



Microwave Synthesis, spectroscopic characterization and DFT investigation of 4-(4-(2-(4-substitutedphenyl)-4-oxothiazolidin-3-yl)benzyl)oxazolidin-2-one derivatives

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ABSTRACT

A series of some novel 4-(4-(2-(4-substitutedphenyl)-4-oxothiazolidin-3-yl)benzyl)oxazolidin-2-one (6-10) derivatives were designed and synthesized under microwave irradiation. The synthesized compound was purified by crystallization using ethanol. The structure of the synthesized compound was assigned on the basis of the spectral data. IR spectrum showed the expected absorption frequencies and signals of this compound. To identify the stable structure, conformational analysis was performed using B3LYP/6-31 G(d,p) level of calculation. For the stable conformer the bond parameters were calculated by the same basis set. Results obtained at this level of theory were used for a detailed interpretation of the FT-IR spectra. The energy gap of the molecule was found using HOMO and LUMO calculation. Atomic charges of the carbon, nitrogen and oxygen were calculated using same level of calculations. The optimized geometric parameters and the theoretical vibrational frequencies were found to be in good agreement with the corresponding experimental data and with the results found in the literature.

Keywords: 2-arylthiazolidine, FT-IR, hyperpolarizability, HOMO–LUMO

1. INTRODUCTION

In recent years, 4-thiazolidinones and 2,4-thiazolidinediones have been among the most widely investigated classes of organic compounds. Thiazolidine derivatives are reported to be evidence for a variety of biological activities. The presence of a thiazolidine ring in penicillin and related derivatives was the first recognition of its occurrence in nature [1]. Literature surveys demonstrate that thiazolinyldrazones exhibit antimycobacterial [2-5], antifungal [6-8], antiviral [9-13], and anticonvulsant [14] activities. Looking towards literature, it was thought that incorporation of all these biologically active moieties might be result in better biological activities and therefore as the part of our continuous research in developing the new heterocycles containing nitrogen and sulfur atom and investigate their molecular structural analysis, vibrational and electronic spectroscopic studies in the gas phase, was taken up with DFT/B3LYP level of theory using 6-31 G(d,p) basis set. As vibrational and electronic spectroscopic studies provided useful information regarding the structure and conformation of molecules if utilized in conjunction with quantum chemical calculations [15,16], a complete description of molecular dynamics and vibrational wavenumber calculations has been administered at the DFT levels of theory. Microwave-assisted technique is a green method in current organic synthesis. It is attractive, offering reduced pollution, low cost, and high yields. The green technique can often shorten the reaction time. On the basis of this, in this work, we calculated the vibrational wavenumbers of the title compound in the ground state and compare the fundamentals from the experimental vibrational wavenumbers, geometric parameters and calculation of HOMO–LUMO and non-linear optical properties of the synthesized compounds. The results of this work are presented herein.

2. EXPERIMENTAL

Measurements

All the solvents were of spectral grade and used as such without further purification. The melting points of all the synthesized compounds were measured in open capillaries and are uncorrected. FT-IR spectra were recorded on an AVATAR-330 FT-IR spectrometer (Thermo Nicolet) using KBr (pellet form). ¹H spectrum was recorded at 400 MHz, Bruker, using DMSO-d₆ as solvent for all the compounds. Tetramethylsilane (TMS) was used as an internal reference for all NMR spectra, with chemical shifts reported in δ units (parts per million) relative to the standard. ¹H NMR splitting patterns are designated as singlet (s), doublet (d), doublet of doublet (dd), triplet (t), quartet (q) and multiplet (m). Coupling constants are expressed in Hertz (Hz).

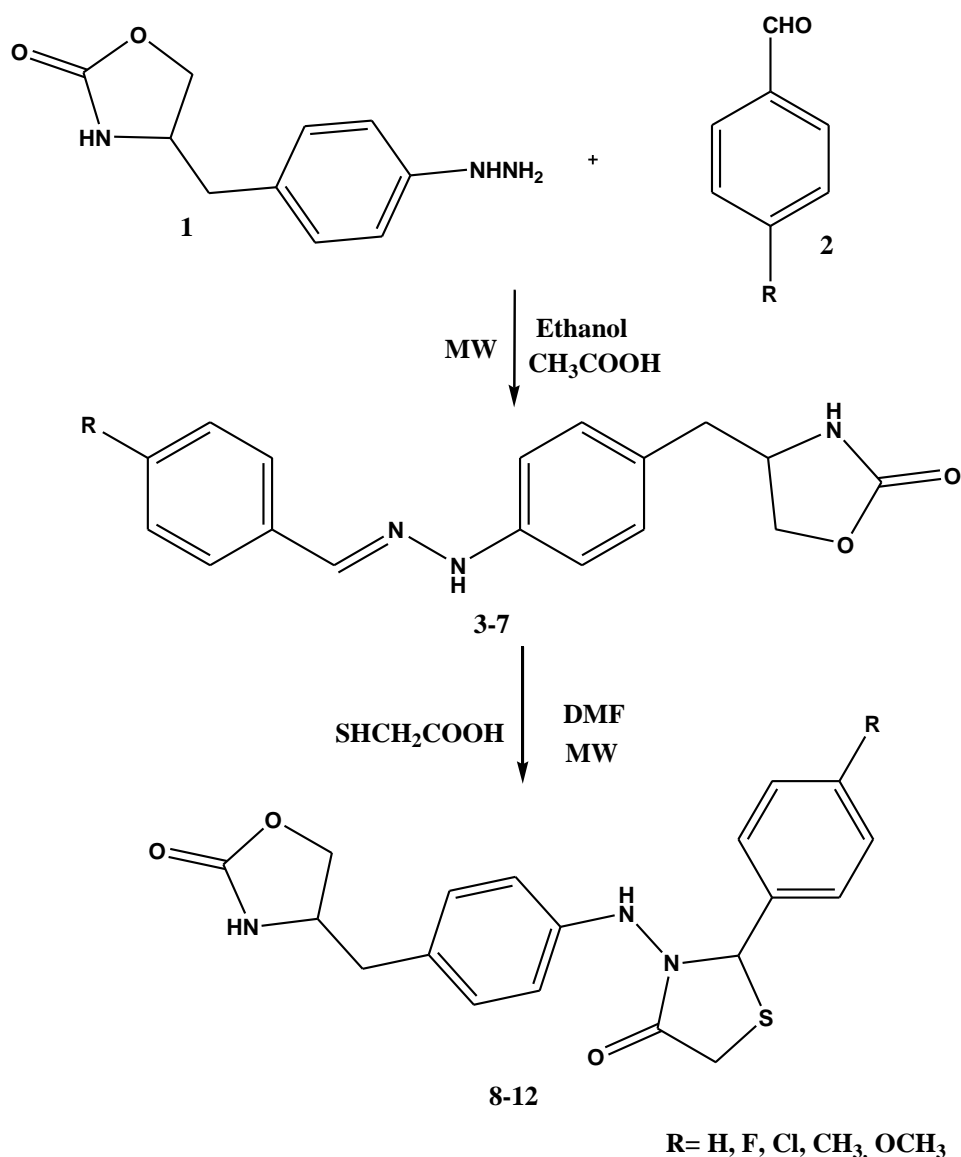
General procedure for preparation of (E)-(4-(4-(2-arylindenehydrazinyl)benzyl)oxazolidin-2-one (3-7)

A mixture of 4-(4-hydrazinylbenzyl)oxazolidin-2-one (0.01 mole) and appropriate aromatic aldehyde (0.01 mole) in absolute ethanol (30 ml). A drop of acetic acid were added and was placed in a small conical flask at room temperature, then the mixture exposed to microwave irradiation at 270 w for 4 min, This reaction was monitored by TLC. The resultant solution was cooled and poured into cold water. The separated solid was filtered, crystallized from ethanol to give crystalline yellow.

