**Original Research Article**

# Comparison of 6-311G(d) and 3-21G(DFT/HF) Methods of 3-Methyl-4-[3-(3-methoxybenzoxy)-benzylidenamino]-4,5-dihydro-1*H*-1,2,4-triazol-5-one


## ABSTRACT

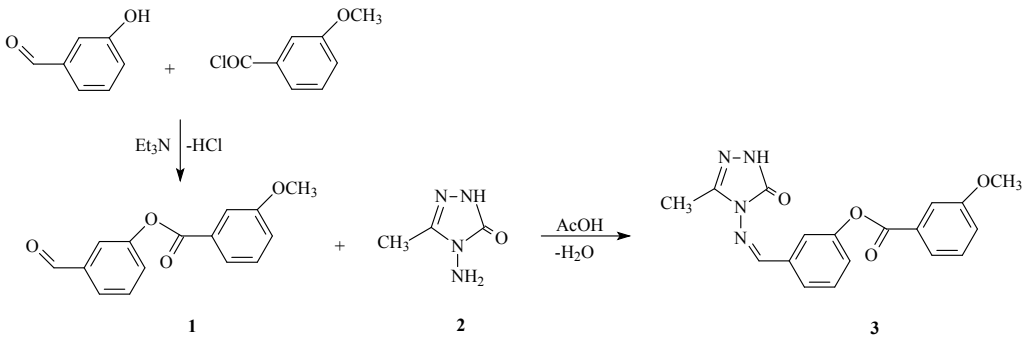
3-Methyl-4-[3-(3-methoxybenzoxy)-benzylidenamino]-4,5-dihydro-1*H*-1,2,4-triazol-5-one was synthesized by the reaction of 3-methyl-4-amino-4,5-dihydro-1*H*-1,2,4-triazol-5-one with 3-(3-methoxybenzoxy)-benzaldehyde which was synthesized by the reaction of 3-hydroxybenzaldehyde with 3-methoxybenzoyl chloride by using triethylamine. This compound was optimized by using B3LYP/6-311G(d) HF/6-311G(d) and B3LYP/3-21G, HF/3-21G basis sets. Electronic properties (total energy, dipole moment), thermodynamic parameters, geometric properties (bond angles and bond lengths), the highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO), Mulliken atomic charges, the molecular electrostatic potential (MEP) of 3-methyl-4-[3-(3-methoxybenzoxy)-benzylidenamino]-4,5-dihydro-1*H*-1,2,4-triazol-5-one have been performed. $^{1}$H-NMR and $^{13}$C-NMR isotropic shift values of 3-methyl-4-[3-(3-methoxybenzoxy)-benzylidenamino]-4,5-dihydro-1*H*-1,2,4-triazol-5-one in the ground state and in DMSO solvent were calculated by using the gauge-including atomic orbital (GIAO) method. The structural and spectroscopic data of the molecule in the ground state have been calculated by using density functional metfelhod (DFT/B3LYP) and Hartree–Fock method (HF) with the 6-311G(d) and 3-21G basis sets. The veda4f program was used for the identification of calculated IR data. The UV-vis values in ethanol were found and compared with experimental results. All experimental data were compared with theoretical data.


*Keywords:* 4,5-Dihydro-1*H*-1,2,4-triazol-5-on, Gaussian 09W, GIAO, B3LYP, HF, 6-311G(d), 3-21G basis sets.

## 1. INTRODUCTION

Many properties of molecules with theoretical calculation methods can be calculated without having to experiment. In fact, some studies are more accurate and reliable results than the experimental method. Theoretical data are always router and informative for experimental studies. Also, it is used as a comparative experimental study with theoretical studies. Heterocyclic compounds containing 1,2,4-triazole and 4,5-dihydro-1*H*-1,2,4-triazol-5-one derivatives have been reported to exhibit diverse biological activities such as antimicrobial, antitumor, anticancer, antifungal, anti-HIV, antiviral, anti-inflammatory, analgesic and antioxidant properties [1–4]. Nowadays many theoretical studies have been published on structure and properties of *N*-arylidenamino-4,5-dihydro-1*H*-1,2,4-triazol-5-one derivatives. The structural and spectroscopic properties with combined computational and experimental tools of some 4,5-dihydro-1*H*-1,2,4-triazol-5-one derivatives have been reported Indeed, the theoretical and experimental spectroscopic properties of some 4,5-dihydro-1*H*-1,2,4-triazol-5-one derivatives of the were investigated [5-12].

In this study, 3-methyl-4-[3-(3-methoxybenzoxy)-benzylidenamino]-4,5-dihydro-1*H*-1,2,4-triazol-5-one (**3**) were obtained from the reaction of compound **(2)** with 3-(3-methoxybenzoxy)-benzaldehyde (**1**) which was synthesized by the reaction of 3-hydroxybenzaldehyde with 3-methoxybenzoyl chloride by using triethylamine (Scheme **1**).




**Scheme1.** Synthetic pathway of compound **3**

3-Methyl-4-[3-(3-methoxybenzoxy)-benzylidenamino]-4,5-dihydro-1*H*-1,2,4-triazol-5-one (**3**) has been optimized by using B3LYP/6-311G (d), HF/6-311G (d) and B3LYP/3-21G, HF/3-21G basis sets [10,11]. Starting from this optimized structure with $^{1}$H-NMR and $^{13}$C-NMR and IR spectral data values according to GIAO method was calculated using the method of Gaussian G09W program package in gas phase and in DMSO solvent [12]. Theoretical and experimental values [13] were plotted according to exp =a +b. δ calc Eq. a and b constants regression coefficients with a standard error values were found using the SigmaPlot program. Theoretically calculated IR data are multiplied with appropriate adjustment factors and the data obtained according to HF and DFT methods are formed using theoretical infrared spectrum. The veda4f program was used for the identification of calculated IR data [14]. Experimental [13] and theoretical UV-vis values in ethanol were calculated and compared. The purpose of this study is to report theoretical results of FT-IR, $^{1}$H-NMR and $^{13}$C-NMR and UV-vis spectra of compound **3**. Additionally, the bond angles, bond lengths, dipole moments, HOMO-LUMO energy, total energies, thermodynamic properties, Mulliken atomic charges, molecular electrostatic potential (MEP) of the molecule were found by both methods.

## 2. MATERIAL AND METHODS

### 2.1. Experimental

*Chemistry*

Chemical reagents and all solvents used in this study were purchased from Merck AG (Darmstadt, Germany), Sigma (Sigma-Aldrich GmbH, Sternheim, Germany) and Fluka (Buchs, Switzerland). The starting compound 3-methyl-4-amino-4,5-dihydro-1*H*-1,2,4- triazol-5-one **2** were prepared from the reactions of the corresponding ester ethoxycarbonylhydrazones with an aqueous solution of hydrazine hydrate as described in the literature [15]. Melting points were determined in open glass capillaries using a WRS-2A Microprocessor melting-point apparatus (Liaoning, mainland China) and are uncorrected. The IR spectra were obtained on an ALPHA-P BRUKER FT-IR (Germany) spectrometer. $^{1}$H and $^{13}$C NMR spectra were recorded in deuterated dimethyl sulfoxide with TMS as an internal standard using a Bruker (Germany) spectrometer at 400 MHz and 100 MHz, respectively. UV absorption spectra were measured in 10 mm quartz cells between 200 and 400 nm using a PG Instruments Ltd T80 UV/VIS (Leicestershire, United Kingdom) spectrometer. Extinction coefficients (ε) are expressed in L mol$^{-1}$ cm$^{-1}$.

*The synthesis of compound **3***

The compound **2** (0.01 mol) was dissolved in acetic acid (20 mL) and treated with 3-(3 methoxybenzoxybenzaldehyde) **1** (0.01 mol). The mixture was refluxed for 2 h and subsequently evaporated at 50-55 °C *in vacuo*. Several recrystallizations of the residue from ethanol gave pure compound **3** as colourless crystals.

*3-Methyl-4-[3-(3-methoxybenzoxy)-benzylidenamino]-4,5-dihydro-1H-1,2,4-triazol-5-one*

Yield: 3.48 g (98%); mp: 188 ºC; IR (KBr, *u*, cm$^{-1}$): 3169 (NH), 1735, 1700 (C=O), 1601, 1578 (C=N), 1268 (COO), 776, 681 (1,3-disubstituted benzenoid ring); $^{1}$H NMR (400 MHz, DMSO-d6): δ 2.29 (s, 3H, $CH_3$), 3.87 (s, 3H, $OCH_3$), 7.33-7.36 (m, 1H, Ar-H), 7.46-7.48 (m, 1H, Ar-H), 7.55 (t, 1H, Ar-H, *J*=7.84), 7.60-7.64(m, 2H), 7.75-7.79(m, 3H), 9.79 (s, 1H, N=CH), 11.87 (s, 1H, NH); $^{13}$C NMR (100 MHz, DMSO-d6): δ 11.08 ($CH_3$), 55.43 ($OCH_3$), 120.22 (2C), 122.13, 124.94, 125.94, 130.03, 130.16, 130.25, 135.21, 151.01, 159.39, 144.31 (triazole C3), 151.15 (N=CH), 152.40 (triazole C5), 164.33 (COO); UV $\lambda_{max}$ (ε): 296 (16.750), 242 (13.213), 220 (23.654) nm.

### 2.2. Theoretical

All the calculations for title compound was performed by using Gaussian G09W program. Firstly, geometry of this compound was obtained at the HF and DFT/B3LYP levels of theory along with standard 6-311G(d) and 3-21G basis sets. The obtained results were visualized by aid of GaussView program [16]. After the vibrational frequencies and their relative intensities had calculated with the aid of B3LYP/6-311G(d), HF/6-311G(d) and B3LYP/3-21G, HF/3-21G basis sets, the obtained results were compared with experimental results. The GIAO (Gauge Including Atomic Orbital) method is the most widely used technique for calculating NMR shielding values [12]. That's why theoretically calculating $^{1}$H NMR and $^{13}$C NMR chemical shifts values was used this method. Also, computing excitation energies and oscillator strengths for electronic transitions from ground to excited states was used time–dependent density functional theory (TD-DFT) [17-19]. Many electronic, geometric and thermodynamic properties, HOMO-LUMO energies, Mulliken atomic charges, the molecular electrostatic potential of title molecule are calculated at the HF/6-311G(d) and DFT/6-311G(d) and HF/3-21G and DFT/3-21G levels.

## 3. RESULTS AND DISCUSSION

The optimized molecular and chemical structure of 3-methyl-4-[3-(3-methoxybenzoxy)-benzylidenamino]-4,5-dihydro-1*H*-1,2,4-triazol-5-one are shown in (Figure **1**). The calculated molecular geometric parameters (bond angles, bond lengths, Mulliken atomic charges) by using the Hartree Fock (HF) and DFT/B3LYP methods with 6-311G(d) and 3-21G basis sets are given in Table **1-3**.

