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## Molecular Geometry and Spectroscopic Investigation on 2-Imino-5-Phenyl-4-Oxazolidinone Using Quantum Computational Methods

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### ABSTRACT

In this work, Fourier Transform Infrared Red and Fourier Transform RAMAN spectra were studied in the range of 4000–400 cm<sup>-1</sup> and 4000–100cm<sup>-1</sup> respectively, for 2-Imino-5-phenyl-4-oxazolidinone compound. The optimized molecular structural parameters, vibrational frequencies and corresponding vibrational intensity of the bands computed using Hartree-Fock and Density Functional Theory with B3LYP/ 6-311+G(d,p) method and basis sets and the result are interpreted. The results of the calculations were used to stimulated vibrational spectra of the title compound and the whole vibrational assignments of all the fundamentals were made, which show outstanding agreement with experimental spectra. The NMR chemical shifts for <sup>1</sup>H and <sup>13</sup>C of the molecule were calculated by gauge independent atomic orbital with B3LYPmethod and 6-311+G(d,p) basis set and the chemical shifts were compared. The frontier molecular orbital energies, UV-Visible wavelengths absorption, corresponding excitation energy, dipole moment were computed by HF and DFT Hartree-Fock and Density Functional Theory methods. The Entropy Enthalpy and heat capacity at different temperatures were computed. In addition, Mullikan charges and molecular electrostatic potential map performed.

**Keywords:** FTIR and FT-Raman B3LYP, GIAO, MEP, HOMO-LUMO.

### INTRODUCTION

The molecular formula for the 2-Imino-5-phenyl-4-oxazolidinone (abbreviated as 2I5P4O) is C<sub>9</sub>H<sub>8</sub>N<sub>2</sub>O<sub>2</sub>. The other name of the title molecule is

Pemoline, 2-Amino-5-phenyl-2-oxazolin-4-one. 2I5P4O is a powdered white crystal, it is insoluble in water, melt at 245°C. 2I5P4O is an oxazolidine compound. Central nervous system is stimulate by

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2I5P4O and used in treatment of attention deficit and hyperactivity complaint and impulsivity in children as well as adults with narcolepsy in case of no response of psychotherapy. Amines derived from  $\beta$ -phenyl ethyl amines and their derivatives are found to be effective in central nervous system stimulation. They also can produce an increase in arterial blood pressure as well as appetite depressions.

Hence, literature survey reveals that, no such work has been reported on 2I5P4O, particularly the spectroscopic analysis such IR, Raman, UV, and NMR analysis were not carried out till now. Hence, the present investigation was undertaken to carry out all these spectral analysis with help of quantum computational theories through ab-initio and density functional methods.

### EXPERIMENTAL DETAILS

The FTIR, FT Raman and FT NMR spectra of the compound under investigation namely 2I5P4O was bought from Spectral Library of M/S Aldrich Chemicals, USA. According to the report, the FT-IR spectrum of the compound was recorded wave number ranging between 4000 and 400  $\text{cm}^{-1}$  with perseverance of  $\pm 2 \text{ cm}^{-1}$  using Perkin-Elmer 180 Spectrometer. The FT-Raman spectrum of the compound was recorded using FRA 106 Raman module equipped with Nd: YAG laser source operating at 1.064  $\mu\text{m}$  line widths with 200 mW powers with scanning speed of 30  $\text{cm}^{-1} \text{ min}^{-1}$  of spectral width 2  $\text{cm}^{-1}$ , wave number ranging between 4000 and 100  $\text{cm}^{-1}$ . The wave numbers of all piercing bands are precise to  $\pm 1 \text{ cm}^{-1}$ . The  $^1\text{H}$  and  $^{13}\text{C}$  NMR spectra were noted using high perseverance Nuclear Magnetic Resonance Spectrometer[1].

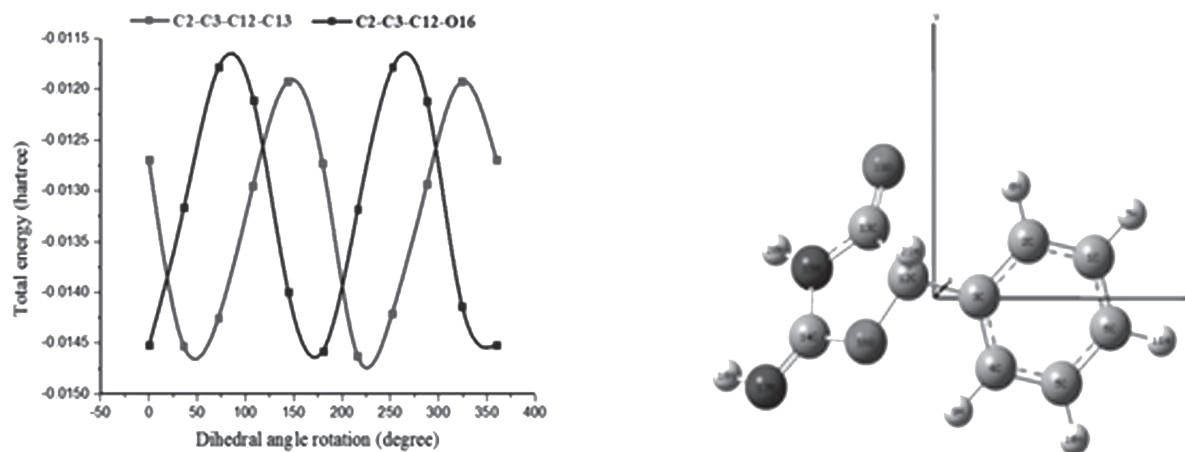
### DETAILS OF COMPUTATION

The Gaussian 09 programing software is used to perform complete quantum chemical calculations [2, 3] on a Pentium IV/3.02GHz PC. The structure of the molecule 2I5P4O was designed using Gauss view program [4]. The same structure is used to get optimized structural parameter and compute the vibrational frequencies by Hartree-Fock and DFT(B3LYP) methods with basis set 6-311+G (d, p). The time-dependent TD-SCF method used to get UV-Visible spectrum, HOMO-LUMO energy gap, in gas, DMSO, and chloroform phases with 6-311+G (d, p) basis set. In the same way NMR chemical shift, NBO, Mulliken charges, NLO properties are also computed.

### OUTCOMES AND DISCUSSION

#### Conformational Structure Investigation

So as to achieve minimum energy arrangement of molecule 2I5P4O, the potential energy surface (PES) scan was done for 2I5P4O using Semi empirical AM1 method. The total energy of atoms as a function of C2-C3-C21-C13 and C2-C3-C12- O16 dihedral angles was taken for rotation. The dihedral angle was rotated in steps of 10 each step with  $36^\circ$ . For this rotation three global minimum positions have been obtained at  $0^\circ$ ,  $180^\circ$  and  $360^\circ$  for C2-C3-C12- O16 shown in the Fig.1 (a) which clearly reveals that these three positions corresponds to the global minimum energy (-0.0146) position. The rotational energies are presented in Table 1(a). For C2-C3-C21-C13 dihedral rotation, the minimum energy positions were obtained for  $36^\circ$  and  $216^\circ$  with energy of -0.0145 and -0.0146. The structure obtained for global minimum energy of -0.0146 is used for other calculations.



**Fig.1(a) : Global Minimum Energy Positions for 2-Imino-5-phenyl-4-oxazolidinone**

**Table 1(a). Angle of Rotation and Rotational Energies for 2-Imino-5-phenyl-4-oxazolidinone**

Angle of Rotation (degree)	Rotational Energy (hartree)	
	C2-C3-C12-C13	C2-C3-C12-O16
0	-0.0127	-0.0146
36	-0.0145	-0.0133
72	-0.0143	-0.0120
108	-0.0129	-0.0123
144	-0.0119	-0.0141
180	-0.0127	-0.0146
216	-0.0146	-0.0133
252	-0.0142	-0.0120
288	-0.0129	-0.0123
324	-0.0119	-0.0142
360	-0.0127	-0.0146

### Structural Analysis

The optimized geometrical parameters like lengths and angles between the atoms are calculated by HF and B3LYP method with 6-311+G (d, p) basis sets. The calculated and experimental values are presented in Table 1(b). The optimised geometrical structure of the title compound 2I5P4O is shown in the Fig 1(b). All the Carbon-Carbon bond lengths are 1.38 Å in HF and 1.39 Å in B3LYP; these demonstrations give no differentiation among the

single and double bond inside the ring. This is due to the overlapping of p-orbitals. Where as in CN bonds, two single bonds and one double bond with values 1.37, 1.40 and 1.25Å respectively. On comparing the results of HF and B3LYP, HF results are somewhat fewer than B3LYP. In the substitution group CC bond length is greater than other CC bond lengths. For C12-C13 and C3-C12 have bond length about 1.53 Å because these carbons are connected with oxygen. All the CH bond lengths are nearly in 1.08 Å.