General procedure for preparation of 4(4((4-oxo-2-arylthiazolidin-3-yl)amino)benzyl)oxazolidin-2-one (8-12)

A mixture of (E)-4-(4-(2-arylindenehydrazinyl)benzyl)oxazolidin-2-one (3-7) (0.01 mole) and mercaptoacetic acid (1.82 g, 0.02 mole) in DMF (30 ml), 2g of zinc chloride was added and placed in a small conical flask at room temperature then the mixture exposed to microwave irradiation at 180 w for 10 min, this reaction was monitored by TLC. The resultant solution was cooled and poured into cold water. The separated solid was filtered, crystallized from ethanol to give crystalline yellow.

Computation details



Scheme 1. Synthetic routes of compounds thiazolidinones

The density functional theory (DFT) with B3LYP level theory using 6-31G(d,p) basis set in Gaussian-03 have been used for theoretical calculations [17-19]. Following the geometry optimizations with B3LYP method, the optimized structural parameters used in the vibrational wavenumber calculation at DFT level to characterize all stationary points while minima. Furthermore, HOMO and LUMO energy values and energy gap for thiazolidinones were calculated by using B3LYP method with 6-31G(d,p) basis set. Moreover, in order to show nonlinear optical (NLO) activity of studied molecules, the dipole moment, linear polarizability and first order hyper polarizability were obtained from molecular polarizabilities based on theoretical calculations. Mulliken atomic charges and Molecular Electrostatic Potentials (MEPs) of thiazolidinones were plotted in 3D by using optimized structures at same level theory.

Molecular geometry

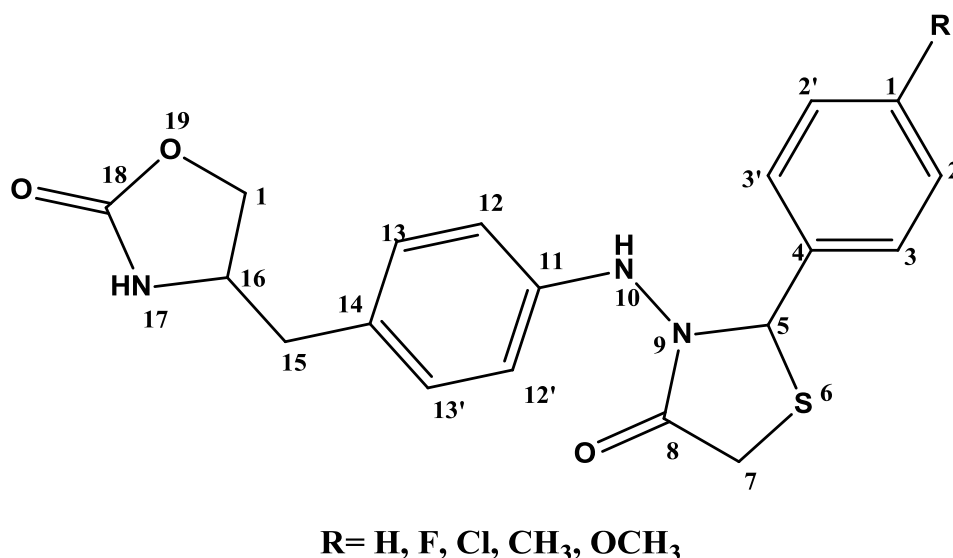
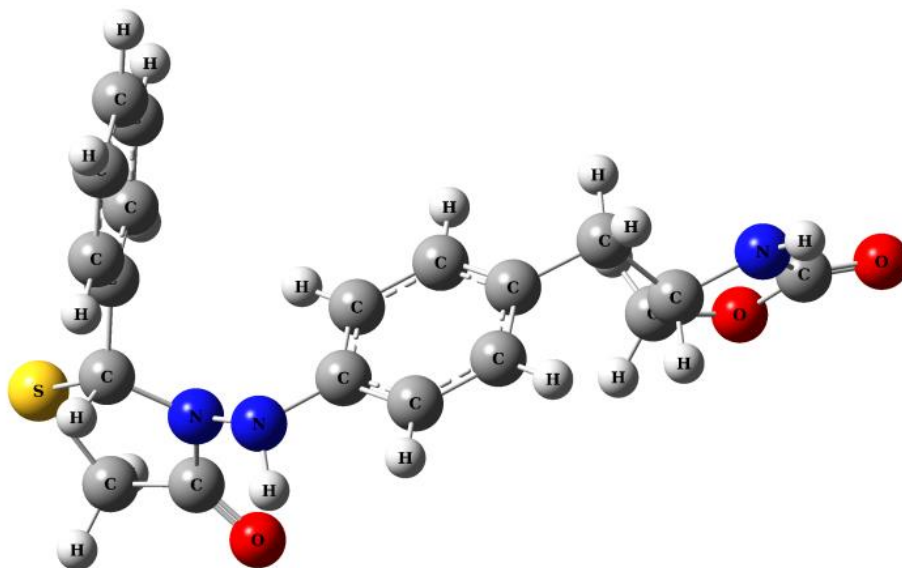


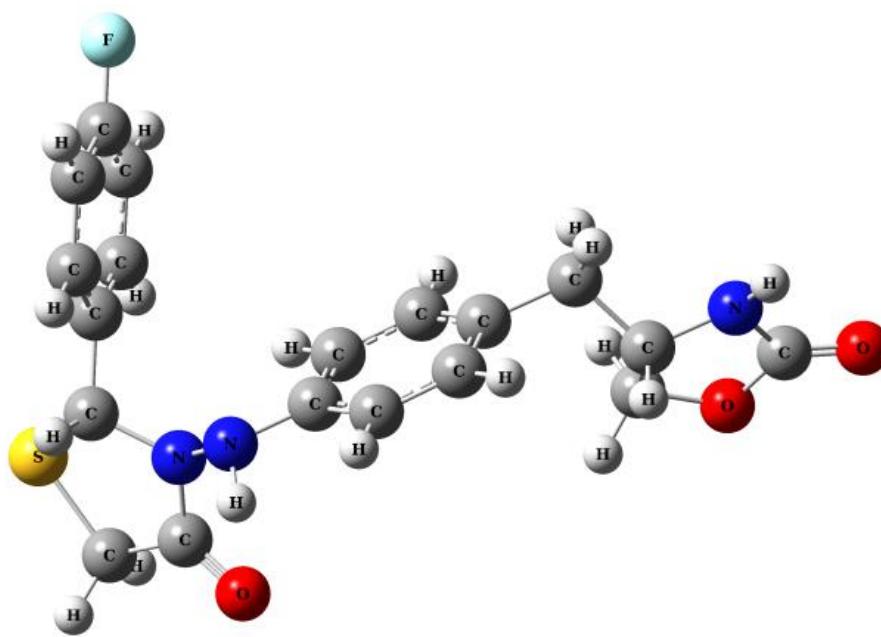
Fig. 1. Numbering Pattern of thiazolidinones.