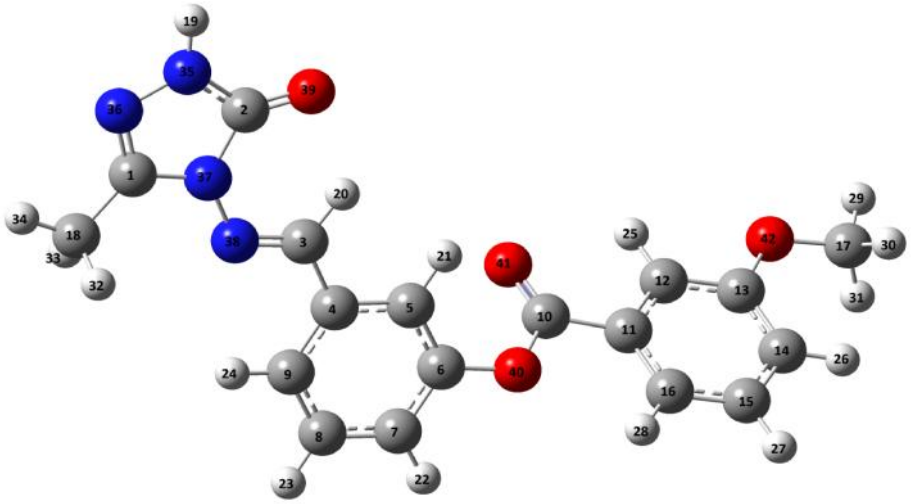



**Figure 1. The optimized molecular structure of 3-methyl-4-[3-(3-methoxybenzoxy)-benzylidenamino]-4,5-dihydro-1*H*-1,2,4-triazol-5-one**

**Table 1. The calculated bond angles ($^{0}$) of compound 3 (6-311G(d) HF/B3LYP, 3-21G HF/B3LYP)**

| | Bond Angles | HF 6-311G(d) | B3LYP 6-311G(d) | HF 3-21G | B3LYP 3-21G |
|---|---|---|---|---|---|
| **1** | C(1)-N(37)-N(38) | 121.062 | 121.276 | 120.430 | 120.701 |
| **2** | C(1)-N(36)-N(35) | 105.020 | 104.750 | 104.094 | 103.327 |
| **3** | C(1)-N(37)-C(2) | 108.082 | 108.260 | 109.216 | 109.287 |
| **4** | C(1)-C(18)-H(32) | 110.647 | 111.137 | 110.144 | 110.380 |
| **5** | C(1)-C(18)-H(33) | 110.649 | 111.158 | 110.144 | 110.380 |
| **6** | C(1)-C(18)-H(34) | 108.624 | 108.723 | 108.983 | 108.909 |
| **7** | H(32)-C(18)-H(34) | 109.546 | 109.258 | 109.799 | 109.765 |
| **8** | H(33)-C(18)-H(32) | 107.814 | 107.259 | 107.962 | 107.632 |
| **9** | H(33)-C(18)-H(34) | 109.548 | 109.270 | 109.799 | 109.765 |
| **10** | N(36)-C(1)-N(37) | 111.302 | 111.401 | 111.725 | 112.206 |
| **11** | N(36)-N(35)-H(19) | 120.841 | 120.313 | 120.148 | 119.487 |
| **12** | N(36)-N(35)-C(2) | 113.777 | 114.490 | 112.860 | 113.973 |
| **13** | N(37)-C(1)-C(18) | 123.272 | 123.480 | 122.367 | 122.485 |
| **14** | H(19)-N(35)-C(2) | 125.382 | 125.197 | 126.992 | 126.540 |

| | | | | | |
|---|---|---|---|---|---|
| **15** | N(35)-C(2)-N(37) | 101.818 | 101.098 | 102.105 | 101.206 |
| **16** | N(35)-C(2)-O(39) | 129.582 | 130.112 | 130.222 | 130.859 |
| **17** | O(39)-C(2)-N(37) | 128.600 | 128.790 | 127.673 | 127.934 |
| **18** | C(2)-N(37)-N(38) | 130.854 | 130.462 | 130.354 | 130.013 |
| **19** | N(37)-N(38)-C(3) | 120.006 | 119.209 | 118.992 | 117.229 |
| **20** | N(38)-C(3)-H(20) | 122.340 | 122.029 | 122.540 | 122.475 |
| **21** | N(38)-C(3)-C(4) | 120.404 | 117.948 | 120.047 | 119.613 |
| **22** | H(20)-C(3)-C(4) | 117.259 | 117.762 | 117.413 | 117.911 |
| **23** | C(3)-C(4)-C(5) | 119.033 | 119.572 | 117.828 | 119.082 |
| **24** | C(3)-C(4)-C(9) | 122.564 | 122.481 | 121.645 | 121.572 |
| **25** | C(4)-C(5)-H(21) | 120.989 | 120.233 | 120.936 | 121.089 |
| **26** | C(4)-C(5)-C(6) | 119.885 | 119.572 | 119.061 | 119.167 |
| **27** | H(21)-C(5)-C(6) | 119.125 | 120.190 | 120.004 | 119.744 |
| **28** | C(5)-C(6)-O(40) | 117.928 | 122.321 | 124.881 | 125.371 |
| **29** | C(5)-C(6)-C(7) | 121.117 | 121.037 | 120.820 | 120.661 |
| **30** | O(40)-C(6)-C(7) | 120.872 | 116.532 | 114.299 | 113.968 |
| **31** | C(6)-C(7)-H(22) | 120.051 | 119.242 | 118.721 | 118.559 |
| **32** | C(6)-C(7)-C(8) | 118.950 | 119.278 | 119.694 | 119.793 |
| **33** | H(22)-C(7)-C(8) | 120.998 | 121.480 | 121.585 | 121.648 |
| **34** | C(7)-C(8)-H(23) | 119.425 | 119.481 | 119.583 | 119.507 |
| **35** | C(7)-C(8)-C(9) | 120.709 | 120.519 | 120.328 | 120.343 |
| **36** | H(23)-C(8)-C(9) | 119.866 | 120.000 | 120.089 | 120.150 |
| **37** | C(8)-C(9)-H(24) | 120.516 | 120.851 | 121.131 | 121.542 |
| **38** | C(8)-C(9)-C(4) | 119.934 | 120.021 | 119.570 | 119.689 |
| **39** | H(24)-C(9)-C(4) | 119.549 | 119.129 | 119.300 | 118.769 |
| **40** | C(9)-C(4)-C(5) | 119.404 | 119.571 | 120.527 | 120.347 |
| **41** | C(6)-O(40)-C(10) | 120.030 | 120.567 | 128.248 | 125.479 |
| **42** | O(40)-C(10)-O(41) | 123.395 | 123.565 | 123.483 | 124.181 |
| **43** | O(40)-C(10)-C(11) | 111.899 | 111.211 | 111.449 | 110.232 |
| **44** | O(41)-C(10)-C(11) | 124.706 | 125.224 | 125.068 | 125.587 |
| **45** | C(10)-C(11)-C(16) | 122.175 | 122.641 | 122.033 | 122.615 |
| **46** | C(10)-C(11)-C(12) | 117.239 | 117.015 | 116.966 | 116.550 |
| **47** | C(11)-C(12)-H(25) | 120.464 | 120.163 | 120.618 | 120.120 |
| **48** | C(11)-C(12)-C(13) | 120.285 | 120.321 | 120.061 | 120.243 |
| **49** | H(25)-C(12)-C(13) | 119.251 | 119.517 | 119.321 | 119.637 |
| **50** | C(12)-C(13)-O(42) | 115.788 | 115.688 | 116.044 | 115.806 |
| **51** | C(12)-C(13)-C(14) | 119.428 | 119.522 | 119.360 | 119.196 |
| **52** | C(13)-O(42)-C(17) | 119.946 | 118.659 | 120.963 | 118.207 |
| **53** | O(42)-C(13)-C(14) | 124.784 | 124.790 | 124.596 | 124.998 |
| **54** | O(42)-C(17)-H(29) | 106.190 | 105.746 | 105.464 | 104.864 |
| **55** | O(42)-C(17)-H(30) | 111.459 | 111.547 | 111.308 | 111.613 |
| **56** | O(42)-C(17)-H(31) | 111.465 | 111.553 | 111.308 | 111.613 |
| **57** | H(29)-C(17)-H(30) | 109.105 | 109.243 | 109.618 | 109.684 |
| **58** | H(29)-C(17)-H(31) | 109.099 | 109.236 | 111.308 | 109.683 |
| **59** | H(30)-C(17)-H(31) | 109.430 | 109.419 | 109.445 | 109.293 |
| **60** | C(13)-C(14)-C(15) | 119.785 | 119.682 | 120.128 | 120.122 |
| **61** | C(13)-C(14)-H(26) | 121.116 | 120.999 | 120.696 | 120.618 |
| **62** | C(14)-C(15)-C(16) | 121.132 | 119.682 | 120.795 | 120.907 |
| **63** | H(26)-C(14)-C(15) | 119.099 | 119.319 | 119.176 | 119.260 |
| **64** | C(14)-C(15)-H(27) | 119.033 | 119.057 | 119.259 | 119.175 |
| **65** | H(27)-C(15)-C(16) | 119.835 | 119.814 | 119.946 | 119.918 |
| **66** | C(15)-C(16)-H(28) | 120.743 | 120.874 | 121.400 | 121.677 |
| **67** | C(15)-C(16)-C(11) | 118.784 | 119.002 | 118.655 | 118.697 |
| **68** | H(28)-C(16)-C(11) | 120.472 | 120.123 | 119.945 | 119.626 |
| **69** | C(16)-C(11)-C(12) | 120.586 | 120.344 | 121.001 | 120.835 |