Table 1(b) : Optimized Bond length and Angle for 2- Imino 5-phenyl 4-oxazolidinone

Bond Length(Å)	B3LYP/ 6-311+G(d,p)	HF/ 6-311+G(d,p)	<sup>a</sup> Experimental
C1-C2	1.3918	1.382	1.384
C1-C6	1.3949	1.3875	1.386
C1-H7	1.084	1.0752	0.95
C2-C3	1.3986	1.3905	1.401
C2-H8	1.084	1.0752	0.95
C3-C4	1.3953	1.3851	1.386
C3-C12	1.5156	1.515	1.504
C4-C5	1.3948	1.3881	1.386
C4-H9	1.0824	1.073	0.95
C5-C6	1.3925	1.3824	1.394
C5-H10	1.0841	1.0752	0.95
C6-H11	1.0841	1.0753	0.95
C12-C13	1.5374	1.5248	1.547
C12-O16	1.4372	1.4113	1.434
C12-H21	1.0949	1.0836	1.0
C13-N15	1.3765	1.3629	1.494
C13-O19	1.2046	1.1811	
C14-N15	1.402	1.3869	1.487
C14-O16	1.3602	1.3351	1.432
C14-N17	1.2592	1.2413	
N15-H20	1.0093	0.9942	
N17-H18	1.016	1.0006	
<b>Bond Angle (°)</b>			
C2C1C6	120.2023	120.1477	119.83
C2C1H7	119.6524	119.6972	
C6C1H7	120.1452	120.1551	
C1C2C3	120.0641	120.1687	120
C1C2H8	119.9723	119.8184	
C3C2H8	119.9589	120.0095	
C2C3C4	119.7638	119.6967	119.4
C2C3C12	119.0388	119.0004	
C4C3C12	121.1974	121.3005	122
C3C4C5	119.9118	119.9341	120
C3C4H9	119.717	120.0516	
C5C4H9	120.3656	120.0094	
C4C5C6	120.3461	120.3452	119.8
C4C5H10	119.522	119.5013	
C6C5H10	120.1317	120.153	
C1C6C5	119.7106	119.7054	119.8
C1C6H11	120.1126	120.1911	
C5C6H11	120.1765	120.1972	
C3C12C13	113.6121	113.7224	112.9

Bond Length(Å)	B3LYP/ 6-311+G(d,p)	HF/ 6-311+G(d,p)	<sup>a</sup> Experimental
C3C12O16	112.2332	112.231	
C3C12H21	110.3271	110.2941	
C13C12O16	104.1893	103.5909	102
C13C12C21	108.2072	108.253	
O16C12H21	107.9323	108.4111	
C12C13N15	104.0855	104.2548	102
C12C13O19	128.2854	128.2586	
N15C13O19	127.6241	127.4771	
N15C14O16	107.3648	107.3301	103
N15C14N17	131.3432	130.4852	
O16C14N17	121.2918	122.1847	
C13N15C14	113.0848	112.5911	106
C13N15H20	123.1186	123.3399	
C14N15H20	123.79	124.0497	
C12O16C14	111.2552	112.203	
C14N17H18	112.3398	112.2642	

<sup>a</sup>x-ray data taken from Reference [Ian Sean Campbell, Kate L. Edler, Raleigh W. Parrott II, Shawn R. Hitchcock and Gregory M. Ferrence\*ActaCrystallographica Section EMarch 2010]

Usually benzene ring has the hexagonal shape it has the bond angle of 120°. Here the benzene ring is substituted with imnooxazolidinone; due to this substitution the bond angle is lowered 1° from the hexagonal angle. Imnooxazolidinone has pentagon shape; it has the different bond angle varying from 104° to 131°. This variation is observed due to the substitution of amine and carboxylic groups. The calculated bond length and angles are compared with available x-ray data.

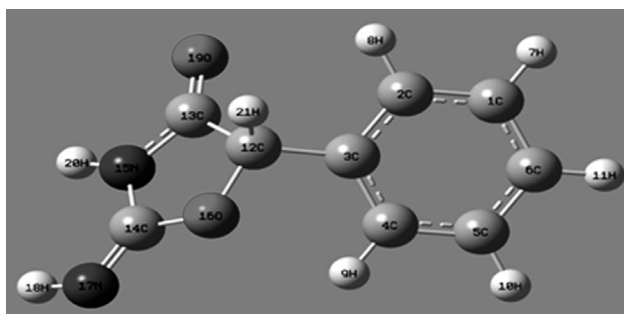


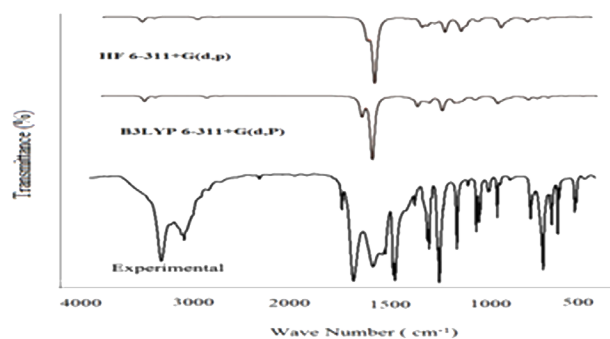
Fig 1(b) : Optimized Structure of 2-Imino-5-phenyl-4-oxazolidinone

## VIBRATIONAL ASSIGNMENTS

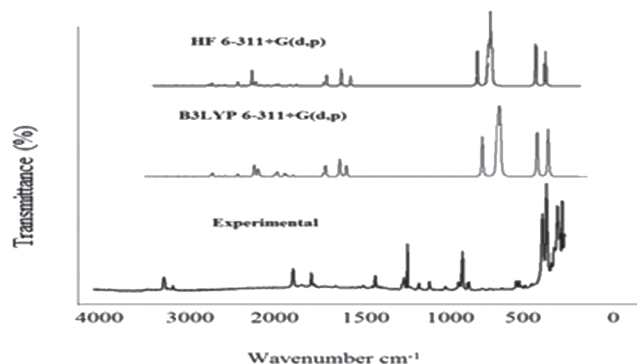
The molecule under study 2I5P4O has 21 atoms so it has 57 fundamental modes of vibrations and belongs to CS point group symmetry. These 57 normal modes are distributed as

$$\Gamma_{\text{Vib}} = 39 A' + 18 A''$$

A' represents the in the plane vibration and A'' represents out plane vibration. All these fundamental modes of vibration are active in both IR and Raman spectra. The experimental and computed frequency by means of HF and B3LYP methods with 6-311+G(d,p), basis sets are reported in the Table 2. For graphical comparison, the experimental and computed spectra are shown in the Fig 2 & 3 for FT-IR and FT-Raman respectively.



