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The Sapience

Vibrational Electronic NBO and NLO Properties of Resorcinol by using DFT Method

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Abstract

In this paper using combination of DFT /6-31G(d) theory and basis set calculations are performed to explore its vibrational structural and optical properties of resorcinol. A good correlation is shown between experimental and calculated vibrational frequencies. Geometry optimization has been done without any symmetry constrain .Using combination of theory and basis set calculate the vibrational spectra, dipole moment (μ), polarizability (α), and the first static hyperpolarizability (β) and NBO analysis of the title molecule, based on the finite field approach. The vibrational frequencies associated with ground state optimized geometry have been evaluated with 6-31G (d).

Keywords: Vibrational Spectra; Density functional theory; NBO analysis, NLO analysis.

1. Introduction

After the decades of theoretical evolution, algorithm improvement, and computational advances, the theoretical investigations of the electronic structure of matter now, offer computational simulation of new materials, a better understanding of the structure, formed by the atoms of materials, in addition to describing the great variety of phenomena observed. Comprehensive understanding of the electronic properties of a solid system has become an indispensable part of materials research nowadays, for the underlying electronic structure, affects the materials properties in a significant way. There has been a major attention in solving chemical problems like molecular geometries, spectroscopic signatures, transition states, and various thermodynamic properties using the tools of Quantum Chemistry over the last three decades [1-11], Quantum chemistry is a branch of theoretical chemistry which applies quantum mechanics and to address problems in chemistry. Quantum chemistry lies on the border between chemistry and physics. Thus, significant contributions have been made by scientists from both fields. It has a strong and active overlap with the field of atomic physics and molecular physics, as well as physical chemistry.

Resorcinol crystallizes from benzene as colorless needles that are readily soluble in water, alcohol, and ether, but insoluble in chloroform and carbon disulfide. It reduces Fehling's solution and ammoniacal silver solutions. It does not form a precipitate with lead acetate solution, as does the isomeric pyrocatechol. Iron (III) chloride colors its aqueous solution a dark-violet, and bromine water precipitates tribromoresorcin. These properties are what give it its use as a colouring agent for certain chromatography experiments. Sodium amalgam reduces it to dihydroresorcin, which when heated to 150 to 160°C with concentrated barium hydroxide solution gives γ-acetylbutyric acid (D. Vorlgnder); when fused with potassium hydroxide, resorcinol yields phloroglucin, pyrocatechol, and diresorcin. It condenses with acids or acid chlorides, in the presence of dehydrating agents, to oxyketones, e.g., with zinc chloride and glacial acetic acid at 145°C it yields resacetophenone (HO)2C6H3~CO.CH3.[12] With the anhydrides of dibasic acids, it yields fluoresines. When heated with calcium Chloride ammonia to 200°C it yields meta-dioxydiphenylamine [13]. With sodium nitrate it forms a water-soluble blue dye, which is turned red by acids, and is used as an indicator, under the name of lacmoid [14]. Title molecule is well known medicinal compound so in the present study, the experimental FT-IR frequencies of the title molecule are compared with theoretical frequencies obtained by DFT/B3LYP method. To gain a better understanding of the performance and limitation of DFT/B3LYP method, as a general approach to the vibrational problems of organic molecules, we calculated harmonic frequencies of title molecule by this method and compared these results with observed fundamental vibrational frequencies. The purpose of this study assumes importance because of the further work on resorcinol in which presumably some alteration by chemical response such as oxidation/reduction on polyfunctional bioactive natural product will engender new reactive site in the molecule.

2. Computational Methods

Initial geometry was generated from standard geometrical parameters and was minimized without any constraint in the potential energy surface. Geometry optimization has been done without any symmetry constrain [15]. The gradient corrected DFT/B3LYP theory along with6-31G(d) basis set has been employed for the computation of molecular structure, vibrational frequencies, HOMO-LUMO, and energies of the optimized structures, using GAUSSIAN 09 [15]by combining the results of the GAUSSVIEW'S program.

3. Results and Discussions

3.1 Geometry Optimization

Optimized parameters of Resorcinol calculated by combination of DFT/6-31 G(d) method and basis set are listed in Table 1 in accordance with the atom numbering scheme as shown in Figures 1. Local minimum energies are obtained -380.4147 for Resorcinol. Resorcinol has C_1 point group symmetry. In Resorcinol contained a benzene ring with two hydrogen replaced by hydroxyl group. For Resorcinol C–C bond distances are found to be in the range from Resorcinol. 1.38 Å while bond length of O-H bond are 0.94 Å In case of C-H bond distances, they lie in the range 1.07 Å The angular changes in benzene ring geometry have also proved to be a sensitive indicator of the interaction between the substituent and the benzene ring [17]. The structural changes in the carbon skeleton involve both, the bond distances and bond angles. The data reflects the well-known trends observed for various substituents: groups with π-acceptor substituent tend to increase in α_{ipso}, decrease α_{ortho} and this results in a small increase in α_{para}, e.g., in the title molecule the bond angle between (α_{ipso})C5-C4-C3 is 120.8^0 and <C4-C5-C6 (α_{ortho}) is 118.6^0.All carbon in benzene ring are SP^2 hybridized so bond angle between all carbon become 120^0 but angular changes in benzene ring geometry have also proved to be a sensitive indicator of the interaction between the O-H substituent and the benzene ring α_{ipso} is increase 120^0 to120.8^0 and α_{ortho} decrease 120^0 to 118.7^0.

