analyzed clearly. Based on the results obtained, the title compound with strong reactivity and polarity has been found to be useful to bond metallically and interact intermolecularly. In conclusion, this study both shows the way to the identification of 1,3-Dibenzoylimidazolidine-2-thione molecule and helps to researchers for the future studies in both the fundamental researches and applications in technology and industry.

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