**Fig 2: Experimental and Computed FT-IR Spectra for 2-imino-5-phenyl-4-oxazolidinone**



**Fig 3: Observed and Computed FT-Raman Spectra for 2-imino-5-phenyl-4-oxazolidinone**

**Table 2: Detailed Vibrational Assignment for 2- Imino 5-phenyl 4-oxazolidinone4**

Modes	Symmetry Species	<sup>a</sup> Experimental		HF 6-311+G(d,p)		B3LYP 6-311G+(d,p)		<sup>b</sup> Vibrational assignment
		IR	Raman	Unscaled	Scaled	Unscaled	Scaled	
1	A'	3300s	-	3877	3516	3635	3573	NH v
2	A'	3200m		3783	3431	3543	3394	NH v
3	A'	3100m		3370	3056	3203	3068	CH v
4	A'	3050m	3060vw	3353	3040	3192	3058	CH v
5	A'	3030m	3030vw	3343	3031	3183	3049	CH v
6	A'		2960vw	3332	3022	3174	3041	CH v
7	A'	2950m	2950vw	3321	3012	3165	3032	CH v
8	A'	2800w		3228	2927	3044	2916	CH v
9	A'	1720w	1720vw	2020	1832	1834	1757	C=O v
10	A'	1700w	1670vw	1931	1752	1771	1697	C=N v
11	A'	1660vs	1620vw	1792	1625	1643	1615	C=C v
12	A'	1560s	1595vw	1766	1602	1625	1557	C=C v
13	A'	1480vs		1652	1498	1526	1462	C=C v
14	A'	1470vs		1598	1449	1481	1419	C-C v
15	A'	1390s	1350vw	1546	1402	1394	1335	C-C v
16	A'	1360m	1310vw	1504	1364	1360	1303	C-C v
17	A'	1290s	1290vw	1476	1339	1356	1299	C-C v
18	A'		1240vw	1448	1313	1341	1285	C-C v
19	A'	1230m		1440	1306	1305	1250	C-O v
20	A'	1220vs		1337	1212	1281	1227	C-Ov
21	A'		1200vw	1334	1210	1217	1196	C-N v
22	A'	1140m		1309	1187	1208	1157	C-N v
23	A'	1095m		1291	1171	1204	1153	NH β
24	A'	1050m	1040vw	1232	1117	1183	1133	NH β
25	A'	1040m		1196	1085	1111	1064	C-H β
26	A'	1030m		1170	1062	1079	1034	C-H β
27	A'	1020m	1010w	1159	1051	1049	1005	C-H β

Modes	Symmetry Species	<sup>a</sup> Experimental		HF		B3LYP		<sup>b</sup> Vibrational assignment
		IR	Raman	6-311+G(d,p)		6-311G+(d,p)		
				Unscaled	Scaled	Unscaled	Scaled	
28	A'		1000w	1118	1014	1045	1001	C-H $\beta$
29	A'	980w		1118	1014	1016	973	C-H $\beta$
30	A'		940vw	1105	1002	1009	967	C-H $\beta$
31	A'	930w		1081	980	993	976	C=O $\beta$
32	A'	910vw		1062	963	961	921	C=N $\beta$
33	A'	890vw		1044	947	943	903	C-O $\beta$
34	A'		870vw	1005	912	922	883	C-O $\beta$
35	A'	780m		951	863	867	831	C-N $\beta$
36	A'		770vw	946	858	861	825	C-N $\beta$
37	A''	700vs	690vw	862	782	766	734	NH $\gamma$
38	A''	670m	650w	826	749	755	723	NH $\gamma$
39	A''	630m	630vw	803	728	737	706	C-H $\gamma$
40	A''	620w	615vw	797	723	712	682	C-H $\gamma$
41	A''	610w		771	700	711	699	C-H $\gamma$
42	A''	540w	540vw	754	684	694	665	C-H $\gamma$
43	A''	530w		702	637	640	613	C-H $\gamma$
44	A''	500w		672	610	631	604	C-H $\gamma$
45	A''	450w		658	597	608	582	C=O $\gamma$
46	A''		490vw	599	544	555	532	C=N $\gamma$
47	A''		410vw	526	477	491	470	C-O $\gamma$
48	A''		320vw	513	466	477	457	C-O $\gamma$
49	A''		300vw	450	408	412	395	C-N $\gamma$
50	A''		270vw	429	389	391	375	C-N $\gamma$
51	A'		230vw	359	326	332	326	CCC $\beta$
52	A'		150m	280	254	259	248	CCC $\beta$
53	A'		140vs	232	211	215	206	CCC $\beta$
54	A''		100w	133	121	130	125	CCC $\gamma$
55	A''		95w	111	101	101	97	CCC $\gamma$
56	A''		60s	61	55	58	56	CCC $\gamma$
57	A''		50s	32	29	32	31	CCC $\gamma$

<sup>a</sup>vs- very strong; s-strong; m-medium; w- weak; vw very weak    <sup>b</sup> : $\nu$ -Stretching ,  $\beta$ -in-plane bending,  $\gamma$ -Out of plane bending

### C-H Vibrations

The expected region for aromatic C-H elongating vibrations lies between 3000-3100  $\text{cm}^{-1}$  [5-7], which is the area for identification of C-H elongating vibrations in aromatic benzene derivatives. The compound 2I5P4O have six bands detected at 3100, 3050, 3030, 2960, 2950 and 2800  $\text{cm}^{-1}$  are

allotted to C-H elongating vibrations. The last three bands is found to be in the lower range. Among the three the first two bands from the aromatic C-H elongation, the last band at 2800  $\text{cm}^{-1}$  is owing to the stretching of C-H present in the substitution of Iminooxazolidinone. From the observations the stretching of C-H is disturbed by the substitution.

Typically, the strongest absorptions for C–H in-plane and out-plane bending of aromatic compounds happen in the region 1300-1000  $\text{cm}^{-1}$  and 1000–675  $\text{cm}^{-1}$  respectively [8-12]. In the present situation, the in-plane bending vibrations of C–H are found at 1040, 1030, 1020, 1000, 980 and 940  $\text{cm}^{-1}$  in FT-IR and FT-Raman. Almost all the C–H in-plane bending vibrations are found to be in the expected region except last two bands. This indicates that the two C-H in-plane bending vibration corresponds to Oxazolidinone group. The out-plane bending vibrations are observed at 630, 620, 610, 540, 530 and 500  $\text{cm}^{-1}$ . The out-plane bending vibration of C-H is likewise affected by the surrounding atoms which lie lower than the characteristic region.

#### Carbon-Carbon modes

The elongating vibrations insidering are significant in benzene and its derivatives are extremely representative of the aromatic compound. The aromatic Carbon double and single bond elongating modes frequently happen in the range 1400-1625  $\text{cm}^{-1}$  [8], predominantly the bands among the range 1590-1650  $\text{cm}^{-1}$  [13] and 1590-1430  $\text{cm}^{-1}$  [14,15]. In the current study, the C=C stretching vibrations are detected at 1660, 1560 and 1480  $\text{cm}^{-1}$  with very strong intensity. The corresponding C-C stretching vibrations are found at 1480, 1390, 1360 1290 and 1240  $\text{cm}^{-1}$  with very strong intensity, which is beneath the predictable range. From these observations it is unblemished that the stretching vibrations inside the ring are disturbed greatly by the  $\text{NH}_2$  and  $\text{O}_2$  group. The Carbon-Carbon in out plane bending modes is appeared at 230, 150 and 140  $\text{cm}^{-1}$  and 100, 95, 60, and 50  $\text{cm}^{-1}$  correspondingly. Entirely the assignments connected to in-plane and out-plane ring bending mode are in coherent with the literature values [8-10].

#### Carbon-Nitrogen Modes

Usually, CN vibration assorted with other modes; hence it is very tricky to recognize CN vibration. Most of the ring C-H bending modes are mixed with CN modes. But in this current study, the CN stretching vibration is recognized undoubtedly with medium intensity at 1700  $\text{cm}^{-1}$  in FTIR and 1670  $\text{cm}^{-1}$  in FT-Raman allotted to Carbon Nitrogen double bond stretching and 1200 and 1140  $\text{cm}^{-1}$  in infrared region are allotted to Carbon Nitrogen single bond stretching modes. The in-plane and out-plane bending vibration of Carbon Nitrogen double bond is observed at 910 and 490  $\text{cm}^{-1}$  and Carbon Nitrogen single bond are observed at 780, 770 and, 300, 270  $\text{cm}^{-1}$  respectively. This observation is supported by the literatures [10]. According to the CN vibrations, there is no interference of other modes of vibrations and also they are in expected range.