The optimized structural parameters such as bond lengths, bond and dihedral angles of thiazolidinones were determined at B3LYP level theory with 6-31G(d,p) basis set and are presented in Table 1 in accordance with the atom numbering scheme of the molecule shown in Fig. 1. To the best of our knowledge, no single crystal X-ray crystallographic data of DDMs has yet been reported. However, the theoretical results obtained are almost comparable with closely related molecules [20,21]. Bond distances in the five independent molecules show little differences (± 0.025 Å). Likewise, bond angles are very similar as well ($\pm 0.2^\circ$). In the ring named thioazolidin in molecule 1, the selected bond distances C₅-S₆, C₅-N₉, C₈-N₉ are 1.8572 Å, 1.4754 Å and 1.3858 Å, which are in agreement with XRD values [20, 21]. The carbonyl carbon atom is sp² hybridised (three σ -bonds and one π -bond), and as a consequence, the carbonyl group is planar and has bond angles of around 111.8° (B3LYP) and 111.4° (XRD). The C=O bond is short (~ 1.2 Å) and rather strong (ca. 690 kJ mol⁻¹). As oxygen is more

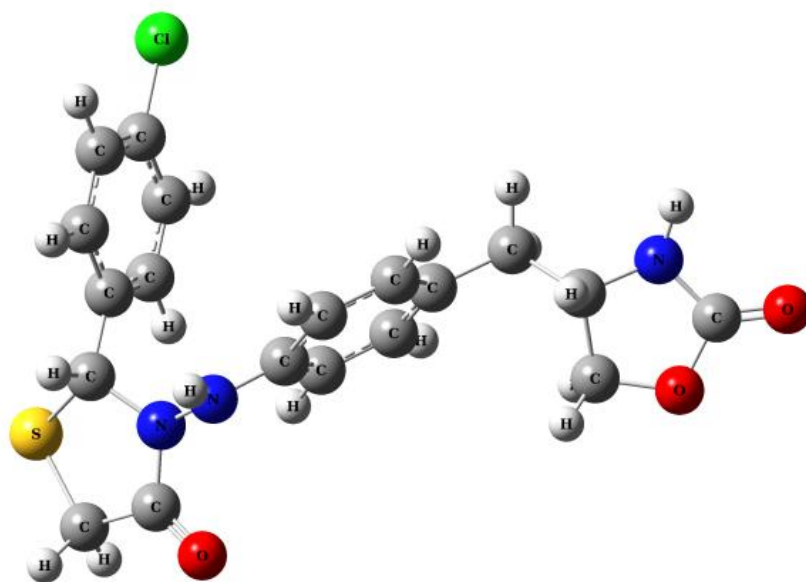
electronegative than carbon, the electrons in the C=O bond are drawn towards the oxygen. This means that carbonyl compounds are polar and have substantial dipole moments. Due to pulling of electron from carbon C₈, the bond strength changes which results in the lengthening of the bond (C₇-C₈ and C₈-N₉) compared with normal bond lengths of C-C and C-N. The selected dihedral angles of the molecule are C₃-C₄-C₅-S₆ (133.54°), C₃-C₄-C₅-N₉ (70.89°), C₁₃-C₁₄-C₁₅-C₁₆ (-101.83°) and C₁₃-C₁₄-C₁₅-C₁₆ (76.70°). These data reveal that the thiazolidine ring at N₉ C₁₅ is lying in the same plane. Whereas, oxazolidin-2-one ring at N₁₇ C₁₅ perpendicular with respect to phenyl group.



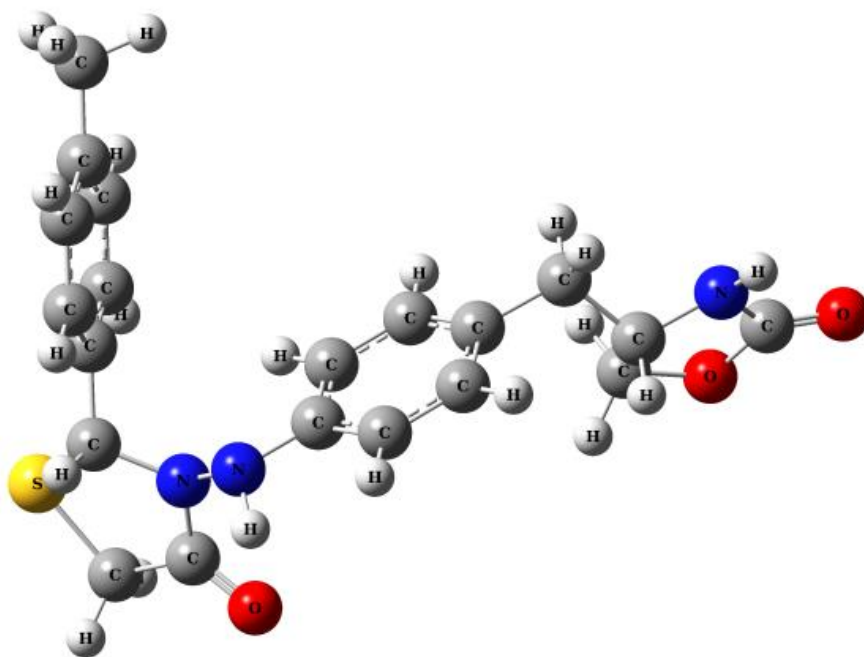
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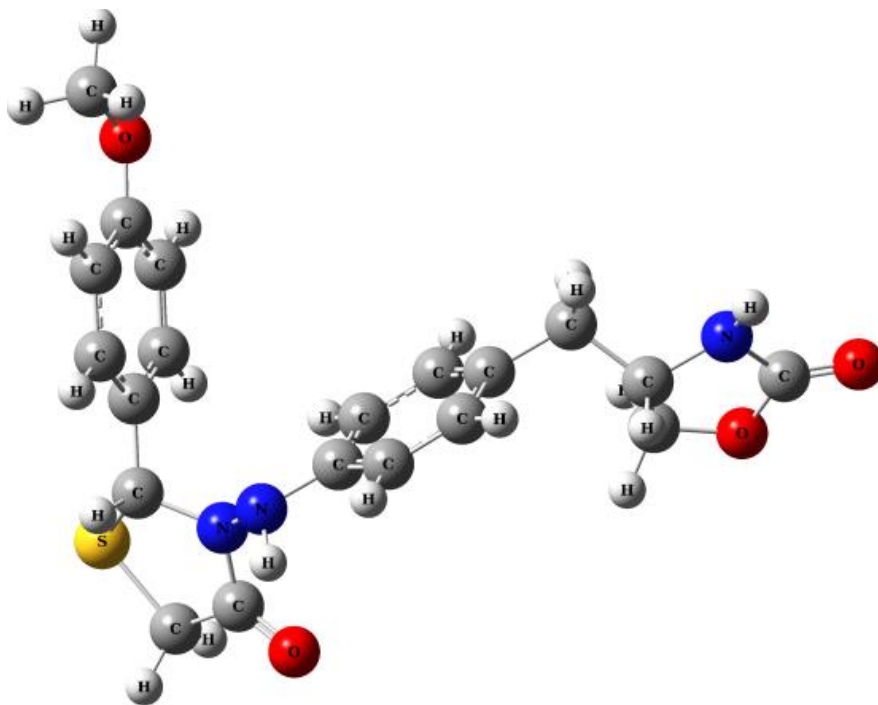
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9



10

Fig. 2. Optimized structures of thiazolidinones.