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114

**Table 2. The calculated bond lenghts ($A^0$) of compound 3 (6-311G(d) HF/B3LYP, 3-21G HF/B3LYP)**

| | **Bond Lenghts** | **HF 6-311G(d)** | **HF 3-21G** | **B3LYP 6-311G(d)** | **B3LYP 3-21G** |
|---|---|---|---|---|---|
| **1** | C(1)-N(36) | 1.2661 | 1.2786 | 1.2957 | 1.3125 |
| **2** | C(1)-N(37) | 1.3793 | 1.3816 | 1.3889 | 1.3890 |
| **3** | C(1)-C(18) | 1.4875 | 1.4840 | 1.4852 | 1.4861 |
| **4** | C(18)-H(32) | 1.0827 | 1.0824 | 1.0927 | 1.0948 |
| **5** | C(18)-H(33) | 1.0827 | 1.0824 | 1.0926 | 1.0948 |
| **6** | C(18)-H(34) | 1.0800 | 1.0749 | 1.0894 | 1.0911 |
| **7** | N(37)-C(2) | 1.3884 | 1.3971 | 1.4209 | 1.4328 |
| **8** | C(2)-O(39) | 1.1960 | 1.2185 | 1.2156 | 1.2372 |
| **9** | N(35)-C(2) | 1.3460 | 1.3543 | 1.3686 | 1.3778 |

| | | | | | |
|---|---|---|---|---|---|
| **10** | N(35)-H(19) | 0.9885 | 0.9919 | 1.0053 | 1.0087 |
| **11** | N(35)-N(36) | 1.3695 | 1.4278 | 1.3798 | 1.4390 |
| **12** | N(37)-N(38) | 1.3629 | 1.3985 | 1.3692 | 1.4099 |
| **13** | N(38)-C(3) | 1.2572 | 1.2669 | 1.2846 | 1.2972 |
| **14** | C(3)-H(20) | 1.0741 | 1.0701 | 1.0866 | 1.0848 |
| **15** | C(3)-C(4) | 1.4767 | 1.4716 | 1.4664 | 1.4653 |
| **16** | C(4)-C(5) | 1.3876 | 1.3884 | 1.4005 | 1.4032 |
| **17** | C(4)-C(9) | 1.3916 | 1.3866 | 1.4038 | 1.4036 |
| **18** | C(5)-H(21) | 1.0748 | 1.0657 | 1.0824 | 1.0778 |
| **19** | C(5)-C(6) | 1.3797 | 1.3807 | 1.3905 | 1.3949 |
| **20** | C(6)-O(40) | 1.3786 | 1.3957 | 1.3937 | 1.4100 |
| **21** | C(6)-C(7) | 1.3767 | 1.3814 | 1.3892 | 1.3974 |
| **22** | C(7)-H(22) | 1.0736 | 1.0694 | 1.0840 | 1.0817 |
| **23** | C(7)-C(8) | 1.3872 | 1.3817 | 1.3958 | 1.3949 |
| **24** | C(8)-H(23) | 1.0747 | 1.0713 | 1.0849 | 1.0834 |
| **25** | C(8)-C(9) | 1.3799 | 1.3811 | 1.3869 | 1.3916 |
| **26** | C(9)-H(24) | 1.0726 | 1.0695 | 1.0830 | 1.0820 |
| **27** | O(40)-C(10) | 1.3400 | 1.3572 | 1.3733 | 1.3940 |
| **28** | C(10)-O(41) | 1.1782 | 1.2048 | 1.2018 | 1.2277 |
| **29** | C(10)-C(11) | 1.4921 | 1.4787 | 1.4891 | 1.4807 |
| **30** | C(11)-C(12) | 1.3802 | 1.3772 | 1.3926 | 1.3923 |
| **31** | C(11)-C(16) | 1.3933 | 1.3884 | 1.4026 | 1.4027 |
| **32** | C(12)-H(25) | 1.0722 | 1.0687 | 1.0829 | 1.0812 |
| **33** | C(12)-C(13) | 1.3902 | 1.3859 | 1.3972 | 1.3986 |
| **34** | C(13)-O(42) | 1.3455 | 1.3689 | 1.3611 | 1.3825 |
| **35** | C(13)-C(14) | 1.3851 | 1.3821 | 1.3986 | 1.3397 |
| **36** | C(14)-H(26) | 1.0726 | 1.0695 | 1.0827 | 1.0815 |
| **37** | C(14)-C(15) | 1.3902 | 1.3879 | 1.3966 | 1.3990 |
| **38** | C(15)-H(27) | 1.0750 | 1.0715 | 1.0851 | 1.0836 |
| **39** | C(15)-C(16) | 1.3770 | 1.3769 | 1.3872 | 1.3903 |
| **40** | C(16)-H(28) | 1.0713 | 1.0673 | 1.0815 | 1.0794 |
| **41** | O(42)-C(17) | 1.3977 | 1.4368 | 1.4193 | 1.4603 |
| **42** | C(17)-H(29) | 1.0785 | 1.0772 | 1.0882 | 1.0899 |
| **43** | C(17)-H(30) | 1.0849 | 1.0831 | 1.0954 | 1.0968 |
| **44** | C(17)-H(31) | 1.0850 | 1.0831 | 1.0954 | 1.0968 |

**Table 3. The calculated Mulliken atomic charges of compound 3 (6-311G(d) HF/B3LYP, 3-21G HF/B3LYP)**

| | **HF 6-311G(d)** | **HF 3-21G** | **B3LYP 6-311G(d)** | **B3LYP 3-21G** |
|---|---|---|---|---|
| **C1** | 0.515 | 0.756 | 0.405 | 0.626 |
| **C2** | 0.787 | 1.249 | 0.583 | 0.940 |
| **C3** | 0.036 | 0.192 | 0.055 | 0.108 |
| **C4** | -0.042 | -0.164 | -0.023 | -0.056 |
| **C5** | -0.272 | -0.246 | -0.209 | -0.212 |
| **C6** | 0.327 | 0.383 | 0.231 | 0.301 |
| **C7** | -0.211 | -0.254 | -0.193 | -0.192 |
| **C8** | -0.207 | -0.227 | -0.201 | -0.183 |
| **C9** | -0.194 | -0.205 | -0.159 | -0.172 |
| **C10** | 0.647 | 1.008 | 0.430 | 0.708 |
| **C11** | -0.203 | -0.246 | -0.157 | -0.107 |
| **C12** | -0.241 | -0.199 | -0.203 | -0.166 |
| **C13** | 0.368 | 0.417 | 0.272 | 0.322 |
| **C14** | -0.300 | -0.267 | -0.259 | -0.207 |
| **C15** | -0.195 | -0.227 | -0.193 | -0.182 |
| **C16** | -0.211 | -0.209 | -0.168 | -0.183 |
| **C17** | -0.416 | -0.273 | -0.454 | -0.336 |
| **C18** | -0.670 | -0.618 | -0.670 | -0.596 |
| **C19** | 0.406 | 0.404 | 0.371 | 0.353 |
| **H20** | 0.306 | 0.330 | 0.261 | 0.262 |
| **H21** | 0.240 | 0.324 | 0.229 | 0.247 |
| **H22** | 0.238 | 0.266 | 0.209 | 0.206 |
| **H23** | 0.227 | 0.251 | 0.200 | 0.195 |
| **H24** | 0.241 | 0.271 | 0.209 | 0.207 |
| **H25** | 0.264 | 0.305 | 0.230 | 0.230 |
| **H26** | 0.242 | 0.255 | 0.216 | 0.196 |

| | | | | |
|---|---|---|---|---|
| **H27** | 0.224 | 0.251 | 0.199 | 0.195 |
| **H28** | 0.244 | 0.274 | 0.213 | 0.205 |
| **H29** | 0.233 | 0.239 | 0.233 | 0.227 |
| **H30** | 0.208 | 0.200 | 0.211 | 0.199 |
| **H31** | 0.207 | 0.200 | 0.211 | 0.199 |
| **H32** | 0.244 | 0.251 | 0.235 | 0.231 |
| **H33** | 0.245 | 0.251 | 0.236 | 0.231 |
| **H34** | 0.251 | 0.250 | 0.239 | 0.226 |
| **H35** | -0.496 | -0.760 | -0.496 | -0.592 |
| **N36** | -0.266 | -0.389 | -0.198 | -0.337 |
| **N37** | -0.468 | -0.849 | -0.363 | -0.622 |
| **N38** | -0.271 | -0.358 | -0.206 | -0.320 |
| **N39** | -0.532 | -0.670 | -0.389 | -0.520 |
| **O40** | -0.509 | -0.815 | -0.373 | -0.600 |
| **O41** | -0.436 | -0.616 | -0.317 | -0.481 |
| **O42** | -0.461 | -0.735 | -0.336 | -0.550 |

3-Methyl-4-[3-(3-methoxybenzoxy)-benzylidenamino]-4,5-dihydro-1*H*-1,2,4-triazol-5-one molecule have 42 atoms and the normal vibrational number is 120. The observed and calculated vibrational frequencies for compound **3** are summarized by using of 6-311G(d) and 3-21G basis sets of B3LYP and HF methods (Table **4** and **5**).

**Table 4. The calculated IR frequencies of compound 3 (6-311G(d))**

| | Vibration Frequencies | HF | B3LYP |
|---|---|---|---|
| **1** | τ NCCC(18), τ CCCC(20), τ COCC(80) | 7 | 10 |
| **2** | τ NCCC(23), τ COCC(21), τ CNNC(34), τ CCCN(28) | 14 | 15 |
| **3** | τ COCC(38), τ NCCC(12), τ CCOC(63) | 18 | 19 |
| **4** | τ COCC(14), τ CCCC(16), δ COC(11) | 41 | 41 |
| **5** | τ CCCC(10), τ COCC(28), τ CCNN(20), τ NCCN(27) | 56 | 50 |
| **6** | δ COC(17), τ CCNN(10), τ NCCN(11), τ NCNN(26),τ NNCN(11), τ COCC(11) | 62 | 63 |
| **7** | δ NCC(13), τ COCC(17), τ HCOC(11) | 70 | 82 |
| **8** | τ COCC(53), δ CNN(22), δ CCN(26) | 78 | 83 |
| **9** | τ NCNN(10), τ CNNC(33), τ CCCN(15) | 110 | 115 |
| **10** | δ CCC(10), δ COC(17), δ CCO(13) | 152 | 134 |
| **11** | τ HCCN(15), τ CNNC(37) | 163 | 162 |
| **12** | τ HCCN(41), τ CNNC(10), τ CCCC(10), δ COC(12) | 169 | 166 |
| **13** | τ CNNC(25), τ HCCN(55) | 181 | 173 |
| **14** | ν CC(10), δ COC(10), δ CCC(11), τ CCCC(13) | 185 | 191 |
| **15** | δ CNN(14), δ CCC(10),δ NNC(17) | 206 | 204 |
| **16** | τ HCOC(18), τ CCCC(12), τ COCC(13), τ OCCC(25), τ CCCN(14), τ NCCN(31) | 225 | 214 |
| **17** | τ NCCC(11), τ NCNN(17), τ CCCC(30), τ HCOC(19), τ OCCC(11) | 226 | 237 |
| **18** | ν CC(12), δ CCN(22), δ COC(11), δ CCO(12) | 245 | 240 |
| **19** | δ COC(23) | 271 | 263 |
| **20** | τ HCOC(45), τ CCCC(25), τ COCC(10) | 293 | 280 |
| **21** | τ HNNC(17), τ HCCN(11), τ CNNC(33), τ NCNN(26) | 293 | 290 |
| **22** | δ COC(21), δ OCO(13) | 307 | 296 |
| **23** | δ CCO(13), δ CCN(36) | 345 | 336 |
| **24** | τ NCNN(16), τ NNCN(18), τ CCNN(36), τ NCCN(11) | 362 | 348 |
| **25** | δ NNC(15), δ OCN(17), δ CCO(13), δ CNN(16) | 403 | 380 |
| **26** | δ OCO(10), δ CCC(39), δ COC(11) | 439 | 426 |
| **27** | τ CCCC(47) | 460 | 439 |
| **28** | τ HNNC(58), τ ONNC(11) | 462 | 451 |
| **29** | τ HNNC(40), τ HCCC(11), τ CCCN(18) | 481 | 454 |
| **30** | τ HNNC(17) | 488 | 463 |
| **31** | δ CCC(21), δ COC(12) | 504 | 492 |
| **32** | δ CCC(12), δ COC(11), τ HCCC(11), τ OCOC(11), τ OCCC(37) | 581 | 551 |
| **33** | δ CCC(14), δ COC(19), τ OCCC(14) | 583 | 567 |
| **34** | δ CCC(10), δ CNN(13) | 598 | 582 |
| **35** | δ CCC(16), δ CNN(14) | 612 | 592 |
| **36** | δ OCN(33), δ CNN(11),δ CCN(12), ν NC(13) | 621 | 594 |
| **37** | τ CCOC(20), τ CCCC(12), δ OCO(10), τ OCCC(11) | 628 | 600 |
| **38** | ν CC(19), ν NC(13), δ OCN(33), δ CCN(12), δ CCC(14) | 664 | 646 |
| **39** | τ HNNC(11), τ NNCN(30), τ CNNC(15), τ HCCN(10), τ NCNN(49) | 692 | 658 |
| **40** | τ HCCC(18), τ CCCC(12), δ CCC(23) | 706 | 683 |
| **41** | δ CCC(20), τ HCCC(28), τ CCCC(17) | 716 | 685 |
| **42** | τ HCCC(38), τ CCCC(15), τ CCCN(20) | 725 | 692 |
| **43** | τ ONNC(80), ν CC(11), δ CCC(10) | 779 | 739 |
| **44** | τ HCCC(24), τ OCOC(43) | 808 | 753 |
| **45** | ν NN(10), δ CCC(12), τ CNNC(10), τ ONNC(83) | 814 | 757 |