#### Nitrogen Hydrogen Modes

The NH stretching vibration detected in the range 3300–3500  $\text{cm}^{-1}$  for all the primary aromatic amines [16]. The molecule under examination has two  $\text{NH}_2$  group in substitution. The NH stretching is perceived at 3300 and 3200  $\text{cm}^{-1}$  these assignment correlate well with the earlier reports [17]. NH In-Plane bending is occurs in 1095, 1090  $\text{cm}^{-1}$  and the Out-Plane NH bending vibrations are observed at 700, 670  $\text{cm}^{-1}$ . The whole N-H vibrations seemed within the prescribed region of the spectra. This interpretation indicates the leading character of the amine group.

#### Carbon Oxygen Modes

The pi bond among carbon and oxygen is responsible for carbon-oxygen double bond. The oxygen loan pair concludes the type of carbonyl group present. A strong absorption in the region 1740-1660  $\text{cm}^{-1}$  conform the presence of carboxylic acid [7]. The ketonic CO stretching bands are significantly less intense than acid. The



typical C=O stretching frequency in the current study seems at  $1720\text{ cm}^{-1}$  in FTIR and FT-Raman with feeble intensity. This observation shows that the wave number well within the expected range; also the intensity is not high as expected. The in-plane and the out-of-plane bending vibrations of CO are found at  $930$  and  $450\text{ cm}^{-1}$  respectively. All these values clearly indicate that C = O modes are not usually get affected by the other functional group, particularly CN or CC. The stretching C-O vibrations are found at  $1230$ ,  $1220\text{ cm}^{-1}$  and the in plane bending vibrations are at  $890$ ,  $870\text{ cm}^{-1}$ . The out of plane bending vibrations are found at  $410$  and  $320\text{ cm}^{-1}$ .

### FMO Analysis

The FMO (Frontier Molecular Orbitals) comprise of the highest occupied molecular orbitals (HOMO) and the lowest unoccupied molecular orbitals (LUMO). The Frontier Molecular Orbitals shows a significant part in the optical and electric properties of molecule, as well as in UV-VIS absorption spectra[18]. The HOMO is the electron donor LUMO is an electron acceptor. The energy gap of HOMO-LUMO determines chemical hardness, softness, reactivity, stability and optical polarizability of a molecule [19, 20]. In order to estimate the energetic activities of the 2I5P4O, quantum computational calculations were carried out in DMSO, chloroform and gas using B3LYP/6-311+G(d,p) basis set and are presented in Fig 4.

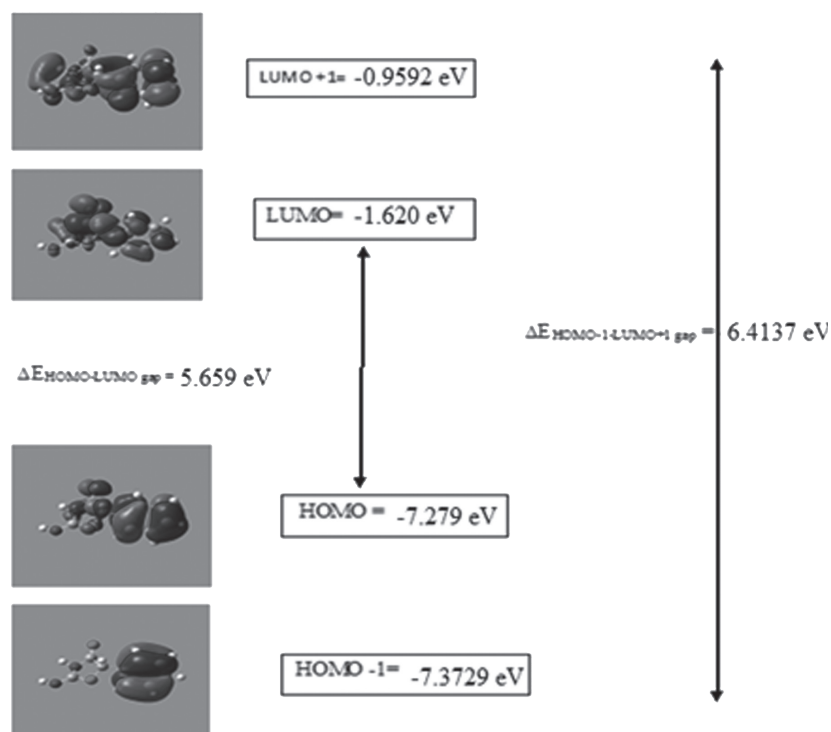


Fig 4 : Molecular Orbitals of 2-imino-5-phenyl-4-oxazolidinone

The computed energy value of HOMO is -7.2727eV in DMSO, -7.2513eV in chloroform, and -7.279eV in gas phase. The computed energy value of LUMO is -1.6324eV in DMSO, -1.6234eV in Chloroform, and -1.620eV in gas phase. The HOMO-LUMO energy gap is 5.640, 5.627, and 5.659eV in DMSO, Chloroform and gas, respectively which are presented in Table 3. The HOMO-LUMO energy gap elucidates the ultimate charge transfer occurs inside the molecule, which is key factor to influence the organic activity of

the molecule. Additionally, the declining value of the energy gap from the gas phase to solvent, expresses the molecular stability. Computed 3D plots at B3LYP/6311+G(d,p) level in gas phase for 2I5P4O are illustrated in Fig 4. This electronic absorption primarily pronounced by an electron excited to LUMO from HOMO, which resembles to the transition to first excited state from the ground state. Thus higher the value of HOMO-LUMO energy gap is basically a consequence of the small stabilization of LUMO.

**Table 3: Computed Energy Values of 2- Imino 5-phenyl 4-oxazolidinonein different phase**

TD-DFT/B3LYP/ 6-311+G(d,p)	DMSO	Chloroform	Gas
Etotal (Hartree)	-607.901	-607.902	-604.266
EHOMO (eV)	-7.272	-7.251	-7.279
ELUMO (eV)	-1.632	-1.623	-1.620
$\Delta$ EHOMO-LUMO gap (eV)	5.64	5.63	5.65
Chemical hardness $\eta$ (eV)	2.82	2.81	2.82
Electronegativity $\chi$ (eV)	4.45	4.43	4.49
Chemical Softness $\xi$ (eV)	11.28	11.25	11.32
Electrophilicity index $\omega$ (eV)	3.52	3.49	3.57
Dipole moment (Debye)	1.1699	1.1012	0.9557

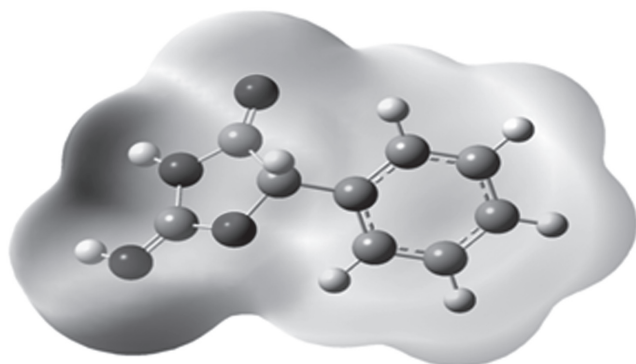
One of the vital electronic properties of the compound is dipole moment, if the molecule having high amount of dipole moment it will have very strong intermolecular interactions. From the Table 3 the computed dipole moment values increase from gas phase (0.9557debye) to solvent phases (1.1012 in chloroform and 1.1699 in DMSO). The chemical hardness, softness, electronegativity and electrophilicity index are presented in Table 3.