Table 1. Selected bond lengths, bond angles and dihedral angles of thiazolidinones.

Bond length (Å)	XRD ^{a,b,c}	6	7	8	9	10
C ₅ -N ₉	1.47	1.4754	1.4758	1.4747	1.4766	1.4779
C ₅ -S ₆	1.77	1.8572	1.8564	1.8559	1.8572	1.8577
S ₆ -C ₇	1.77	1.8327	1.8327	1.8329	1.8324	1.8323
N ₉ -C ₈	1.47	1.3858	1.3857	1.3953	1.3854	1.3849
C ₈ -O ₈	1.207	1.2172	1.2171	1.2108	1.2175	1.2178
N ₉ -N ₁₀	-	1.4003	1.4004	1.3784	1.4007	1.4006
N ₁₀ -C ₁₁	1.476	1.4204	1.4210	1.3963	1.4200	1.4202
C ₁₅ -C ₁₄	1.519	1.5141	1.5141	1.5141	1.5142	1.5374
C ₁₅ -C ₁₆	1.507	1.5376	1.5377	1.5371	1.5377	1.5374

C ₁₆ -N ₁₇	1.47	1.4574	1.4573	1.4567	1.4576	1.4576
N ₁₇ -C ₁₈	1.466	1.3835	1.3837	1.3829	1.3837	1.3835
C ₁₈ -O ₁₈	1.207	1.2056	1.2055	1.2058	1.2056	1.2056
C ₁₈ -O ₁₉	1.207	1.3708	1.3710	1.3709	1.3709	1.3708
O ₁₉ -C ₂₀	-	1.4377	1.4376	1.4376	1.4378	1.4379
Bond angle (°)						
C ₅ -S ₆ -C ₇	92.3	92.66	92.64	92.34	92.70	92.71
S ₆ -C ₇ -C ₈	110.9	107.58	107.59	108.26	107.58	107.55
S ₆ -C ₅ -N ₉	112.4					
C ₇ -C ₈ -N ₉	111.4	111.83	111.80	111.14	111.84	111.86
C ₅ -N ₉ -C ₈	115.8	117.20	117.15	117.81	117.19	117.19
C ₄ -C ₅ -N ₉	111.4	114.29	114.25	114.47	114.40	114.63
C ₃ -C ₄ -C ₅	-	118.82	118.78	119.24	118.98	119.20
C ₅ -N ₉ -N ₁₀	-	116.00	116.01	118.22	116.06	115.96
C ₈ -N ₉ -N ₁₀	-	116.99	117.04	118.08	116.87	116.85
N ₁₀ -C ₁₁ -C ₁₂	-	123.20	123.20	122.11	123.14	123.20
N ₁₀ -C ₁₁ -C ₁₂ '	-	177.40	117.66	118.92	117.73	117.68
Dihedral (°)						
C ₁₃ -C ₁₄ -C ₁₅ -C ₁₆	-	-101.83	-102.13	-104.27	-101.62	-103.14
C ₁₃ '-C ₁₄ -C ₁₅ -C ₁₆	-	76.70	76.20	74.37	76.62	178.40
C ₂₀ -C ₁₆ -C ₁₅ -C ₁₄	-	64.69	64.84	64.40	65.19	64.80
N ₁₇ -C ₁₆ -C ₁₅ -C ₁₄	-	177.11	177.27	176.77	177.64	177.23
C ₃ -C ₄ -C ₅ -S ₆	-	133.54	136.84	124.80	135.94	134.73
C ₃ '-C ₄ -C ₅ -N ₉	-	70.89	74.01	63.74	73.42	72.16
C ₁₂ '-C ₁₁ -N ₁₀ -N ₉	-	-163.59	-163.14	161.00	-161.46	-163.85
C ₁₂ -C ₁₁ -N ₁₀ -N ₉	-	19.46	19.92	-21.72	21.72	19.30
C ₅ -C ₉ -N ₈ -C ₇	-	19.79	19.99	15.56	19.97	19.90

C ₅ -S ₆ -C ₇ -C ₈	-	-13.39	-13.39	-14.96	-13.25	-13.55
C ₁₆ -N ₁₇ -C ₁₈ -O ₁₉	-	14.83	14.96	14.57	14.98	14.92
C ₁₆ -C ₂₀ -O ₁₉ -C ₁₈	-	-18.84	-18.97	-18.54	-18.98	-18.94

a,b,c -Values are taken from Ref 20, 21

FT-IR Vibrational analysis

The computational study was extended to FT-IR spectroscopy for frequency analysis in order to support the assigned experimental values of the vibration bands for the synthesized compounds 6-10. In the present study, frequencies were scaled by using scaled quantum mechanics [19] with scaling factor of 0.9608. Representative simulated vibrational FT-IR spectra are given in Figs. 2.

In Table 1, we have presented the calculated vibrational wavenumbers and IR intensity along with experimental vibrational wavenumbers. The N-H stretching vibration [22,23] appears as a broad band in the region 3500-3100 cm⁻¹. The N-H stretching lies at 3458-3477 cm⁻¹ in FT-IR, but the theoretically calculated frequencies are in the range 3464-3483 cm⁻¹, which are in agreement with the experimental values. It is due to the presence of strong hydrogen bonding in solid phase. The carbonyl stretching frequency is found in the region of 1750-1650 cm⁻¹ [24]. In the FT-IR spectrum, a sharp intense band appear at 1693 cm⁻¹ can be assigned to C=O stretching vibration of the title compounds. The intensity of these bands can increase which may be due to the formation of inter and intra molecular hydrogen bonds. From the DFT calculations, the band at 1696 cm⁻¹ is correlated well with the experimental data.

Table 2. FT-IR vibrational assignments of compound thiazolidinones.