| | | | |
|---|---|---|---|
| **46** | δ OCO(10), τ HCCC(31) | 830 | 788 |
| **47** | ν NC(16), ν CC(10), δ CNN(18), τ HCCC(11) | 834 | 799 |
| **48** | δ CNN(18), ν NC(14), τ HCCC(50), τ OCOC(29) | 861 | 802 |
| **49** | δ OCO(12), τ HCCC(15) | 863 | 815 |
| **50** | δ NNC(14), δ NCC(17),δ CCN(12) | 887 | 846 |
| **51** | ν OC(19), τ HCCC(17) | 926 | 876 |
| **52** | τ HCCC(42), τ CCCC(10) | 966 | 891 |
| **53** | ν OC(11), τ HCCC(34) | 967 | 896 |
| **54** | τ HCCC(40) | 982 | 917 |
| **55** | ν OC(10), ν CC(11), τ HCCC(37) | 984 | 917 |
| **56** | ν CC(13), ν OC(11), δ CCC(12), τ HCCC(38) | 995 | 956 |
| **57** | ν CC(30), δ CCC(23), τ HCCC(55) | 1027 | 961 |
| **58** | ν CC(19), δ CCC(39), τ HCCC(58) | 1035 | 967 |
| **59** | δ HCH(13), δ NNC(14), τ HCCN(37) | 1043 | 990 |
| **60** | ν CC(30), δ CCC(20), τ HCCC(46) | 1044 | 1002 |
| **61** | τ HCNN(86), τ HCCC(57), τ CCCC(10) | 1049 | 1005 |
| **62** | ν CC(17), δ CCC(24), τ HCNN(88) | 1082 | 1008 |
| **63** | ν OC(32), δ HCH(21), τ HCCN(55) | 1117 | 1061 |
| **64** | ν OC(23), δ NNC(19) | 1125 | 1062 |
| **65** | δ HCH(25), τ HCCN(56), ν OC(32) | 1126 | 1066 |
| **66** | ν CC(12), ν OC(11), δ HCC(25) | 1130 | 1085 |
| **67** | ν CC(15), ν OC(13), δ HCC(16) | 1138 | 1098 |
| **68** | ν NN(20), ν CC(18), δ HCC(21), τ HCCN(15) | 1142 | 1100 |
| **69** | ν CC(20), δ HCC(22) | 1151 | 1110 |
| **70** | δ HCC(32), ν NN(28), δ HNN(14), τ HCCN(15) | 1165 | 1164 |
| **71** | ν CC(26), δ HCH(25), τ HCOC(28) | 1168 | 1172 |
| **72** | δ HCC(46) | 1211 | 1180 |
| **73** | δ HCC(28), δ HCH(25), τ HCOC(26) | 1232 | 1185 |
| **74** | δ HCH(12), τ HCOC(22), δ HCC(20) | 1251 | 1199 |
| **75** | ν CC(12), ν NN(18), ν NC(23),δ OCN(11), δ HCC(17) | 1261 | 1205 |
| **76** | ν CC(11), δ HCC(12) | 1268 | 1223 |
| **77** | ν NC(26), ν NN(14), δ CNN(14) | 1276 | 1255 |
| **78** | ν OC(15), ν CC(22) | 1313 | 1282 |
| **79** | ν OC(43), ν CC(12), ν NN(14), δ NCN(12) | 1326 | 1291 |
| **80** | δ HCC(17), ν OC(18) | 1368 | 1310 |
| **81** | δ HCC(26) | 1373 | 1311 |
| **82** | ν CC(21), δ HCC(68) | 1374 | 1343 |
| **83** | ν CC(35), δ HCC(16), ν NN(13), δ CNN(28) | 1386 | 1350 |
| **84** | ν NC(21), δ HCN(35), δ HCH(14) | 1443 | 1373 |
| **85** | δ HNN(63), δ HCN(14), δ HCH(51) | 1475 | 1396 |
| **86** | ν OC(11), ν NC(11), δ HCN(17), δ HCH(55), δ HNN(47) | 1484 | 1417 |
| **87** | δ HCH(10), ν CC(17), δ HNN(11) | 1505 | 1440 |
| **88** | δ HCN(12), ν CC(17), δ HCC(12) | 1524 | 1459 |
| **89** | ν CC(12), δ HCC(11), δ HCH(27), δ HCN(10) | 1529 | 1465 |
| **90** | δ HCH(77), τ HCCN(21) | 1530 | 1475 |
| **91** | δ HCH(58), δ HCC(10) | 1546 | 1481 |
| **92** | δ HCH(54), δ HCN(10), τ HCCN(19) | 1551 | 1489 |
| **93** | δ HCH(74), τ HCOC(14) | 1562 | 1499 |
| **94** | δ HCH(71), τ HCOC(12) | 1570 | 1509 |
| **95** | δ HCC(41), δ HCH(18), δ CCC(13) | 1574 | 1511 |
| **96** | δ HCC(27), δ CCC(14) | 1577 | 1515 |
| **97** | ν CC(33), δ HCC(10), δ CCC(12) | 1691 | 1609 |
| **98** | ν CC(33), δ HCC(11), δ CCC(11) | 1696 | 1610 |
| **99** | ν CC(22), δ HCC(13) | 1717 | 1629 |
| **100** | ν CC(36), δ HCC(10) | 1719 | 1638 |
| **101** | ν NC(47) | 1779 | 1640 |
| **102** | ν NC(58) | 1802 | 1655 |
| **103** | ν OC, ν NC | 1864 | 1787 |
| **104** | ν NC(12), ν OC(85) | 1903 | 1793 |
| **105** | ν CH(91) | 3030 | 2982 |
| **106** | ν CH(93) | 3057 | 3022 |
| **107** | ν CH(50) | 3086 | 3040 |
| **108** | ν CH(100) | 3114 | 3074 |
| **109** | ν CH(93) | 3146 | 3116 |
| **110** | ν CH(63) | 3149 | 3116 |
| **111** | ν CH(52) | 3188 | 3138 |
| **112** | ν CH(54) | 3190 | 3145 |
| **113** | ν CH(33) | 3199 | 3146 |
| **114** | ν CH(42) | 3216 | 3168 |
| **115** | ν CH(66) | 3218 | 3177 |

| | | | |
|---|---|---|---|
| **116** | ν CH(67) | 3220 | 3180 |
| **117** | ν CH(40) | 3226 | 3183 |
| **118** | ν CH(57) | 3236 | 3185 |
| **119** | ν CH(48) | 3239 | 3195 |
| **120** | ν NH(100) | 3771 | 3656 |

ν, stretching; δ, bending; $\delta_s$, scissoring; ρ, rocking; γ, out-of-plane bending; τ, torsion