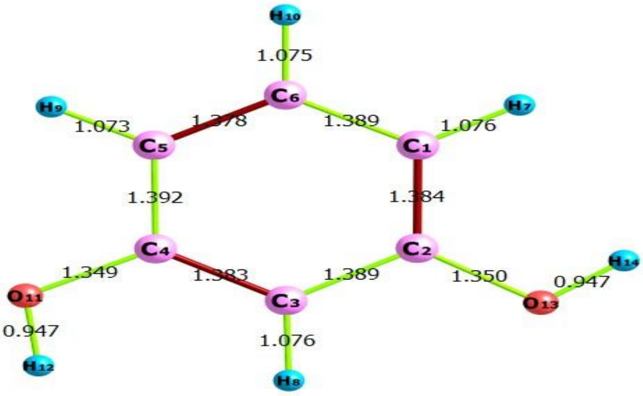


Fig.1: Optimized Structure of Title Molecule

3.2 NLO (Polarizability, Hyper polarizability) Properties

The Mullikan atomic charges for all atoms of the Resorcinol are calculated by combination of DFT, methods and 6-31G (d) as basis set in gas phase and are listed in table–2.

Hyperpolarizability and Polarizability label the account of a system in a functional electric field [18]. Theses Hyperpolarizability and Polarizability are resolute strength of molecular communication and collision process as well as nonlinear optical properties (NLO) of the scheme [19-20]. Hyperpolarizability of first order labelled by 3×3×3 matrix of is a third rank tensor. The 3D matrix contain27 mechanisms can be reduced to 10 mechanisms due to the Kleinman symmetry [21]. It can be given in the lower tetrahedral arrangement. The components of β are constants in the Taylor series extension of the energy in the external electric field. When the external electric field is weak and regular, this extension becomes:

$E = E^0 – \mu_\alpha F_\alpha – 1/2_{\alpha\alpha}\beta F_\alpha F_\beta – 1/6\beta_\alpha\beta_\gamma F_\alpha F_\beta F_\gamma$

Where E^0 is the energy of the unperturbed molecules, Fα the field at the origin $\mu_{\alpha,}$ $_{\alpha\alpha\beta}$, and $\beta_{\alpha\beta}$are the components of dipole moment, polarizability and the first hyperpolarizabilities respectively. Dipole moment (μ), polarizability $<\alpha>$and total first static hyper polarizability $\beta$are also calculated (In Table 2 and 3) by using density functional theory. They can be expressed in terms of *x*, *y*, *z* components and are given by following equations 1, 2 and 3-

$\mu = (\mu_x^2 + \mu_y^2 + \mu_z^2)^{1\backslash 2}$ (1)

$<\alpha> = 1\backslash 3\ [\alpha_{xx} + \alpha_{yy} + \alpha_{zz}]$ (2)

$\beta_{\text{Total}} = (\beta_x^2 + \beta_y^2 + \beta_z^2)^{1\backslash 2}$

$= [(\beta_{xxx} + \beta_{xyy} + \beta_{xzz})^2 + (\beta_{yyy} + \beta_{yxx} + \beta_{yzz})^2 + (\beta_{zzz} + \beta_{zxx} + \beta_{zyy})^2]^{1\backslash 2}$ (3)

The β components of Gaussian output are reported in atomic units.

Where (1 a.u. = $8.3693 X 10^{-33}$ e.s.u.).

For Resorcinol, the dipole moment is calculated by above mentioned method is 1.4505. Debye which is less than dipole moment than water (2.16 Debye), Resorcinol can be used as better solvent. As we see a greater contribution of α_{zz} in molecule which shows that molecule is elongated more towards Z direction and more contracted to Y direction. $\beta_{xxx,}$ β_{xzz} contribute larger part of hyper polarizibity in the molecule. This shows that X axis plane and XZ plane are more optical active in these directions.