### ELECTROSTATIC POTENTIAL MAP ANALYSIS

The ultimate extensive usage of computed molecular electrostatic potentials has been in relation to reactive behaviour. Molecular electrostatic potentials have been extensively used in biochemistry and pharmacology to recognize

specific patterns of positive and negative potentials that either stimulate or prevent specific natures of biological activities. Nucleophilic region of each molecule would interact favourably with the regions of most positive electrostatic potential on the other, exclusively the surface indigenous maxima. The 3D plots of molecular electrostatic potential (MEP) of 2I5P4O is illustrated in Fig 5. In MEP, negative region represented as red colour which is favoured location for electrophilic attack, the positive region represented as green colour which favoured site for nucleophilic attack. The significance of MEP is the fact that it concurrently displays molecular properties in relations of colour code, and is most valuable parameter in investigation of molecular dynamics with its physical and chemical property [21-24]. The various electrostatic potential surface are represented by various colours, potential

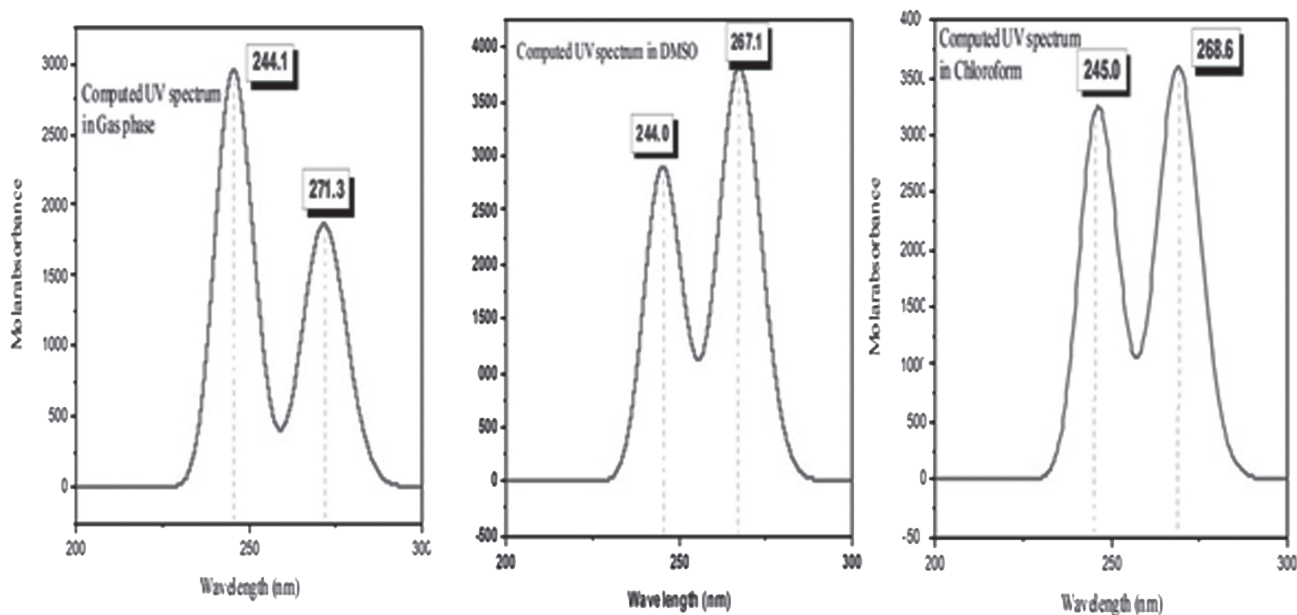
decreases in the order blue > green > yellow > orange > red. The colour code of for 2I5P4O maps is in the range between -0.02731 a.u. (deep red) to 0.02731 a.u. (deep blue). In 2I5P4O molecule electrophilic attack prone to the region around the atoms O19 and N17 and the nucleophilic attack prone to region around H18 and H20. The neutral regions are found around the benzene ring.



**Fig 5: MEP surface of 2-imino-5-phenyl 4-oxazolidinone**

## UV-VISIBLE SPECTRAL ANALYSIS

The time dependent self-consistent field (TD-SCF) calculations are performed for 2I5P4O using B3LYP method with 6-311+G (d, p) basis set, to understand electronic transitions. The computed excitation energies with absorption wavelengths corresponding oscillator strengths and dipole moments are specified in Table 4. The strong transitions observed at 271.32, 268.68 and 267.15 nm with an oscillator strength 0.0172, 0.0073 and 0.066 in gas, chloroform and in DMSO phase respectively are allotted to  $\pi-\pi^*$  transition. The other calculated counterparts are tabulated in Table 4. The stimulated UV-Visible absorption band for 2I5P4O is revealed in Fig 6.



**Fig 6: The UV-VIS Absorption Spectrum of 2-imino-5-phenyl 4-oxazolidinone in Gas and Solvent Phase.**

Table 4: Theoretical UV-VIS Absorption Parameters of 2- Imino 5-phenyl 4-oxazolidinone Computed Using TD-SCF Method in Different Phases

Phase	Absorption Wavelength $\lambda$ (nm)	Excitation Energy E (eV)	Oscillator Strength (f)	Major Contributions
Gas	271.32	4.5697	0.0172	H $\rightarrow$ L 45% H-2 $\rightarrow$ L 38%
	248.53	4.9887	0.0078	H-1 $\rightarrow$ L 61%
	244.16	5.0779	0.0213	H $\rightarrow$ L 35% H-2 $\rightarrow$ L 31%
Chloroform	268.68	4.6146	0.0330	H $\rightarrow$ L 55% H-2 $\rightarrow$ L 32%
	249.95	4.9604	0.0073	H-1 $\rightarrow$ L 79%
	245.04	5.0597	0.0248	H-2 $\rightarrow$ L 43% H-1 $\rightarrow$ L 11%
DMSO	267.15	4.6409	0.0351	H $\rightarrow$ L 57% H-2 $\rightarrow$ L 29%
	249.34	4.9726	0.066	H-1 $\rightarrow$ L 80%
	244.05	5.0803	0.0224	H-2 $\rightarrow$ L 45% H $\rightarrow$ L 35%

H $\rightarrow$  HOMO: L $\rightarrow$  LUMO

### MULLIKEN CHARGE DISTRIBUTION

The distribution of Mulliken charge is the important parameters of the molecule and it stipulates how the electronic assembly varies in atomic movement, so it is directly connected to the type of chemical bonds existing in the molecule. It influences electronic structure of the molecular system by affecting the dipole moment, Polarizability, etc., In Table 5 Mulliken charge distribution of 2I5P4O molecule is calculated using HF and B3LYP level's with same basis sets are tabulated in Table 5. Comparative illustrations of charges distribution on each atom are exposed in Figure 7.

Among the carbon atoms, C13, C14 and C3 are positive than the other carbon atoms. In the case of C14; two methods have predicted contrary results and C3 is most positively charged. In C3 position the substitutional group attached which is the reason for its high positivity of atom C3. Among the negative carbon atoms, C2, C5 and C12 are comparatively more negative than the other atoms. Among the hydrogen atoms, H18, H20, H21 are more positive than other atoms. Among these hydrogen atoms H20 has highest value, which is connected with Nitrogen atom.

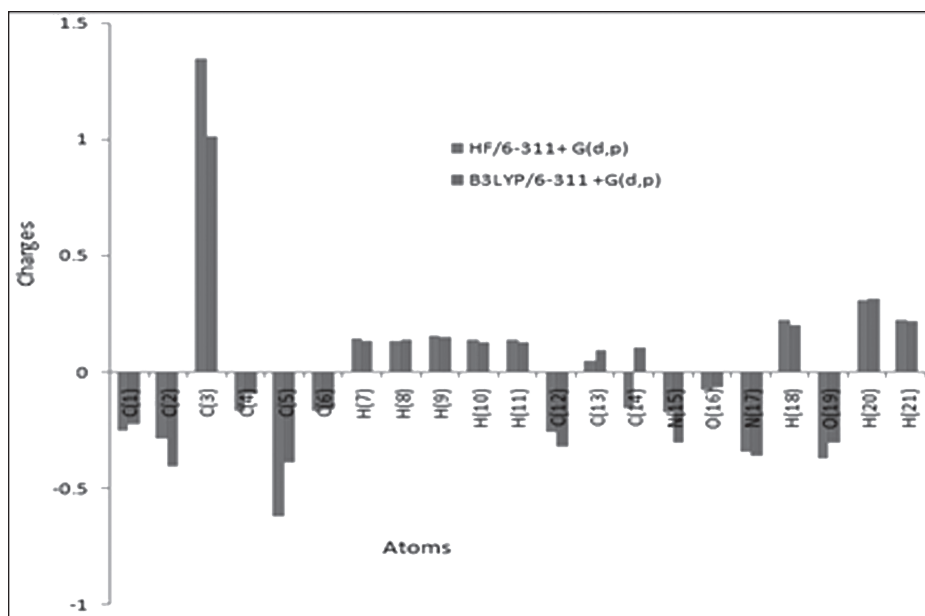


Fig 7: Graphical Illustrations of Charges Distribution of 2-imino-5-phenyl 4-oxazolidinone