**Table 5. The calculated IR frequencies of compound 3 (3-21G)**

| | Vibration Frequencies | HF | B3LYP |
|---|---|---|---|
| **1** | τ CNNC(22), τ NCNC(20), τ COCC(20), τ CCOC(15) | 14 | 16 |
| **2** | τ CCCC(21), τ COCC(43), τ CCOC(20) | 17 | 22 |
| **3** | δ NCC(15), δ CCO(14), δ CCC(25), δ COC(27), δ NNC(12), τ CNNC(12), τ CCOC(30) | 31 | 31 |
| **4** | δ NCC(14), δ COC(27), δ CCC(20), δ NNC(11), τ CNNC(12), τ CCOC(30), τCOCC(41) | 31 | 35 |
| **5** | τ NCNN(11), τ NNCC(38), τ CCNN(10), τ COCC(15), τ CCCC(14) | 62 | 61 |
| **6** | δ NCC(13), δ CCC(20), δ COC(25), δ NNC(18), τ COCC(51) | 67 | 77 |
| **7** | τ CCCC(10), τ COCC(52), δ NCC(14), δ COC(14), δ CCO(17), δ NNC(19) | 76 | 78 |
| **8** | τ CCCC(19), τ COCC(31) | 87 | 94 |
| **9** | τ NCNC(20), τ NCNN(18), τ CCCC(12), τ CNNC(14) | 124 | 122 |
| **10** | δ CCO(12), δ CCC(10), δ COC(15) | 128 | 129 |
| **11** | τ HCCN(74), τ CCCC(15) | 159 | 150 |
| **12** | τ CCCC(28) | 173 | 169 |
| **13** | ν CC(10), δ COC(11), τ NCNC(22), τ CNNC(24), τ CCNN(14) | 183 | 181 |
| **14** | δ CCC(10), δ COC(16), τ NCNC(25), τ CNNC(23, τ CCNN(10) | 185 | 185 |
| **15** | τ HCOC(40), τ COCC(14), τ OCCC(17), δ CNN(10), δ COC(17), δ CCC(15) | 208 | 208 |
| **16** | δ CCC(11), δ COC(24), τ HCOC(45), τ CCCC(13), τ OCCC(10) | 210 | 210 |
| **17** | ν CC(12), δ CCN(27), δ COC(11) | 244 | 242 |
| **18** | τ CCCC(23), τ CNNC(14) | 263 | 258 |
| **19** | τ HCOC(19), τ CCCC(24), δ COC(36) | 270 | 268 |
| **20** | δ CCO(11), δ CCC(12), δ COC(32), τ HCOC(11), τ CCCC(29) | 273 | 271 |
| **21** | τ NCNC(12), τ CNNC(32), τ CCCC(17) | 281 | 287 |
| **22** | δ OCO(14), δ COC(19), δ CCN(20) | 327 | 324 |
| **23** | τ NCNC(10), τ NCNN(33), τ CNNC(31) | 348 | 330 |
| **24** | τ NCNN(13), τ NNCC(22), τ CCNN(28), δ OCN(12), δ CNN(13), δ CCN(10), δ COC(10) | 363 | 354 |
| **25** | δ OCO(10), δ OCN(12), δ CCO(10), τ NCNN(14), τ NNCC(23), τ NNCC(23) | 370 | 356 |
| **26** | δ OCN(11), δ CCC(15) | 422 | 416 |
| **27** | δ COC(11), δ CCC(30) | 439 | 435 |
| **28** | τ CCCC(49) | 464 | 447 |
| **29** | τ CCOC(14), τ HCCC(20), τ CCCC(42), τ OCCC(10) | 485 | 466 |
| **30** | δ CCC(19) | 492 | 486 |
| **31** | τ HNNC(88), δ CCC(16), δ COC(18) | 557 | 536 |
| **32** | τ HCCC(13), τ CCCC(11), τ OCOC(15), τ OCCCC(39) | 572 | 551 |
| **33** | δ CCC(16), δ COC(21), ν NC(14), ν CC(13), δ OCN(26), δ CCN(10) | 578 | 553 |
| **34** | ν NC(12), δ OCN(32), δ CCN(11), τ HNNC(92) | 579 | 565 |
| **35** | ν CC(14), δ CCC(15), δ CNN(22) | 581 | 572 |
| **36** | δ COC(18), δ CCC(26), δ CCO(15) | 594 | 584 |
| **37** | δ CCC(10), ν NC(16), ν CC(15), τ CCOC(35), τ CCCC(16) | 637 | 609 |
| **38** | ν NC(11), ν CC(18), δ CCC(14), τ OCCC(23), τ CCCC(26) | 638 | 629 |
| **39** | τ NCNC(23), τ CNNC(14), τ CCNN(15), τ NCNN(11) | 674 | 642 |
| **40** | ν CC(14), δ OCO(10), δ CCC(28) | 694 | 683 |
| **41** | τ HCCC(31), τ CCCC(19) | 727 | 702 |
| **42** | τ CCCC(31), ν NN(12), τ HCCC(42) | 735 | 711 |
| **43** | ν NN(12), δ CCC(10), τ HCCC(42), τ CCCC(18) | 737 | 723 |
| **44** | ν OC(10), ν NC(12), ν CC(13), δ NCN(36), δ CNN(14), τ ONNC(76), τ CCNN(12) | 776 | 735 |
| **45** | τ HCCC(13), τ OCOC(55) | 784 | 744 |
| **46** | ν NC(11), ν CC(12), δ NCN(34), δ CNN(15), δ OCO(27) | 792 | 761 |
| **47** | ν OC(11), δ OCO(27), τ ONNC(74), τ CCNN(13) | 795 | 771 |
| **48** | δ NCC(23), δ NNC(11) | 821 | 801 |
| **49** | τ HCCC(34), τ CCCC(13) | 861 | 809 |
| **50** | τ HCCC(62), τ OCOC(10) | 865 | 812 |
| **51** | ν CC(13), ν OC(19) | 876 | 857 |
| **52** | ν CC(14), ν OC(10), δ CCC(15), δ NCN(31), δ CNN(22) | 932 | 919 |
| **53** | δ NCN(28), δ CNN(12), τ HCCC(62) | 947 | 920 |
| **54** | ν CC(15), ν OC(11), τ HCCC(51) | 995 | 925 |
| **55** | ν CC(15), ν OC(11), τ HCCC(51) | 997 | 926 |
| **56** | ν CC(28), δ CCC(10), τ HCCC(38) | 1002 | 945 |
| **57** | ν CC(12), δ CCC(23),τ HCCC(26) | 1011 | 977 |
| **58** | ν NC(26), τ HCCC(34) | 1017 | 985 |
| **59** | ν CC(23), ν NC(34), ν OC(16), δ CNN(15) | 1032 | 986 |

| | | | |
|---|---|---|---|
| **60** | τ HCCC(59), τ CCCC(16), τ HCNN(14) | 1041 | 995 |
| **61** | ν OC(54), τ HCCC(51) | 1050 | 995 |
| **62** | ν CC(13), δ CCC(39), τ HCCC(62) | 1073 | 997 |
| **63** | ν OC(36), δ CCC(21), τ HCCC(47) | 1077 | 1012 |
| **64** | ν NC(11), δ HCC(13), τ HCNN(83), τ HCCN(36) | 1090 | 1047 |
| **65** | ν NC(11), δ HCH(15), δ HCC(13), τ HCCN(40) | 1090 | 1060 |
| **66** | ν CC(18), ν OC(13), δ HCC(17), δ CCC(11) | 1099 | 1070 |
| **67** | ν CC(18), δ HCC(15), δ HCH(22), τ HCCN(59) | 1100 | 1075 |
| **68** | ν CC(12), δ HCC(19), δ HCH(19), τ HCNN(12), τ HCCN(49) | 1100 | 1087 |
| **69** | ν CC(17), δ HCC(20), τ HCNN(61), τ HCCN(14) | 1108 | 1091 |
| **70** | ν NC(27), ν NN(16), ν CC(14) | 1142 | 1116 |
| **71** | ν CC(30), δ HCH(24), τ HCOC(26) | 1155 | 1120 |
| **72** | ν OC(13), ν CC(30), δ HCC(11), δ HCH(24), τ HCOC(26) | 1156 | 1137 |
| **73** | ν CC(25), δ HCC(12), δ HCH(16), τ HCOC(28) | 1158 | 1149 |
| **74** | ν OC(12), δ HCC(15) | 1172 | 1173 |
| **75** | δ HCH(13), δ HCC(31), τ HCOC(24) | 1184 | 1183 |
| **76** | ν CC(12), δ HCC(26) | 1218 | 1189 |
| **77** | ν CC(14), δ HCC(41) | 1219 | 1202 |
| **78** | ν CC(18), ν OC(14), δ HCC(13) | 1245 | 1241 |
| **79** | ν CC(19), ν OC(12), ν NN(16), δ CNN(14) | 1264 | 1257 |
| **80** | ν CC(26), ν OC(35) | 1279 | 1279 |
| **81** | ν CC(15), δ HCC(10), ν OC(23) | 1295 | 1294 |
| **82** | ν CC(14), δ HCC(41) | 1334 | 1309 |
| **83** | ν NC(12), δ HNN(57), δ HCN(10), δ HCC(30) | 1345 | 1310 |
| **84** | δ HCC(67), δ HNN(44) | 1353 | 1323 |
| **85** | δ HNN(17), δ HCN(32), δ HCC(16) | 1367 | 1341 |
| **86** | ν NC(12), δ HCN(34) | 1418 | 1390 |
| **87** | ν CC(15), δ HCC(11), δ HCH(97) | 1444 | 1417 |
| **88** | δ HCH(87), δ HCN(17), δ HCC(10) | 1453 | 1419 |
| **89** | ν CC(12), δ HCC(15) | 1458 | 1432 |
| **90** | δ HCC(10), δ HCH(72) | 1483 | 1452 |
| **91** | δ HCH(66), τ HCCN(25) | 1490 | 1473 |
| **92** | δ HCC(22), δ HCH(75), τ HCCN(24) | 1498 | 1482 |
| **93** | δ HCC(47), δ CCC(10) | 1508 | 1483 |
| **94** | ν CC(19), δ HCC(25), δ HCH(76), τ HCCN(24) | 1513 | 1490 |
| **95** | δ HCH(76), τ HCOC(11) | 1525 | 1502 |
| **96** | δ HCH(74), τ HCOC(10) | 1534 | 1514 |
| **97** | ν NC(44), ν CC(26), δ HCC(10), δ CCC(10) | 1598 | 1535 |
| **98** | ν NC(41), δ HCH(16), ν CC(41), δ HCC(17) | 1600 | 1550 |
| **99** | ν CC(25), δ HCC(20), δCCC(10) | 1613 | 1557 |
| **100** | ν CC(33), δ HCC(14) | 1623 | 1567 |
| **101** | ν NC(40), ν CC(32), δ CCC(18) | 1638 | 1572 |
| **102** | ν CC(22), δ HCC(11), ν NC(45) | 1671 | 1585 |
| **103** | ν OC(84) | 1733 | 1675 |
| **104** | ν OC(85) | 1745 | 1710 |
| **105** | ν CH(91) | 2907 | 2923 |
| **106** | ν CH(92) | 2932 | 2965 |
| **107** | ν CH(50) | 2956 | 2976 |
| **108** | ν CH(100) | 2983 | 3013 |
| **109** | ν CH(92) | 3015 | 3050 |
| **110** | ν CH(92) | 3016 | 3056 |
| **111** | ν CH(51) | 3061 | 3076 |
| **112** | ν CH(52) | 3063 | 3092 |
| **113** | ν CH(36) | 3080 | 3094 |
| **114** | ν CH(68) | 3090 | 3120 |
| **115** | ν CH(67) | 3092 | 3122 |
| **116** | ν CH(31) | 3097 | 3126 |
| **117** | ν CH(55) | 3108 | 3134 |
| **118** | ν CH(48) | 3119 | 3150 |
| **119** | ν CH(28) | 3138 | 3167 |
| **120** | ν NH(100) | 3540 | 3515 |

ν, stretching; δ, bending; $\delta_s$, scissoring; ρ, rocking; γ, out-of-plane bending; τ, torsion

The $^{1}H$ and $^{13}C$ NMR chemical shifts of title compound in gase phase and in DMSO solvent have been calculated by using the DFT (B3LYP) and Hartree Fock (HF) methods with 6-311G(d) and 3-21G basis sets (Figure **2**). $^{1}H$- and $^{13}C$-NMR chemical shift values of this compound given in Table **6** and **7**.