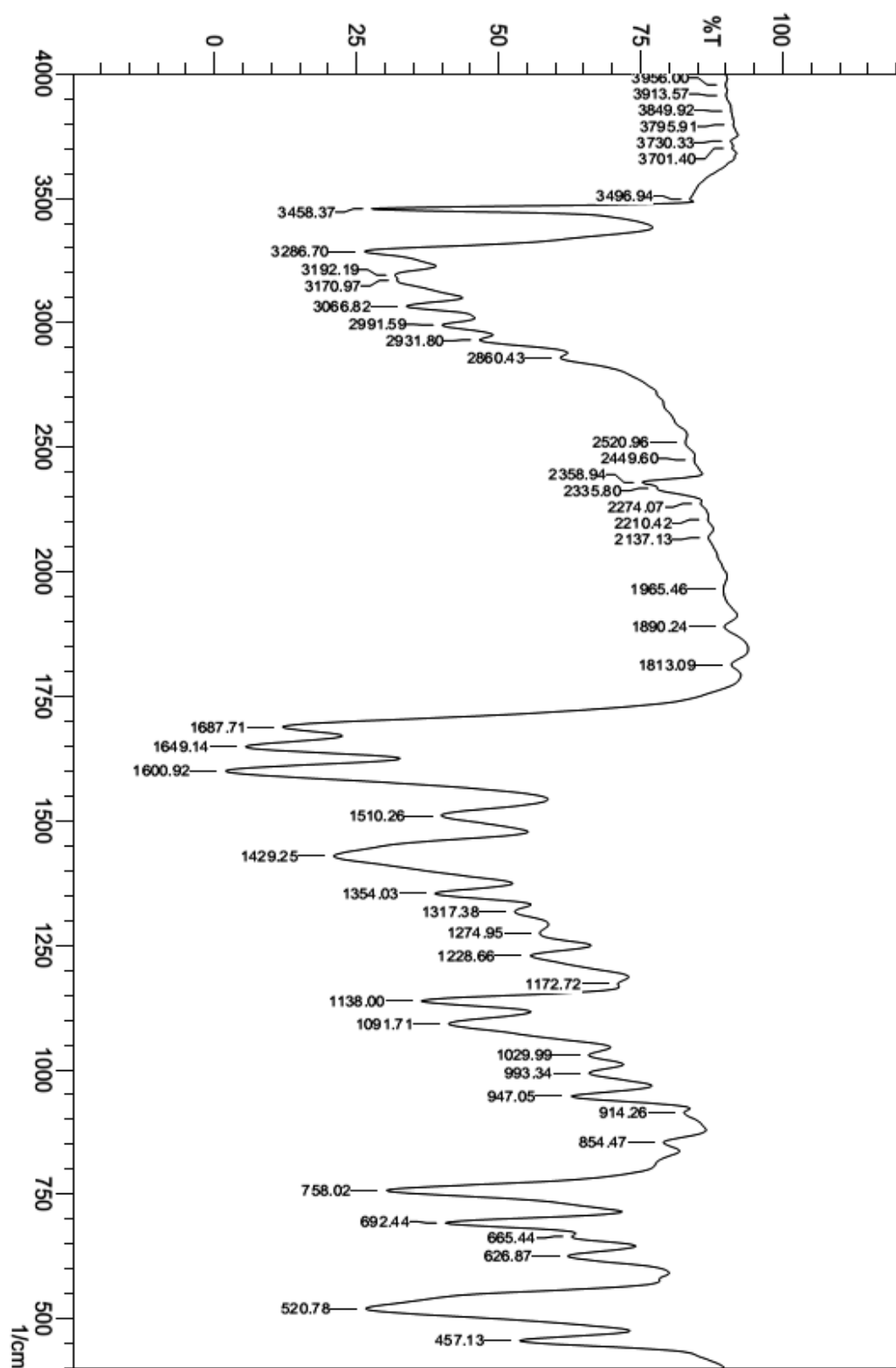
Assignments	6		7		8		9		10						
	Expt.	B3LYP		Expt.	B3LYP		Expt.	B3LYP		Expt.	B3LYP				
		Scaled Values	Intensity		Scaled Values	Intensity		Scaled Values	Intensity		Scaled Values	Intensity			
vN -H	3458	3481	34.54	3477	3481	34.66	3464	3489	34.3	3464	3470	34.19	3462	3483	34.08

$\nu\text{C-N}$	$\nu\text{C-O}$	$\nu\text{C=C}$	$\nu\text{C=O}$	$\nu\text{Ali-H}$	$\nu\text{ArC-H}$
1091	1138	1429	1687	2991	3192
1109	1143	1465	1691	3071	3199
7.54	30.79	42.31	262.56	20.99	10.53
1028	1112	1411	1674	2976	3147
1138	1121	1468	1694	3051	3166
5.85	5.32	10.12	274.21	4.6	18.98
1076	1128	1436	1693	2993	3170
1077	1125	1440	1696	3067	3180
1.77	2.02	60.35	321.73	321.73	24.24
1095	1155	1427	1658	2962	3157
1105	1140	1435	1691	3027	3161
7.81	50.09	61.35	283.45	3.43	18.42
1026	1126	1423	1656	2920	3151
1055	1123	1492	1682	2930	3166
7.12	8.24	56.23	283.35	3.71	19.93

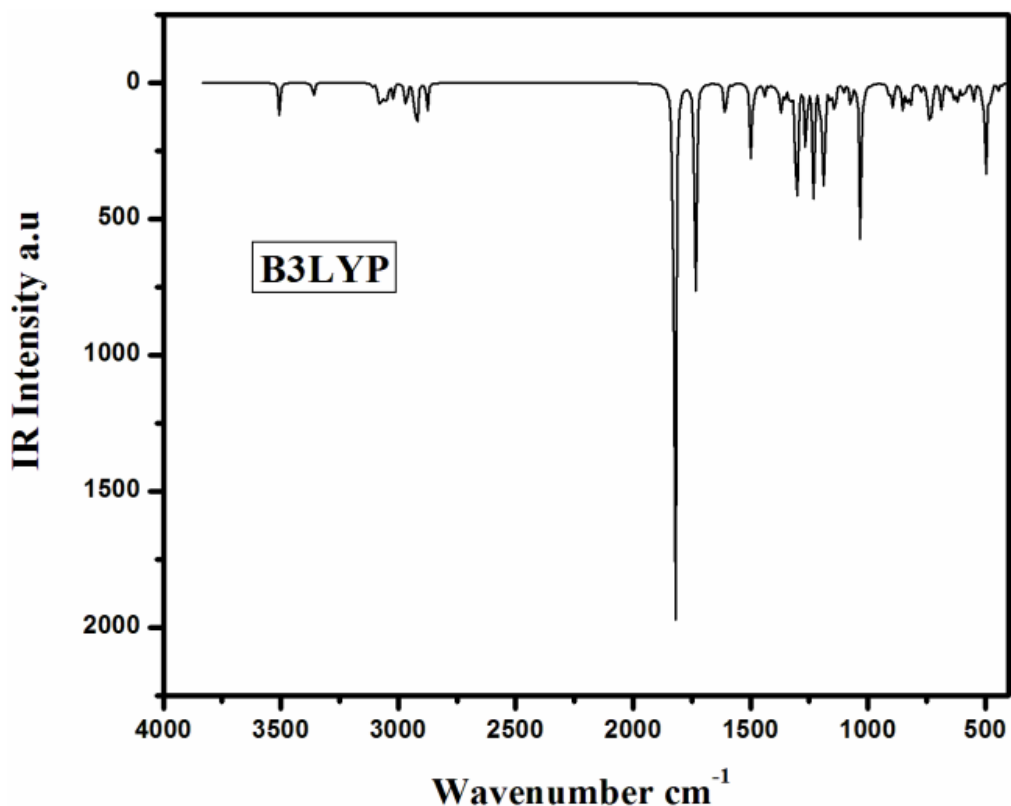
The C–H stretching vibrations in aromatic and hetero aromatic rings appear in the range 3200-3000 cm^{-1} which is the characteristic region for the ready identification of such C–H stretching vibrations [25]. In the present case, the C–H stretching frequency is observed at $\sim 3192 \text{ cm}^{-1}$ in the FT-IR spectrum whereas the computed C–H stretching vibrations of thiazolidinones ring obtained around $\sim 3199 \text{ cm}^{-1}$.

The methyl and methylene groups stretching are expected at 2980-2870 cm^{-1} [26]. The C-H stretching of these groups appeared around 2993 cm^{-1} as very strong bands in FT-IR and the DFT values ranges from 2930 to 3071 cm^{-1} .