Table 5: Mulliken Atomic Charges of 2-Imino-5-phenyl-4-oxazolidinone

Atoms	HF/6-311+ G(d,p)	B3LYP/6-311 +G(d,p)
1C	-0.248881	-0.222088
2C	-0.285665	-0.407174
3C	1.34661	1.014018
4C	-0.164220	-0.094537
5C	-0.620375	-0.385436
6C	-0.167783	-0.163210
7H	0.142358	0.131192
8H	0.131254	0.137913
9H	0.155456	0.151671
10H	0.141824	0.130448
11H	0.139431	0.128740
12C	-0.259661	-0.319590
13C	0.051424	0.091877
14C	-0.158095	0.102791
15N	-0.174015	-0.303863
16O	-0.077192	-0.065885
17N	-0.344172	-0.360139
18H	0.226796	0.203874
19O	-0.368200	-0.302595
20H	0.310875	0.314677
21H	0.222232	0.217317

## NON -LINEAR OPTICAL STUDIES

Non Linear Optic (NLO) parameters the polarizability and first order hyperpolarizability of the 2I5P4O compound were computed using the B3LYP method with 6-311+G(d,p) basis set to investigate the relationships among molecular structures.

The  $\alpha_{xx}$ ,  $\alpha_{xy}$ ,  $\alpha_{yy}$ ,  $\alpha_{xz}$ ,  $\alpha_{yz}$ ,  $\alpha_{zz}$  and  $\beta_{xxx}$ ,  $\beta_{xxy}$ ,  $\beta_{xyy}$ ,  $\beta_{yyy}$ ,  $\beta_{xxz}$ ,  $\beta_{xyz}$ ,  $\beta_{yyz}$ ,  $\beta_{xzz}$ ,  $\beta_{yzz}$ ,  $\beta_{zzz}$  are tensors related to polarizability and

hyperpolarizability. They acquired from frequency output file of Gaussian. The  $\alpha$  and  $\beta$  values has been converted into electro static units (esu), they are in atomic unit (a.u). The total dipole moment ( $\mu$ ) of molecule, linear polarizability ( $\alpha$ ) and first-order hyperpolarizability ( $\beta$ ) have been explained in detail previous studies [25,26] and Density Functional Theory has been comprehensively used as technique to examine the organic NLO properties of the materials [27-31].

$$\alpha_{tot} = \frac{1}{3} (\alpha_{xx} + \alpha_{yy} + \alpha_{zz})$$

$$\langle \beta \rangle = \left[ (\beta_{xxx} + \beta_{xxy} + \beta_{xxz})^2 + (\beta_{yyy} + \beta_{yyz} + \beta_{yxx})^2 + (\beta_{zzz} + \beta_{zxx} + \beta_{zyy})^2 \right]^{\frac{1}{2}}$$

$$\mu_{tot} = (\mu_x^2 + \mu_y^2 + \mu_z^2)$$

The NLO properties of the molecule depend on the value of dipole moment, molecular polarizability and first hyper polarizability. In Table 6, the calculated polarizability and hyper polarizability and the electronic dipole moment  $\mu_x$ ,  $\mu_y$ ,  $\mu_z$  and total dipole moment for 2I5P4O are listed. The  $\mu_{tot}$  is measured using  $\mu_x$ ,  $\mu_y$ ,  $\mu_z$  [32]. From the table, it has been found that polarizability and hyperpolarizability and dipole moment of the 2I5P4O are active. So that 2I5P4O can be used to make NLO materials.

**Table 6: NLO Parameters of 2-Imino-5-phenyl-4-oxazolidinone**

Parameter	a.u.	Parameter	a.u.
$\alpha_{xx}$	-60.9836	$\beta_{xxx}$	-30.6564
$\alpha_{yy}$	-10.6163	$\beta_{yyy}$	-13.9614
$\alpha_{zz}$	-2.9038	$\beta_{zzz}$	1.6249
$\alpha_{xy}$	-4.9883	$\beta_{xyy}$	19.9622
$\alpha_{yz}$	6.3783	$\beta_{xxy}$	24.0561
$\alpha_{xz}$	9.031	$\beta_{xxz}$	-36.2679
$\alpha_{tot}$	-24.8346	$\beta_{xzz}$	-6.1858
$\Delta\alpha$	58.5336	$\beta_{yzz}$	6.4327
$\mu_x$	0.3176	$\beta_{yyz}$	-0.8659
$\mu_y$	0.3189	$\beta_{xyz}$	-0.5282
$\mu_z$	0.8430	$\beta_{tot}$	42.6494
$\mu_{tot}$	0.9556		

## THERMODYNAMIC PROPERTIES

The values of thermodynamical factors like zero point vibrational energy etc., of 2I5P4O at 298.15 K in lower energy state are tabulated in Table 7. The significant difference in Zero-Point

Vibrational Energies (ZPVEs) found. The HF method shows higher ZPVE than DFT/B3LYP method. The highest value of ZPVE of 2I5P4O is 453600.2 joule mol<sup>-1</sup> computed by HF/6-311++G(d,p) while the lowest value is 421428.7 joule mol<sup>-1</sup> computed by B3LYP/6-311++G(d,p).

**Table 7: The computed Thermodynamical Properties of 2- Imino 5-phenyl 4-oxazolidinone Molecule at 298.15K**

Thermodynamical Factors	DFT	HF
SCF Energy	-607.90158(a.u)	-604.26658(a.u)
ZPVE (joule mol <sup>-1</sup> )	421428.7(joule mol <sup>-1</sup> )	453600.2(joule mol <sup>-1</sup> )
Rotational Constants A	1.65176(GHz)	1.68706(GHz)
Rotational Constants B	0.56131(GHz)	0.56923(GHz)
Rotational Constants C	0.45083(GHz)	0.45765(GHz)
Specific heat capacity (C <sub>v</sub> )	39.822(cal mol <sup>-1</sup> K <sup>-1</sup> )	36.525(cal mol <sup>-1</sup> K <sup>-1</sup> )
Entropy (S)	102.175(calorie mole <sup>-1</sup> K <sup>-1</sup> )	99.785(calorie mole <sup>-1</sup> K <sup>-1</sup> )
Dipole Moment	1.3593(Debye)	1.3822(Debye)
Enthalpy (KCal/Mol)	107.167	114.438

Dipole moment replicates the charge distribution in a molecule and is assumed as a vector quantity. Consequently, it is the significant factor to demonstration of charge drive through the molecule. The centre of positive and negative charge decides the position of the dipole moment vector in a molecule. The result obtained from HF and DFT computation shows lowest dipole moment was observed for DFT than HF for 2I5P4O. Based on vibration, the statistical thermodynamic functions like heat capacity (C), entropy (S), and enthalpy changes ( $\Delta H$ ) for 2I5P4O were computed and tabulated in Table 8. From the Table 8, it can be observed that these functions are increasing with increase in temperature in steps of 50K upto 250

K. This is due to the molecular vibration increase with temperature [33]. The relationships between thermodynamic functions are fitted by quadratic equations.

$$C = 5.2446 + 0.07596T - 1.65886 \times 10^{-4} T^2$$

(R<sup>2</sup> = 0.9999)

$$S = 51.0506 + 0.2057T - 1.66514 \times 10^{-4} T^2$$

(R<sup>2</sup> = 0.9995)

$$H = 99.3134 + 0.0026T - 6.05714 \times 10^{-5} T^2$$

(R<sup>2</sup> = 0.9998)

The comparable fitting factors (R<sup>2</sup>) are 0.9999, 0.9995 and 0.9998. The graphical relationships are shown in Fig. 8.