**Table 6. The calculated $^{1}H$ and $^{13}C$ NMR isotropic chemical shifts of compound 3 (with respect to TMS, all values in ppm) (6-311G(d)).**

| | $\delta_{Exp.}$ | $\delta_{cal.}$ HF (Vacum) | $\delta_{cal.}$ HF (DMSO) | Different | Different (DMSO) | $\delta_{cal.}$ B3LYP (Vacum) | $\delta_{cal.}$ B3LYP (DMSO) | Different | Different (DMSO) |
|---|---|---|---|---|---|---|---|---|---|
| **C1** | 144.31 | 148.18 | 150.14 | -3.87 | -5.83 | 138.83 | 141.20 | 5.48 | 3.11 |
| **C2** | 151.15 | 152.45 | 153.50 | -1.30 | -2.35 | 141.66 | 142.64 | 9.49 | 8.51 |
| **C3** | 151.01 | 152.37 | 152.73 | -1.36 | -1.72 | 142.17 | 142.77 | 8.84 | 8.24 |
| **C4** | 135.21 | 140.01 | 139.53 | -4.80 | -4.32 | 126.65 | 126.43 | 8.56 | 8.78 |
| **C5** | 125.94 | 130.17 | 129.44 | -4.23 | -3.50 | 117.84 | 118.28 | 8.10 | 7.66 |
| **C6** | 152.40 | 157.69 | 157.43 | -5.29 | -5.03 | 142.81 | 141.26 | 9.59 | 11.14 |
| **C7** | 124.94 | 125.83 | 127.17 | -0.89 | -2.23 | 118.66 | 118.85 | 6.28 | 6.09 |
| **C8** | 130.03 | 131.55 | 133.08 | -1.52 | -3.05 | 120.34 | 121.10 | 9.69 | 8.93 |
| **C9** | 120.22 | 123.51 | 123.93 | -3.29 | -3.71 | 114.18 | 114.81 | 6.04 | 5.41 |
| **C10** | 164.33 | 166.45 | 168.01 | -2.12 | -3.68 | 151.05 | 152.85 | 13.28 | 11.48 |
| **C11** | 130.25 | 134.84 | 133.83 | -4.59 | -3.58 | 122.86 | 121.81 | 7.39 | 8.44 |
| **C12** | 122.13 | 124.76 | 122.85 | -2.63 | -0.72 | 115.20 | 113.22 | 6.93 | 8.91 |
| **C13** | 159.39 | 165.16 | 165.39 | -5.77 | -6.00 | 149.51 | 149.42 | 9.88 | 9.97 |
| **C14** | 114.31 | 114.94 | 117.77 | -0.63 | -3.46 | 103.99 | 106.58 | 10.32 | 7.73 |
| **C15** | 130.16 | 131.60 | 133.23 | -1.44 | -3.07 | 120.80 | 122.37 | 9.36 | 7.79 |
| **C16** | 120.22 | 124.19 | 124.31 | -3.97 | -4.09 | 113.43 | 113.70 | 6.79 | 6.52 |
| **C17** | 55.43 | 53.55 | 54.11 | 1.88 | 1.32 | 35.28 | 35.76 | 20.15 | 19.67 |
| **C18** | 11.08 | 12.18 | 12.15 | -1.10 | -1.07 | 0.51 | 0.57 | 10.57 | 10.51 |
| **H19** | 11.87 | 6.23 | 6.72 | 5.64 | 5.15 | 5.42 | 5.86 | 6.45 | 6.01 |
| **H20** | 9.79 | 9.59 | 9.53 | 0.20 | 0.26 | 8.98 | 8.96 | 0.81 | 0.83 |
| **H21** | 7.61 | 7.11 | 7.14 | 0.50 | 0.47 | 6.64 | 6.85 | 0.97 | 0.76 |
| **H22** | 7.47 | 6.79 | 7.04 | 0.68 | 0.43 | 6.65 | 6.84 | 0.82 | 0.63 |
| **H23** | 7.77 | 7.08 | 7.35 | 0.69 | 0.42 | 6.85 | 7.11 | 0.92 | 0.66 |
| **H24** | 7.78 | 7.74 | 7.85 | 0.04 | -0.07 | 7.56 | 7.70 | 0.22 | 0.08 |
| **H25** | 7.75 | 7.53 | 7.35 | 0.22 | 0.40 | 7.44 | 7.24 | 0.31 | 0.51 |
| **H26** | 7.34 | 6.34 | 6.73 | 1.00 | 0.61 | 6.05 | 6.47 | 1.29 | 0.87 |
| **H27** | 7.55 | 7.04 | 7.30 | 0.51 | 0.25 | 6.79 | 7.09 | 0.76 | 0.46 |
| **H28** | 7.63 | 7.45 | 7.55 | 0.18 | 0.08 | 7.19 | 7.32 | 0.44 | 0.31 |
| **H29** | 3.87 | 3.69 | 3.77 | 0.18 | 0.10 | 3.07 | 2.72 | 0.80 | 1.15 |
| **H30** | 3.87 | 3.20 | 3.38 | 0.67 | 0.49 | 2.51 | 3.14 | 1.36 | 0.73 |
| **H31** | 3.87 | 3.20 | 3.38 | 0.67 | 0.49 | 2.51 | 2.71 | 1.36 | 1.16 |
| **H32** | 2.29 | 1.98 | 2.10 | 0.31 | 0.19 | 1.50 | 1.65 | 0.79 | 0.64 |
| **H33** | 2.29 | 1.98 | 2.09 | 0.31 | 0.20 | 1.50 | 1.64 | 0.79 | 0.65 |
| **H34** | 2.29 | 1.70 | 1.76 | 0.59 | 0.53 | 1.30 | 1.35 | 0.99 | 0.94 |

**Table 7. The calculated $^{1}H$ and $^{13}C$ NMR isotropic chemical shifts of compound 3 (with respect to TMS, all values in ppm) (3-21G).**

| | $\delta_{Exp.}$ | $\delta_{cal.}$ HF (Vacum) | $\delta_{cal.}$ HF (DMSO) | Different | Different (DMSO) | $\delta_{cal.}$ B3LYP (Vacum) | $\delta_{cal.}$ B3LYP (DMSO) | Different | Different (DMSO) |
|---|---|---|---|---|---|---|---|---|---|
| **C1** | 144.31 | 113.63 | 114.92 | 30.68 | 29.39 | 111.44 | 113.33 | 32.87 | 30.98 |
| **C2** | 151.15 | 115.48 | 115.98 | 35.67 | 35.17 | 114.77 | 115.31 | 36.38 | 35.84 |
| **C3** | 151.01 | 117.40 | 117.48 | 33.61 | 33.53 | 115.29 | 115.56 | 35.72 | 35.45 |
| **C4** | 135.21 | 100.74 | 100.09 | 34.47 | 35.12 | 93.44 | 92.69 | 41.77 | 42.52 |
| **C5** | 125.94 | 90.32 | 89.58 | 35.62 | 36.36 | 84.10 | 83.37 | 41.84 | 42.57 |
| **C6** | 152.40 | 120.82 | 120.82 | 31.58 | 31.58 | 111.03 | 110.91 | 41.37 | 41.49 |
| **C7** | 124.94 | 87.72 | 88.74 | 37.22 | 36.20 | 83.48 | 84.47 | 41.46 | 40.47 |
| **C8** | 130.03 | 93.45 | 94.74 | 36.58 | 35.29 | 88.71 | 90.01 | 41.32 | 40.02 |
| **C9** | 120.22 | 87.29 | 87.51 | 32.93 | 32.71 | 82.97 | 83.35 | 37.25 | 36.87 |
| **C10** | 164.33 | 133.14 | 133.82 | 31.19 | 30.51 | 128.36 | 129.28 | 35.97 | 35.05 |
| **C11** | 130.25 | 96.56 | 95.72 | 33.69 | 34.53 | 90.29 | 89.36 | 39.96 | 40.89 |
| **C12** | 122.13 | 88.41 | 86.90 | 33.72 | 35.23 | 85.48 | 83.67 | 36.65 | 38.46 |
| **C13** | 159.39 | 124.15 | 124.27 | 35.24 | 35.12 | 115.68 | 115.39 | 43.71 | 44.00 |
| **C14** | 114.31 | 82.57 | 85.08 | 31.74 | 29.23 | 78.11 | 80.32 | 36.20 | 33.99 |
| **C15** | 130.16 | 94.30 | 95.63 | 35.86 | 34.53 | 88.90 | 90.43 | 41.26 | 39.73 |
| **C16** | 120.22 | 88.14 | 88.15 | 32.08 | 32.07 | 83.97 | 84.42 | 36.25 | 35.80 |
| **C17** | 55.43 | 33.37 | 32.02 | 22.06 | 23.41 | 15.55 | 16.17 | 39.88 | 39.26 |
| **C18** | 11.08 | -6.57 | -6.80 | 17.65 | 17.88 | -17.57 | -17.70 | 28.65 | 28.78 |
| **H19** | 11.87 | 5.46 | 5.98 | 6.41 | 5.89 | 4.51 | 4.95 | 7.36 | 6.92 |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| **H20** | 9.79 | 9.38 | 9.30 | 0.41 | 0.49 | 8.78 | 8.69 | 1.01 | 1.10 |
| **H21** | 7.61 | 7.75 | 7.64 | -0.14 | -0.03 | 7.35 | 7.22 | 0.26 | 0.39 |
| **H22** | 7.47 | 5.73 | 6.03 | 1.74 | 1.44 | 5.69 | 6.03 | 1.78 | 1.44 |
| **H23** | 7.77 | 6.05 | 6.39 | 1.72 | 1.38 | 5.86 | 6.25 | 1.91 | 1.52 |
| **H24** | 7.78 | 6.87 | 6.99 | 0.91 | 0.79 | 6.77 | 6.94 | 1.01 | 0.84 |
| **H25** | 7.75 | 6.69 | 6.51 | 1.06 | 1.24 | 6.81 | 6.56 | 0.94 | 1.19 |
| **H26** | 7.34 | 5.22 | 5.67 | 2.12 | 1.67 | 4.93 | 5.44 | 2.41 | 1.90 |
| **H27** | 7.55 | 5.99 | 6.31 | 1.56 | 1.24 | 5.74 | 6.13 | 1.81 | 1.42 |
| **H28** | 7.63 | 6.64 | 6.78 | 0.99 | 0.85 | 6.49 | 6.69 | 1.14 | 0.94 |
| **H29** | 3.87 | 3.37 | 3.51 | 0.50 | 0.36 | 2.72 | 2.81 | 1.15 | 1.06 |
| **H30** | 3.87 | 2.72 | 2.96 | 1.15 | 0.91 | 1.73 | 2.03 | 2.14 | 1.84 |
| **H31** | 3.87 | 2.72 | 2.96 | 1.15 | 0.91 | 1.73 | 2.03 | 2.14 | 1.84 |
| **H32** | 2.29 | 1.50 | 1.63 | 0.79 | 0.66 | 0.80 | 0.96 | 1.49 | 1.33 |
| **H33** | 2.29 | 1.50 | 1.63 | 0.79 | 0.66 | 0.80 | 0.96 | 1.49 | 1.33 |
| **H34** | 2.29 | 0.97 | 1.07 | 1.32 | 1.22 | 0.43 | 0.53 | 1.86 | 1.76 |