The ring C–C stretching vibrations usually occur in the region 1625-1430 cm^{-1} [27]. In the present work, the C–C vibrations observed experimentally at 1429, 1411, 1436, 1427 and 1423 cm^{-1} for 6-10, respectively and are in agreement with the theoretical values that range from 1435-1492 cm^{-1} . As seen from Table 2, the C-O frequency in the range 1112-1155 cm^{-1} (IR) corresponds to the computed value of 1121-1143 cm^{-1} . According to some investigators [28,29], the C–N stretching occurs in the region $1050 \pm 60 \text{ cm}^{-1}$. For the title compounds, the FT-IR, C–N stretching vibration observed in the range 1026-1091 cm^{-1} and the values calculated by B3LYP method are 1055-1109 cm^{-1} . The out-of-plane bending mode such as wagging and twisting modes of $-\text{CH}_2-$ groups are observed in the lower part of the spectrum



(A)



(B)

Fig. 2(A,B). FT-IR spectrum of Compound 6.

Mulliken charge analysis

The total atomic charges of synthesized compounds 6-10 obtained by using B3LYP/6-31G (d,p) method are listed in Table 3. The corresponding Mulliken plot is shown in Fig. 4 and it gives us information about the charge shifts. Considering the method used in the atomic charge calculation, C₅, C₇, O₈, N₉, N₁₀, C₁₅, N₁₇, O₁₈ and O₁₉ atoms exhibit a substantial negative charge, which are donor atom. The more positive values on C₈, H₁₀, C₁₁, H₁₇ and C₁₈ accommodate higher negative charge, which is an acceptor atom. Therefore it can be concluded that both electrophilic and nucleophilic substitution reactions are favoured in the title compounds.

Table 3. Mulliken atomic charges of thiazolidinones.

Atom	6	7	8	9	10
C ₄	0.134	0.131	0.139	0.130	0.132
C ₅	-0.145	-0.147	-0.157	-0.147	-0.148
S ₆	0.124	0.124	0.127	0.122	0.120

C ₇	-0.424	-0.424	-0.429	-0.423	-0.423
C ₈	0.577	0.577	0.594	0.577	0.577
O ₈	-0.482	-0.481	-0.458	-0.483	-0.485
N ₉	-0.328	-0.328	-0.331	-0.328	-0.327
N ₁₀	-0.436	-0.438	-0.452	-0.436	-0.436
H ₁₀	0.268	0.268	0.258	0.267	0.267
C ₁₁	0.300	0.299	0.355	0.301	0.299
C ₁₄	0.116	0.116	0.114	0.116	0.116
C ₁₅	-0.253	-0.253	-0.253	-0.253	-0.253
C ₁₆	0.056	0.056	0.057	0.056	0.056
N ₁₇	-0.554	-0.554	-0.554	-0.554	-0.554
H ₁₇	0.271	0.271	0.271	0.271	0.270
C ₁₈	0.753	0.754	0.754	0.753	0.753
O ₁₈	-0.403	-0.493	-0.493	-0.493	-0.493
O ₁₉	-0.477	-0.477	-0.477	-0.477	-0.477
C ₂₀	0.060	0.061	0.061	0.060	0.060

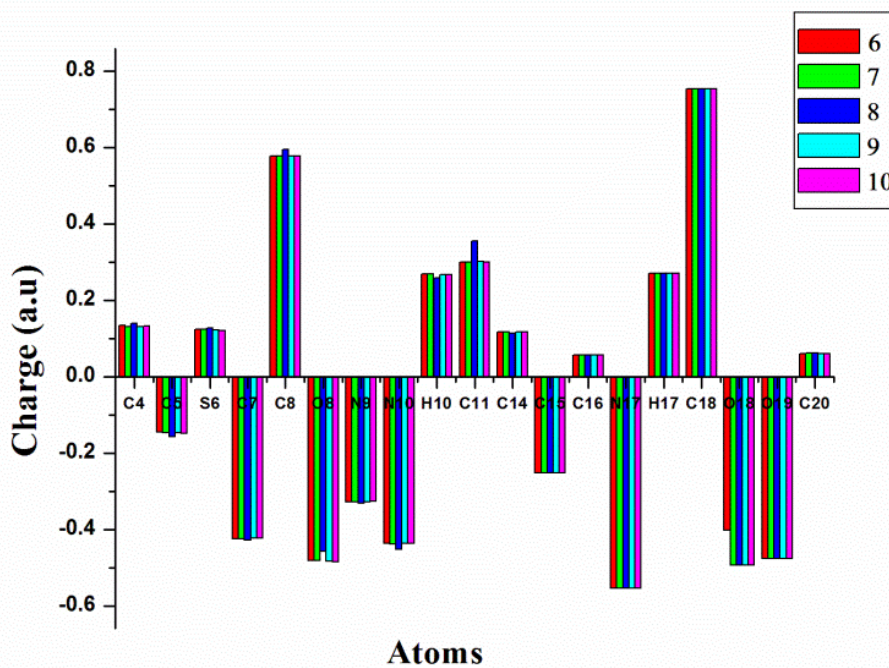
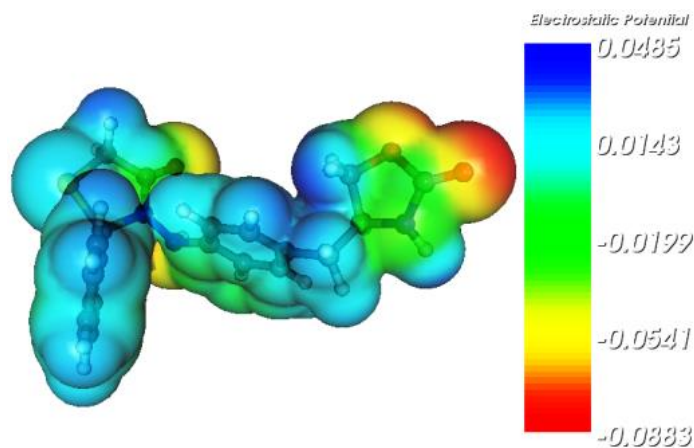


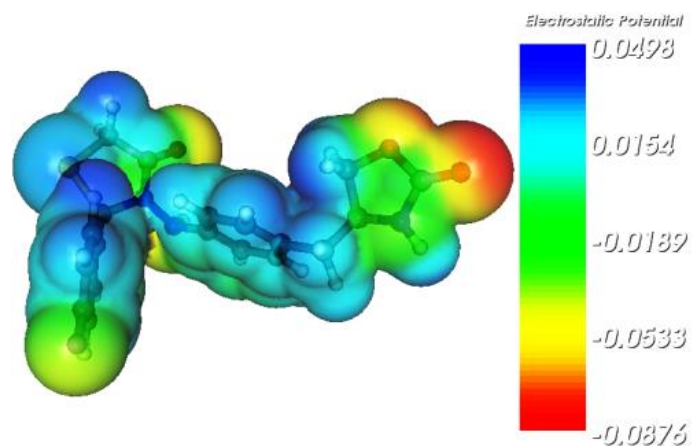
Fig. 4. Mulliken atomic charges of thiazolidinones.

MEP analysis

The molecular electrostatic potential (MEP) are related to the electron density and may be a helpful descriptor in understanding sites for electrophilic and nucleophilic attacks and also hydrogen bonding interactions [30,31]. The 3D plot of electro molecular electrostatic potential (MEP) of 6-10 are shown in Fig. 5. The MEP is a useful property to study the reactivity of a system given that an approaching electrophile will be attracted to negative regions (where the electron density is maximum and shown as red colour). The maximum positive regions are preferred sites for nucleophilic attacks are shown as blue colour. Thus MEP displays molecular size, shape as well as positive, negative and neutral electrostatic potential regions.