Table 8: Thermodynamic Properties of 2-Imino-5-phenyl-4-oxazolidinone at Various Temperatures T(K)

Temperature (kelvin)	Heat Capacity (calorie mole <sup>-1</sup> K <sup>-1</sup> )	Entropy (calorie mole <sup>-1</sup> K <sup>-1</sup> )	Enthalpy Change (kcalorie mole <sup>-1</sup> )
50	9.478	60.737	99.581
100	14.476	70.351	100.206
150	20.316	78.095	101.072
200	27.168	85.239	102.224
250	34.563	92.239	103.766

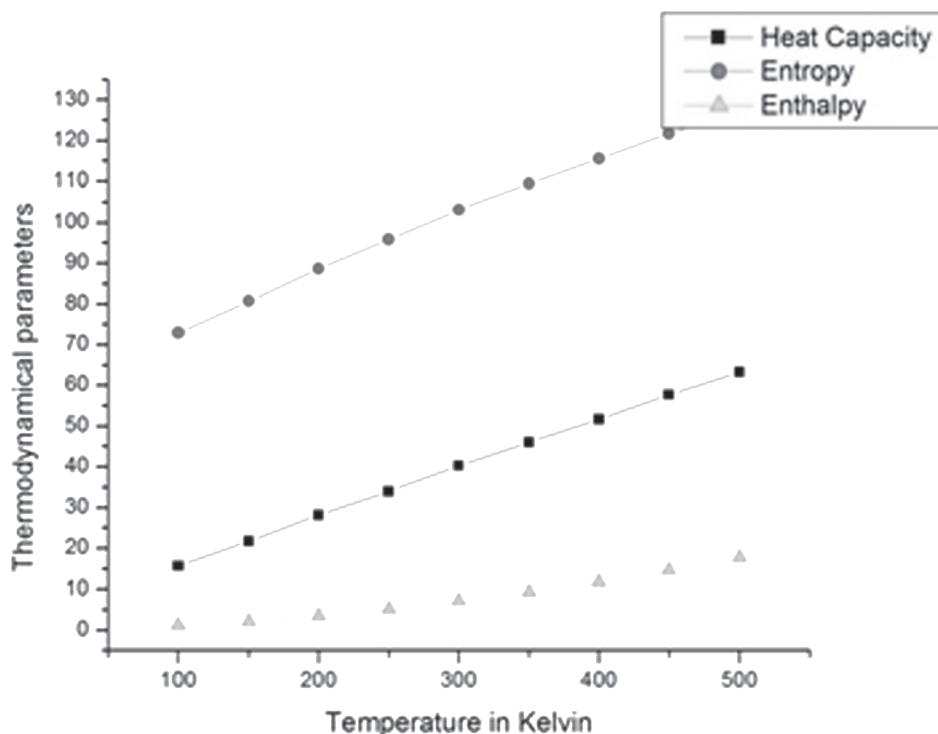


Fig :8 Thermo Dynamical Properties of 2-imino-5-phenyl 4-oxazolidinone

This thermodynamic relation gives valuable information for the additional study on the 2I5P4O. According to the second law of thermodynamics these thermodynamic relations, estimate directions of chemical reactions in thermo chemical field. And they can also be used to compute the other thermodynamic energies. Entropy (S), Enthalpy changes ( $\Delta H$ ) and Heat capacity (C) are increased with respect to temperature is shown in the Fig.8. Hence in the form of vibrational energy the 2I5P4O is capable of storing the kinetic energy

## NMR SHIFT EXAMINATION

The proton i.e. hydrogen H and Carbon13 chemical shift of the title molecule were performed with different solvents like DMSO, ETHANOL, METHANOL and GAS phase by B3LYP/6-311+G(d,p) method. The experimental proton and carbon13 NMR spectrum of the compound 2I5P4O is shown in Fig 9 and 10. Corresponding proton and carbon 13 NMR values for 2I5P4O are given in Table 9. Chemical shifts were calculated in parts per million (ppm) compare to Trimethylsilane



(TMS) for proton and carbon 13 NMR spectra. Affording to results obtained is in correlation with the experimental outcomes.

The maximum chemical shift is observed for the Carbon atom at 13 positions which is attached to the oxygen atom has shift of 202.631ppm in solvent phase and 174.4ppm for gas phase. C14 also have the maximum value 179.679 ppm

which is connected with electronegative nitrogen and oxygen atoms. The minimum chemical shift is observed at C12 is attached to oxygen with single bond having the chemical shift of 89.5438 ppm. The remaining carbon atoms are having the chemical shift values around 130 to 140 ppm.

**Table 9: Computed and Experimental NMR Shift (1H and 13C NMR) of 2- Imino 5-phenyl 4-oxazolidinone**

Atom	Observed Chemical Shift	Computed chemical Shift (ppm)			
		B3LYP/6-311+G(2d,p)			
		GAS	ETHANOL	METHANAL	DMSO
C1	134.46	132.926	135.237	134.901	135.257
C2	126.18	130.12	132.595	132.594	132.593
C3	134.46	139.183	144.29	144.295	144.3
C4	126.18	127.571	130.865	130.858	130.855
C5	128.60	132.926	134.888	135.976	135.987
C12	82.33	85.0345	89.543	89.5438	89.5442
C13	186.35	174.404	202.583	202.631	202.678
C14	176.72	158.43	179.646	179.679	179.712
H7	7.15	7.5242	7.6309	7.6342	7.6375
H8	7.58	7.7248	7.5812	7.5838	7.5633
H9	7.58	7.9202	7.8808	7.882	7.8837
H10	7.15	7.5575	7.6557	7.6587	7.6618
H11	7.15	7.5012	7.5567	7.56	7.5863
H18	8.63	5.7442	8.5408	8.5449	8.5489
H20	5.713	5.7385	6.3659	6.3797	6.3934
H21	5.713	5.6453	5.357	5.3617	5.3661

Among the hydrogen atoms H18 is 8.5449 ppm which is attached to nitrogen atom (N17) so the shift is large. The lowest value is obtained for 21H and 20H as 5.3617 & 6.3797 ppm respectively

because of the attachment of C-O & C-N. The remaining hydrogen atoms have the values from 7.56 to 7.888 ppm.

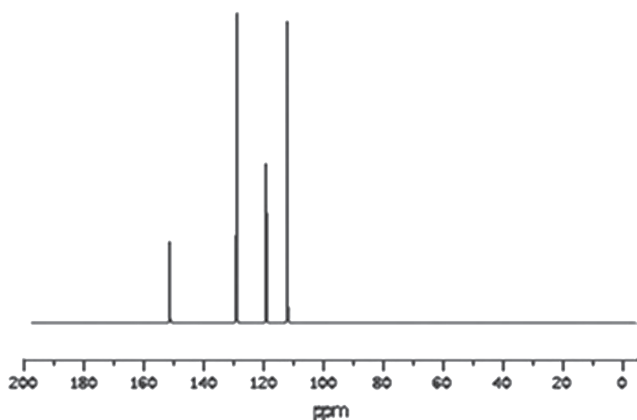


Fig 9: C 13 NMR for 2-Imino-5-phenyl 4-oxazolidinone

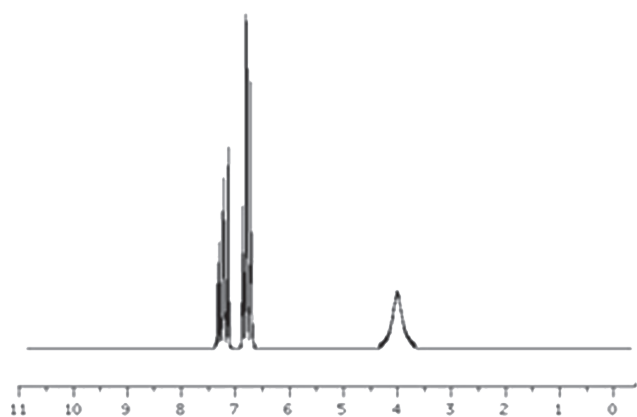


Fig 10: H1 NMR for 2-Imino-5-phenyl 4-oxazolidinone

## NATURAL BOND ORBITAL STUDY

To explain charge transfer and orbital interaction among the bonds in a molecular system natural bond analysis is required. From earlier report [34,35], orbitals of electron donor and acceptor and their interrelating energies are obtained by the second order perturbation theory of Fock matrix. The larger the value of stabilization energy, the more intensive is the interaction between electron donors and acceptor levels. The Lewis type bonding orbital and Non-Lewis type antibonding orbital resemble to donor-acceptor stabilization interaction due the delocalization of electron density between them.