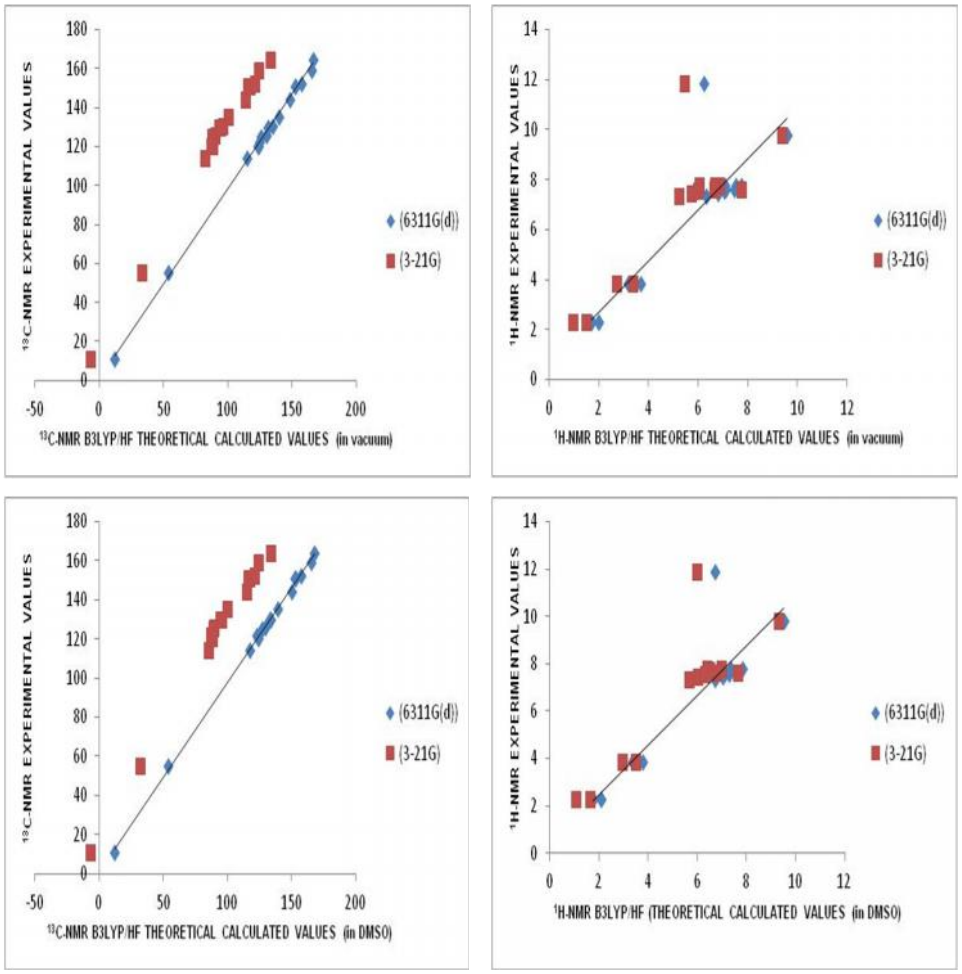
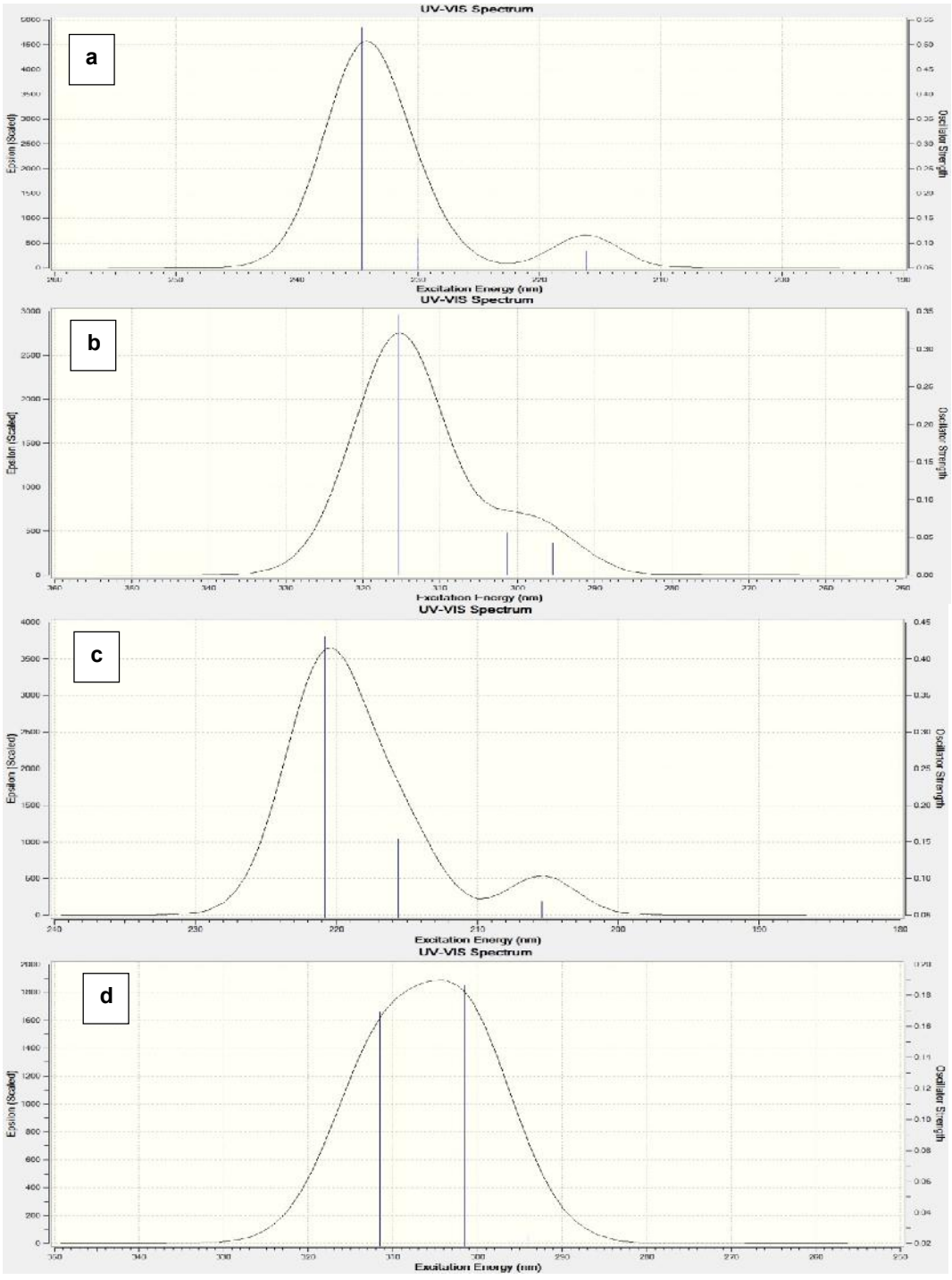



**Figure 2. Comparison of experimental and theoretical $^{13}$C- and $^{1}$H-NMR chemical shifts values of compound 3 with 6-311G(d)(a)/B3LYP, HF, B3LYP(DMSO) ve HF(DMSO) ve 3-21G(b)/B3LYP, HF, B3LYP(DMSO) ve HF(DMSO) methods.**

The excitation energies, oscillator strengths ($f$) and absorption wavelengths (λ) of UV–Vis electron absorption spectroscopy of the title molecule have been calculated in ethanol solvent by using B3LYP/HF methods with 6-311G(d) and 3-21G basis sets and presented in Figure **3** [20]. Futhermore, the highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO) have been simulated for this compound have been determined. In our study, HOMO and LUMO energies and their 3D plots of this compound are shown in Figure **4**. The molecular electrostatic potential (MEP) of this compound have been performed both two methods (Figure **5**).




| λ (nm) HF/B3LYP 6-311G(d) | λ (nm) HF/B3LYP 3-21G | Excitation Energy (eV) HF/B3LYP 6-311G(d) | Excitation Energy (eV) HF/B3LYP 3-21G | *f* (osillatör strengths) HF/B3LYP 6-311G(d) | *f* (osillatör strengths) HF/B3LYP 3-21G |
|---|---|---|---|---|---|
| 234.62/315.39 | 220.82/311.51 | 5.2845/3.9311 | 5.6148/3.9802 | 0.5356/0.3449 | 0.4306/0.1692 |
| 230.06/301.32 | 215.61/301.50 | 5.3893/4.1147 | 5.7503/4.1122 | 0.1096/0.0559 | 0.1543/0.1862 |
| 216.12/295.38 | 205.40/294.03 | 5.7369/4.1975 | 6.0363/4.2166 | 0.0836/0.0427 | 0.0682/0.0260 |

**Figure 3. The calculated absorption wavelength (λ), excitation energies and oscillator strengths (*f*) and UV-vis spectrums (B3LYP/HF 6-311G(d), 3-21G) of compound 3**

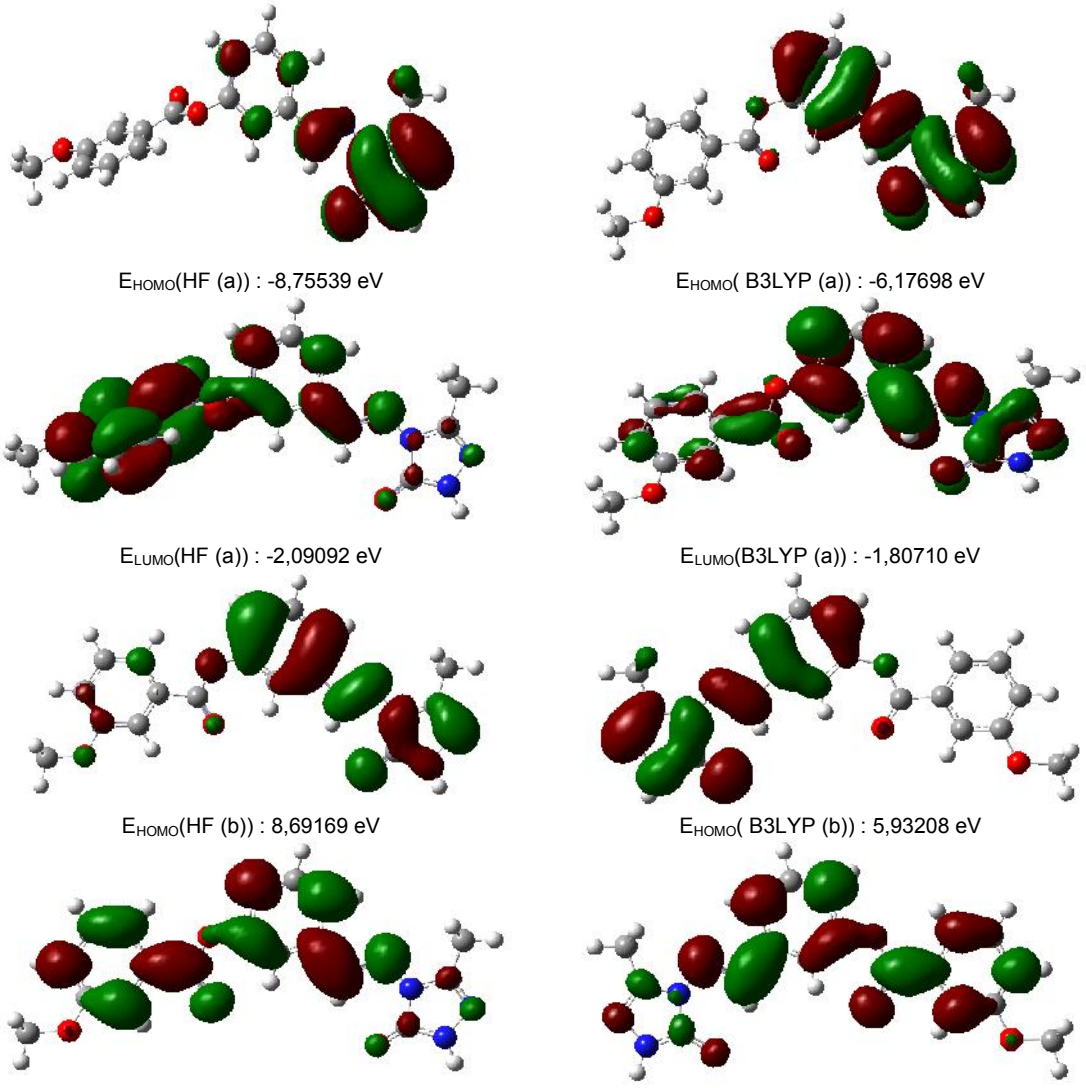



**Figure 4. 3D plots of HOMO and LUMO energies of compound 3 at the HF/B3LYP 6-311G(d) and 3-21G levels**

Total energy values, dipole moments, thermodynamic properties and electronic structure values of above mentioned compound were calculated by using B3LYP/HF 6-311G(d) and 3-21G methods and given in Table **8, 9** and **10.** Using HOMO and LUMO energy values for title molecule have been calculated the following parameters: Ionization potential (*I*), Electron affinity (*A*), Electronegativity(χ), hardness (η), softness (*S*) are given in Table **11**.