6



7

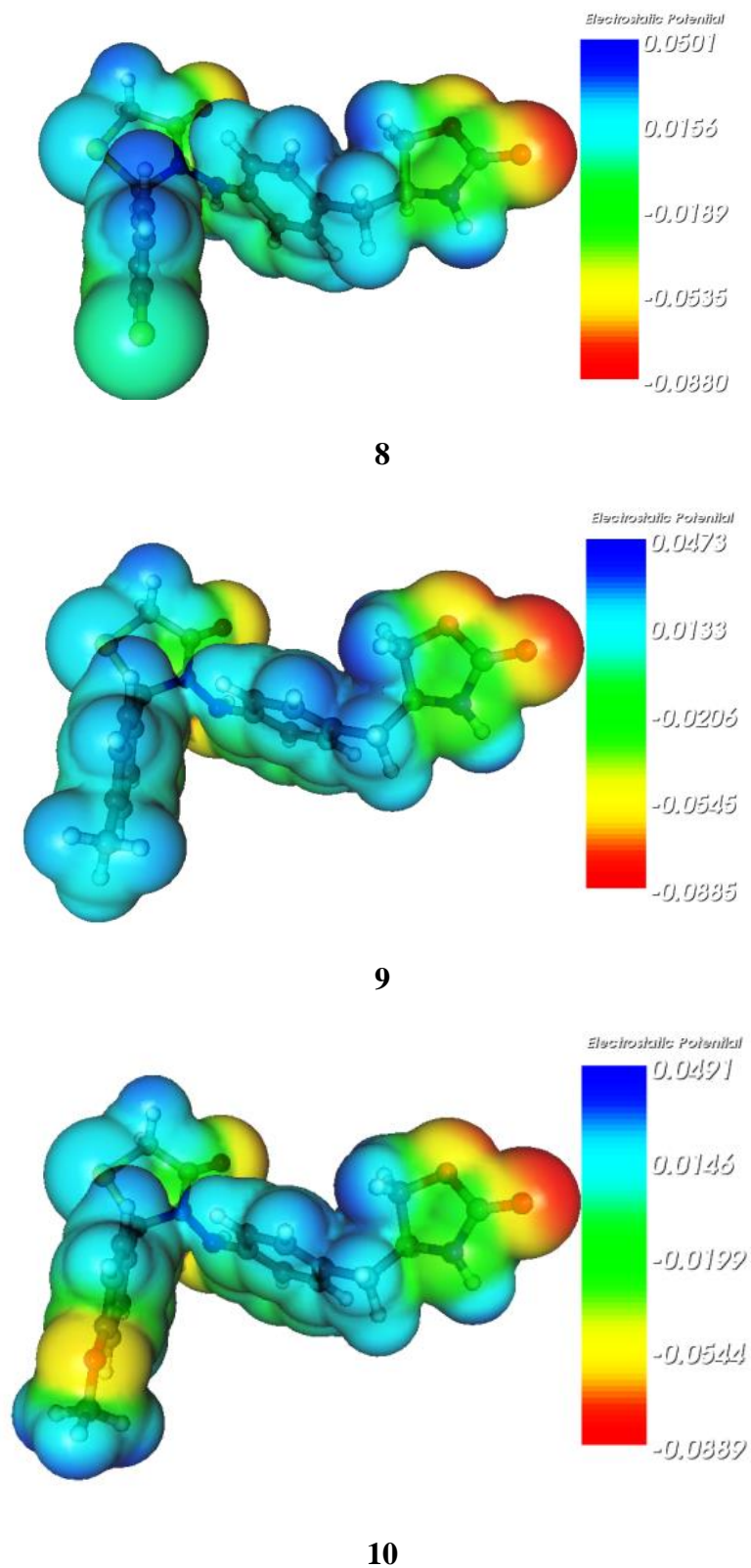


Fig. 5. MEP diagrams of thiazolidinones.

The MEP map of thiazolidinones shows that, regions having the negative potential are over the electronegative N and O atoms and the regions having the positive potential are over the hydrogen atoms.

HOMO-LUMO Energies

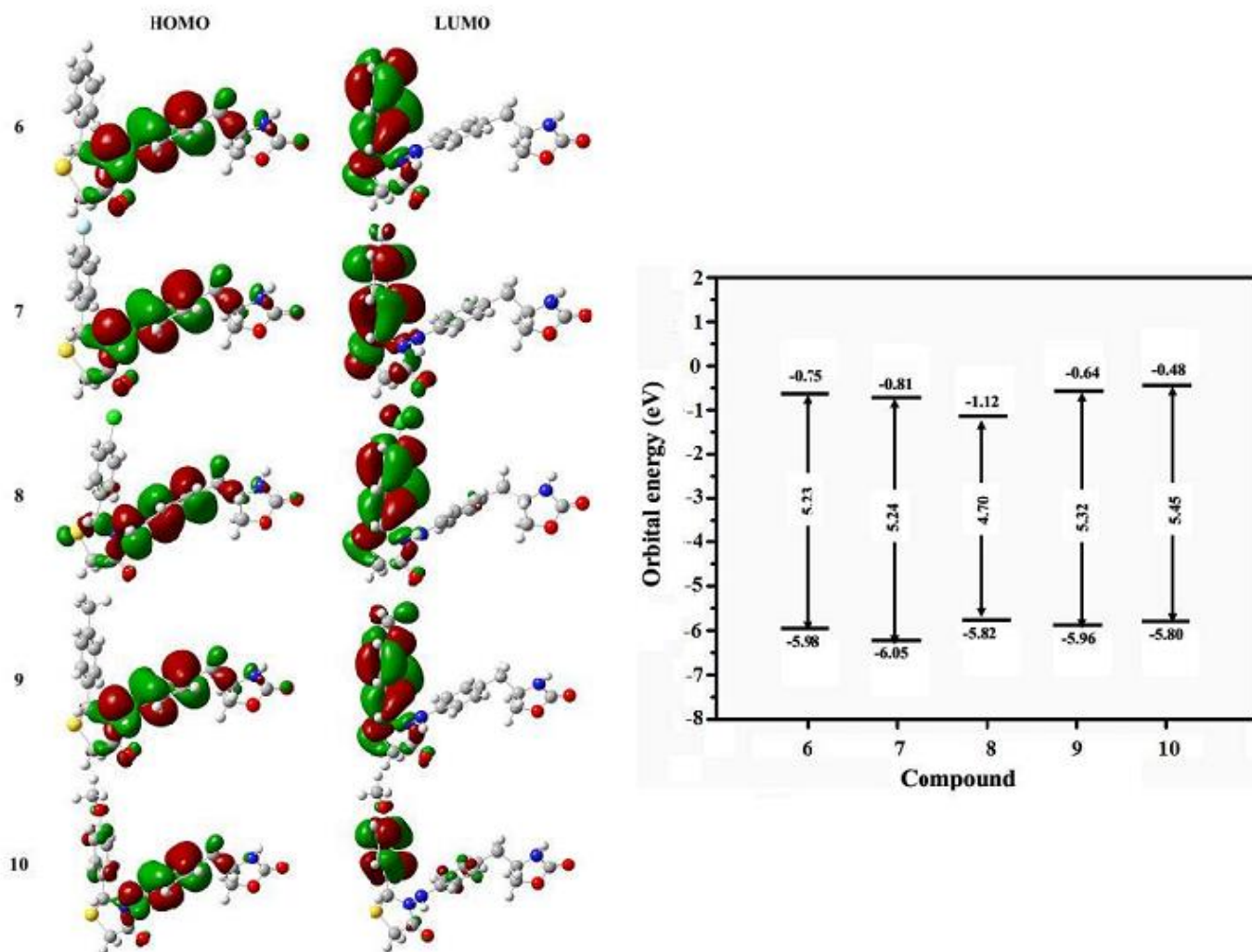


Fig. 6. Molecular orbitals and energies for compound thiazolidinones.