The various conceivable donor and acceptor orbitals, bond types and their occupancy value for 2I5P4O are presented in Table 10. The probability of transitions indicates the stabilisation energy E2 values of different transitions. Affording to energy values E(2) the subsequent transitions are most possible; 1. C1-C6  $\rightarrow$  C2-C3 gives 20.78 Kcal/mol, ( $\pi$ - $\pi^*$ ), 2. C2-C3  $\rightarrow$  C4-C5 gives 20.08 Kcal/mol, ( $\pi$ - $\pi^*$ ), 3. C4-C5  $\rightarrow$  C2-C3 gives 21.18 Kcal/mol, ( $\pi$ - $\pi^*$ ). 4. Lone Pair N15  $\rightarrow$  C13-O19 (23.17 Kcal/mol, n- $\sigma^*$ ) 5. Lone Pair O19  $\rightarrow$  C13-N15 (25.07 Kcal/mol, n- $\pi^*$  type).

Table 10: Natural Bonding Orbital of 2- Imino 5-phenyl 4-oxazolidinone

Donor	Bond type	Occupancy	Acceptor	Bond type	Occupancy	Energy E(2) kcal/mol	Energy difference E(j)-E(i) a.u.	Polarized energy F(i,j) a.u.
C 1 - C 2	$\sigma$	1.97778	C 1 - C 6	$\sigma^*$	0.01548	2.41	1.26	0.049
C 1 - C 2			C 2 - C 3	$\sigma^*$	0.02153	3.32	1.26	0.058
C 1 - C 2			C 2 - H 8	$\sigma^*$	0.01274	1.05	1.15	0.031
C 1 - C 2			C 3 - C 12	$\sigma^*$	0.03404	3.74	1.06	0.056
C 1 - C 6	$\sigma$	1.98043	C 1 - C 2	$\sigma^*$	0.01474	2.47	1.26	0.05
C 1 - C 6			C 5 - C 6	$\sigma^*$	0.01600	2.61	1.28	0.052
C 1 - C 6	$\pi$	1.65495	C 2 - C 3	$\pi^*$	0.02153	20.78	0.28	0.068
C 1 - C 6			C 4 - C 5	$\pi^*$	0.31883	19.65	0.28	0.066

Donor	Bond type	Occupancy	Acceptor	Bond type	Occupancy	Energy E(2) kcal/mol	Energy difference E(j)-E(i) a.u.	Polarized energy F(i,j) a.u.
C 2 - C 3	$\sigma$	1.97473	C 1 - C 2	$\sigma^*$	0.01474	2.81	1.27	0.053
C 2 - C 3			C 3 - C 4	$\sigma^*$	0.02314	3.79	1.27	0.062
C 2 - C 3			C 3 - C 12	$\sigma^*$	0.03404	1.14	1.06	0.031
C 2 - C 3			C 12 - O 16	$\sigma^*$	0.02509	0.88	0.93	0.026
C 2 - C 3	$\pi$	1.66520	C 1 - C 6	$\pi^*$	0.32572	19.19	0.28	0.066
C 2 - C 3			C 4 - C 5	$\pi^*$	0.015	20.08	0.28	0.068
C 2 - C 3			C 12 - C 13	$\sigma^*$	0.03283	3.29	0.58	0.042
C 2 - C 3			C 12 - O 16	$\sigma^*$	0.03001	1.61	0.48	0.027
C 3 - C 4	$\sigma$	1.97372	C 2 - C 3	$\sigma^*$	0.02314	3.74	1.27	0.062
C 3 - C 4			C 3 - C 12	$\sigma^*$	0.03404	1.23	1.06	0.032
C 3 - C 4			C 4 - C 5	$\sigma^*$	0.015	2.86	1.27	0.054
C 3 - C 12	$\sigma$	1.96506	C 1 - C 2	$\sigma^*$	0.01474	2.14	1.2	0.046
C 3 - C 12			C 2 - C 3	$\sigma^*$	0.02153	1.31	1.2	0.036
C 3 - C 12			C 3 - C 4	$\sigma^*$	0.02314	2.56	1.28	0.051
C 3 - C 12			C 4 - C 5	$\sigma^*$	0.015	2.2	1.21	0.046
C 3 - C 12			C 12 - C 13	$\sigma^*$	0.07286	0.78	0.96	0.025
C 3 - C 12			C 13 - N 15	$\sigma^*$	0.08338	0.59	0.95	0.021
C 3 - C 12			C 13 - O 19	$\sigma^*$	0.01378	2.63	0.61	0.037
C 3 - C 12			C 14 - O 16	$\sigma^*$	0.0718	1.13	0.87	0.028
C 4 - C 5	$\sigma$	1.65675	C 3 - C 4	$\sigma^*$	0.02314	3.36	1.26	0.058
C 4 - C 5			C 3 - C 12	$\sigma^*$	0.03404	3.38	1.06	0.056
C 4 - C 5			C 5 - C 6	$\sigma^*$	0.01568	2.43	1.26	0.049
C 4 - C 5	$\pi$	1.65371	C 1 - C 6	$\pi^*$	0.32572	20.36	0.28	0.067
C 4 - C 5			C 2 - C 3	$\pi^*$	0.36058	21.18	0.28	0.069
C 5 - C 6	$\sigma$	1.97995	C 1 - C 6	$\sigma^*$	0.01548	2.43	1.26	0.049
C 5 - C 6			C 4 - C 5	$\sigma^*$	0.015	2.47	1.26	0.05
C 12 - C 13	$\sigma$	1.97463	C 2 - C 3	$\sigma^*$	0.02153	0.05	1.3	0.22
C 12 - C 13			C 3 - C 12	$\sigma^*$	0.03404	1.2	0.7	0.32
Lp(1) - N 15	n	1.75114	C 13 - O 19	$\sigma^*$	0.01378	23.17	0.36	0.082
Lp(1) - N 15			C 14 - N 17	$\sigma^*$	0.0487	9.54	0.45	0.06
Lp(2) - O 16	n	1.86211	C 14 - N 17	$\pi^*$	0.1671	10.87	0.41	0.06
Lp(1) - N 17	n	1.89887	C 14 - N 17	$\sigma^*$	0.0487	17.13	0.65	0.095
Lp(2) - O 19	n	1.97952	C 12 - C 13	$\pi^*$	0.20163	16.91	0.06	0.092
Lp(2) - O 19			C 13 - N 15	$\pi^*$	0.08338	25.07	0.59	0.011

## CONCLUSION

Structural parameters of the 2I5P4O is analysed using HF and B3LYP methods with 6-311+G (d,p) basis sets. The CC bonds around phenyl ring are same. The other C-C bond lengths in substitution are different and also is higher than that the ring CC. A complete vibrational study of the title molecule is performed and also proper assignments were made. From the assignments it is found that Carbon-Hydrogen stretching and bending modes are altered by the substitution. Nitrogen-Hydrogen stretching vibrations are not altered by other modes. The very small difference observed between experimental and calculated wave numbers. Therefore, the outcomes obtained for 2I5P4O indicates that B3LYP methods is trustworthy for the prediction of both infrared and Raman spectra.

Theoretically computed entropy, heat capacity and enthalpy for 2I5P4O are increasing with increase in temperature. This is due to the molecular vibration increases with increase in temperature. So as to understand electronic transitions for 2I5P4O, TD-SCF calculations performed in gas and solvent (DMSO and chloroform) phase. The electronic spectrum corresponds to the  $\pi$ - $\pi^*$  transition. NBO analysis is also done for the title molecule which is used predict the charge transferring occurs between bonding and antibonding orbitals. NMR chemical shift were computed and compared with experimental chemical shift. Using MEP, the reactive site of the molecule was predicted. NLO property of the title molecule also analysed. The outcomes of this investigation aid researchers to make additional investigation and synthesis of new compound.

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