**Table 8. The calculated dipole moment of compound 3 (6-311G(d) HF/B3LYP, 3-21G HF/B3LYP)**

| Dipole Moment | HF 6-311G(d) | HF 3-21G | B3LYP 6-311G(d) | B3LYP 3-21G |
|---|---|---|---|---|
| $\mu_x$ | 1.9302 | 1.5181 | 1.4471 | 0.9850 |
| $\mu_y$ | 5.8613 | 5.4600 | 4.0492 | 3.3631 |
| $\mu_z$ | 1.7752 | 1.8080 | 1.3723 | 1.2629 |
| $\mu_{Toplam}$ | 6.4212 | 5.9486 | 4.5136 | 3.7250 |

**Table 9. The calculated total energy of 3-methyl-4-[3-(3-methoxybenzoxy)-benzylidenamino]-4,5-dihydro-1H-1,2,4-triazol-5-one molecule (6-311G(d) HF/B3LYP, 3-21G HF/B3LYP)**

| Energy | HF 6-311G(d) | HF 3-21G | B3LYP 6-311G(d) | B3LYP 3-21G |
|---|---|---|---|---|
| (a.u.) | -1208.419 | -1201.421 | -1208.419 | -1215.710 |

175

176 **Table 10. The calculated thermodynamic properties of 3-methyl-4-[3-(3-methoxybenzoxy)-benzylidenamino]-4,5-**
177 **dihydro-1H-1,2,4-triazol-5-one molecule (6-311G(d) HF/B3LYP, 3-21G HF/B3LYP)**

| Parameters | Value 6-311G(d) | Value 3-21G |
|---|---|---|
| Termal energy, E (cal/mol K) | Dft/Hf | Dft/Hf |
| Elektronic | 0.000/0.000 | 0.000/0.000 |
| Transnational | 0.889/0.889 | 0.889/0.889 |
| Rotational | 0.889/0.889 | 0.889/0.889 |
| Vibrational | 214.199/228.881 | 215.431/230.308 |
| Total | 215.977/230.659 | 217.208/232.085 |
| Zero-Point Vibrational energy (kcal/mol) | Dft/Hf 201.50569/216.99618 | Dft/Hf 203.06408/218.81690 |
| Sum of electronic and zero-point Energy (Hartree/Particle) | Dft/Hf -1215.389135/-1208.073597 | Dft/Hf -1208.404572/-1201.072346 |
| Sum of electronic and thermal Energies (Hartree/Particle) | Dft/Hf -1215.366074/-1208.051824 | Dft/Hf -1208.382032/-1201.051202 |
| Sum of electronic and thermal Enthalpies (Hartree/Particle) | Dft/Hf -1215.365130/-1208.050880 | Dft/Hf -1208.381087/-1201.050257 |
| Sum of electronic and thermal Free Energies (Hartree/Particle) | Dft/Hf -1215.445778/-1208.129698 | Dft/Hf -1208.459254/-1201.126235 |
| Rotational constants (GHZ) | Dft/Hf | Dft/Hf |
| A | 0.4977683/0.54730 | 0.4977683/0.4977683 |
| B | 0.0596771/0.05970 | 0.0596771/0.059677 |
| C | 0.0538654/0.05623 | 0.0538654/0.0538654 |

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179 **Table 11. Electronic structure parameters calculated for compound 3**

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| | HF/B3LYP 6-311G(d) | HF/B3LYP 3-21G |
|---|---|---|
| $E_{HOMO}$ (eV) | -8,77539/-6,17698 | 8,69169/5,93208 |
| $E_{LUMO}$ (eV) | -2,09092/-1,80710 | 2,17746/1,57390 |
| $\Delta E= E_{LUMO}-E_{HOMO}$ (eV) | 6,68447/4,36988 | -6,51423/-4,35818 |
| I (eV) | 8,77539/6,17698 | -8,69169/-5,93208 |
| A(eV) | 2,09092/1,80710 | -2,17746/-1,57390 |
| $\chi$ (eV ) | 5,433155/3,99204 | -5,434575/-3,75299 |
| $\eta$ (eV ) | 3,342235/2,18494 | -3,257115/-2,17909 |
| S ($eV^{-1}$) | 0,14960/2,22883 | -0,15351/-0,22945 |

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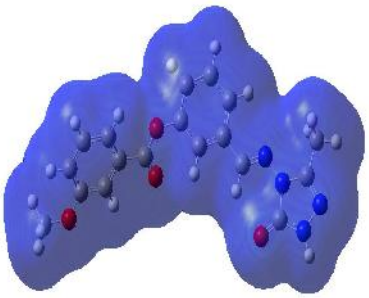
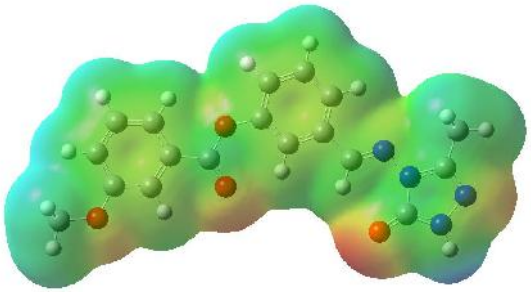
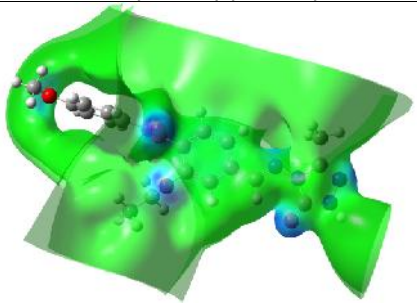
**TOTAL DENSITY (6-311G(d)/B3LYP)**



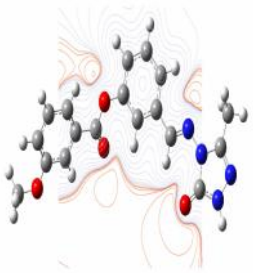
**MEP (6-311G(d)/B3LYP)**



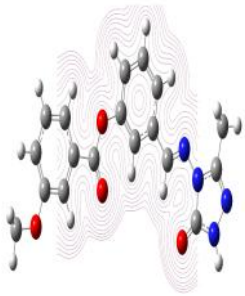
**ESP(6-311G(d)/B3LYP)**



**CONTOUR (6-311G(d)/B3LYP)**

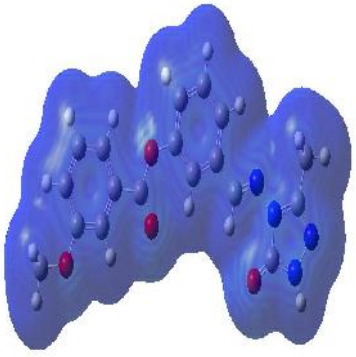


**Electrostatic Potential (6-311G(d))**

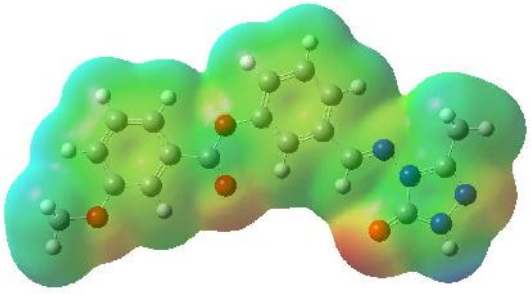


**Electron Density (6-311G(d))**

**TOTAL DENSITY (3-21G/B3LYP)**



**MEP (3-21G/B3LYP)**



**ESP (3-21G/B3LYP)**

**CONTOUR (3-21G/B3LYP)**

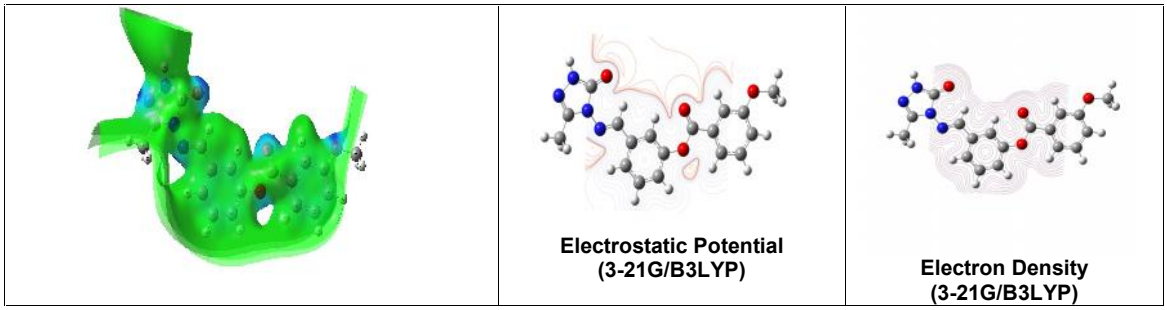



**Figure 5. The calculated molecular surfaces for this compound**

## 4. CONCLUSION

The calculated geometric parameters (bond lengths (Å) and bond angles (˚) of the molecule are listed in Table **1** and **2**. These results show that bond lengths calculated by B3LYP method are generally longer than bond lengths calculated by HF method. The atoms exposed interactions between molecules of the optimized structure with different methods have been found to have different bond lengths (Å) and bond angles (˚).The experimental spectroscopic values were compared with the data of two different methods The best results were found at DFT(B3LYP)/6-311G. Heat generation in thermochemical properties is one of the most important parameters Table **10**. The values of heat generation are not known for most organic compounds. The difficulty of studying heat effects increases the importance of quantum chemical calculations. From the thermodynamic point of view, it can be decided whether or not there is a chemical reaction. Thermodynamic quantum chemical reagents are widely used studying the reaction mechanisms of organic compounds. HOMO energy is known as the ability of the molecule to give electrons ($\pi_{donor}$), the ability of the LUMO energy molecule to accept electrons ($\pi_{Acceptor}$). The space between HOMO and LUMO energy values is known as the chemical stability of the molecule The closer energy levels of the interacting molecular orbitals are the easier the interaction will be. So the smaller the ΔE energy difference, the easier the interaction and reactivity of the reactants will be.

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