HOMO-LUMO energies were calculated theoretically according to DFT method using B3LYP/6-31G(d,p) level theory and the values of thiazolidinones are given in Table 4. Conjugated molecules are characterized by small HOMO-LUMO gaps. The small energy difference between the HOMO and LUMO for the title compound facilitates the intra molecular charge transfer taking place within the molecule through π -conjugated path. This electronic absorption corresponds to the transition from the ground state to the first excited

state and is one electron excitation from the highest occupied molecular orbital to the lowest unoccupied molecular orbital. While the energy of HOMO is directly related to ionization potential and LUMO energy is to electron affinity. Recently, the energy gap between HOMO and LUMO has been used to confirm the bioactivity from ICT [32,33]. The atomic orbital compositions of the frontier molecular orbitals are shown in Fig. 6.

For a system lower value of HOMO-LUMO gap makes it more reactive or less stable and also has a direct influence on the electron density difference for the stabilizing ICT process. In this sense, it seems that the selection of a chloro- containing substituent has a beneficial effect among the designed candidate. As a result, the trend of ΔE gap of inspected compounds becomes **10>9>7>6>8**. We can observe from this Table 4, the introduction of different substituent at 1- site of the phenyl core significantly change the ΔE value.

The absolute electronegativity (χ), hardness (η), electrophilicity index (ψ) and softness (s) were calculated using the following equations [34]

$$\begin{aligned}\eta &= (\text{IP}-\text{EA})/2 \approx (\text{E}_{\text{LUMO}}-\text{E}_{\text{HOMO}})/2 \\ \chi &= (\text{IP}+\text{EA})/2 \approx -(\text{E}_{\text{LUMO}}+\text{E}_{\text{HOMO}})/2 \\ \psi &= \mu^2/2 \eta \\ s &= 1/2 \eta\end{aligned}$$

Global electronegativity values of the investigated molecules are given in Table 4. According to Table 4, compound 10 has higher electronegativity, it carries a methoxy group in the *para*-position and it may affect the entire molecular structure. Larger the electronegativity the interaction level of the molecule with the medium increases [34]. If a molecule has higher electron affinity and ionization potential values, it has unstable molecular structure. Thus, molecule must come in different interactions, which is hydrogen bonding or other different interactions (van der Waals interactions). Molecular softness is a measure of molecular reactivity, while molecular hardness is a measure of molecular stability[34]. From Table 4 that the lowest active molecules are 10, 9, 6 and 7, whereas the bigger stable one is 8.

Table 4. Calculated energy values (eV) of thiazolidinonesin gas phase.

DFT/B3LYP/6-31G(d,p)	6	7	8	9	10
E_{HOMO}	-5.98	-6.05	-5.82	-5.96	-5.93
E_{LUOMO}	-0.75	-0.81	-1.12	-0.64	-0.48
$E_{\text{LUMO-HOMO}}$	5.23	5.24	4.70	5.32	5.45
Electronegativity (χ)	-3.37	-3.43	-3.47	-3.30	-3.21
Hardness (η)	2.62	2.62	2.35	2.66	2.73
Electrophilicity index (ψ)	2.17	2.24	2.57	2.05	1.89
Softness (s)	141.56	141.26	157.57	139.22	135.77

NLO property

NLO is at the forefront of recent research because it provides the key functions of frequency shifting, optical modulation, optical switching, optical logic and optical memory for the emerging are as such as signal processing, telecommunications and optical interconnections [35,36]. The dipole moment (μ), mean polarizability (α) and the total first static hyperpolarizability (β_0) are related directly to the nonlinear optical efficiency of the molecule. In discussing nonlinear optical properties, the polarization of the molecule by an external radiation field is often approximated as the creation of an induced dipole moment by an external electric field. The first hyperpolarizability (β_0) of a molecular system is calculated using B3LYP/6-31G(d,p) method, based on the finite field approach. The total static dipole moment (μ), the Mean polarizability (α), Anisotropy of the polarizability ($\Delta\alpha$) and the first order hyperpolarizability (β_0) using the x, y, z components are calculated using the following equations.

$$\begin{aligned}\mu &= (\mu_x^2 + \mu_y^2 + \mu_z^2)^{1/2} \\ \alpha_{tot} &= \frac{1}{3} \alpha_{xx} + \alpha_{yy} + \alpha_{zz} \\ \Delta\alpha &= \frac{1}{\sqrt{2}} \left[(\alpha_{xx} - \alpha_{yy})^2 + (\alpha_{yy} - \alpha_{zz})^2 + (\alpha_{zz} - \alpha_{xx})^2 + 6(\alpha_{xy}^2 + \alpha_{yz}^2 + \alpha_{xz}^2) \right]^{1/2} \\ \beta_0 &= [(\beta_{xxx} + \beta_{xyy} + \beta_{xzz})^2 + (\beta_{yyy} + \beta_{yzz} + \beta_{yxx})^2 + (\beta_{zzz} + \beta_{zxx} + \beta_{zyy})^2]^{1/2}\end{aligned}$$

Table 5. Non-linear optical properties of thiazolidinones calculated using B3LYP method using 6-31 G(d,p) basis set.

NLO behavior	6	7	8	9	10
Dipole moment (μ) D	7.34	7.05	7.99	7.47	8.52
Mean polarizability (α) $\times 10^{-23}$ esu	2.50	2.60	2.80	2.60	2.70
Anisotropy of the Polarizability ($\Delta\alpha$) $\times 10^{-24}$ esu	1.02	1.10	1.22	1.05	0.99
First order polarizability (β_0) $\times 10^{-30}$ esu	4.33	4.65	5.03	4.56	5.64

Results from Table 5, the general ranking of NLO properties should be as follows: 10>8>7>9>6. From the above results we can concluded that the presence of an electron donating group (methoxy) in the *para* position at the phenyl ring contributes to increase the dipole moments and first order hyper polarizability of the thiazolidinones probably because of an inductive competition between the methoxy and the electronic density available in the

molecule. Therefore, the compound 10 has a potential use in the development of non-linear optical materials.

3. CONCLUSIONS

The geometry optimization and vibrational spectra have been obtained for the compound thiazolidinones by using DFT/B3LYP/6-31G(d,p) level and the optimized results are in good agreement with available single crystal data character. The experimental vibrational spectra are in good agreement with the theoretical spectra. The HOMO–LUMO energy gap has a substantial influence on the ICT. The lowering of HOMO–LUMO energy gap, a quantum–chemical descriptor, explains the ease with which charge transfer interactions take place within the molecule. The MEP map shows that oxygen and nitrogen atoms are the negative potential sites and the positive potential sites are around the hydrogen atoms. The total dipole moment, polarizability and hyperpolarizability of the compounds were calculated and the results show that the molecule 10 could be a good NLO material.

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