3.3 Electronic properties

The interaction with other species in a chemical system is also determined by frontier orbitals, HOMO and LUMO. It can also be determined by experimental data. The frontier orbital gap helps to distinguish the chemical reactivity and kinetic stability of the molecule. A molecule which has a larger orbital gap is more polarized having more reactive part as far as reaction is concerned [22-24]. The frontier orbital gap in case of the given molecules is 8.4561 eV, for Resorcinol given in Table (3). The contour plots of the HOMO, LUMO and

MESP structures of the molecule are shown in figure 2. The importance of MESP lies in the fact that it simultaneously displays molecular size, shape as well as positive, negative, and neutral electrostatic potential region in terms of grading and is very useful in the investigation of molecular structure with its physiochemical property relationship [25-27]. The different values of the electrostatic potential at the surface are represented by different colours: red represents regions of most negative electrostatic potential, blue represents regions of most positive electrostatic potential, and green represents regions of zero potential. Potential increases in the order: red < orange < yellow < green < blue. In all cases, the shape of the electrostatic potential surface is influenced by the structure and charge density distributions in the molecule with sites close to the oxygen atom, showing regions of most negative electrostatic potential. The transition from HOMO→LUMO in given molecule indicates charge transfer Benzene ring.

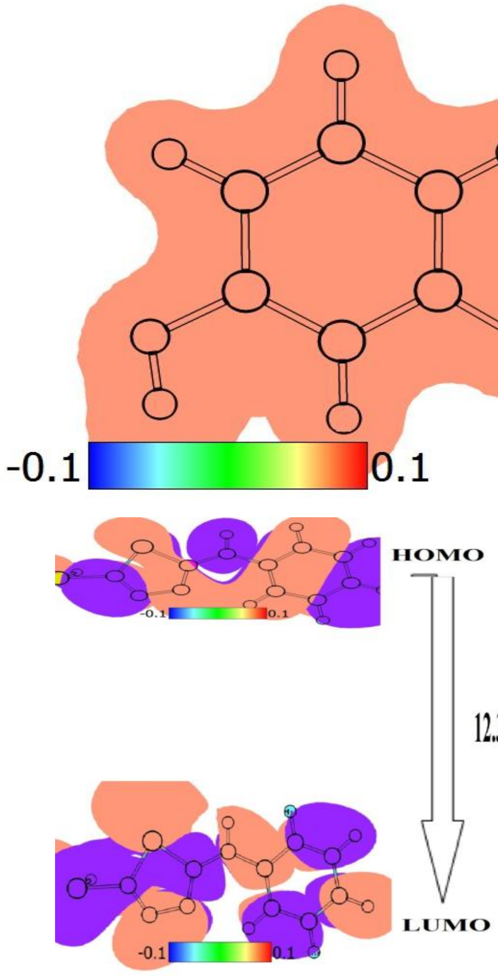


Fig.2: MESP, HOMO-LUMO and Plot of Resorcinol.

3.4 Other Molecular Properties

Several calculated Thermodynamic properties Based on the vibrational analysis at DFT/ 6-31G (d) level, statistical Thermodynamics, the standard Thermodynamic functions internal thermal energy (E), constant volume heat capacity Cv and entropy S have been calculated and listed in Table 5. At the room temperature conduction band is almost empty so electronic contribution in total energy is negligible. Thermodynamic parameters clearly indicate that vibration motion plays a crucial role in order to assess the Thermo dynamical behaviour of title compounds. Based on the vibrational analysis at DFT/ 6-31G (d) level and statistical Thermodynamics, the standard thermodynamic functions internal thermal energy (E), constant volume dipole moment, zero point energy calculated by DFT method are at larger value than water molecule however entropy S and heat capacity gave reverse result.

3.5 Assignment of Fundamentals

Resorcinol has 14 atoms with 36 normal modes of vibration. These normal modes of frequencies are divided in two parts, above 1000 cm-1 are called functional region and below 1000 cm-1 are called fingerprint region. Detailed description of vibrational modes can be given by means of normal coordinate analysis. It is well known that vibrational frequencies obtained by quantum chemistry calculation are typically larger than that of their experimental counterpart and thus experimental scaling factors of .96 are usually employed to have better agreement with the experimental vibrational frequencies [28]. Gauss View 3.0 program has been considered to get visual animation Some important mode are discuss below in Fromour calculated data and experimental FTIR spectra, we observe similarities and differences between the experimental and the calculated u by DFT/6-31G(d) method. Assignments are done using the animated view of normal mode description. A good agreement is found between the theoretical and experimental data. Here we are discussing only important modes.

3.6 Vibrational Modes Description

C–H Vibrations

We have seen in literature that the C–H stretching vibrations are usually observed in 2800–3200 cm^{-1} region [29]. In the study of Resorcinol, the (C–H) functional group is present at 1.07 cm^{-1} in calculated spectra which is in good agreement with the experimental data as given in table 6 Some in plane bending modes of vibration are obtained at 1377 cm^{-1}with significant IR intensity as well as out of plane bending modes are 1167cm^{-1}.

O-H Vibrations

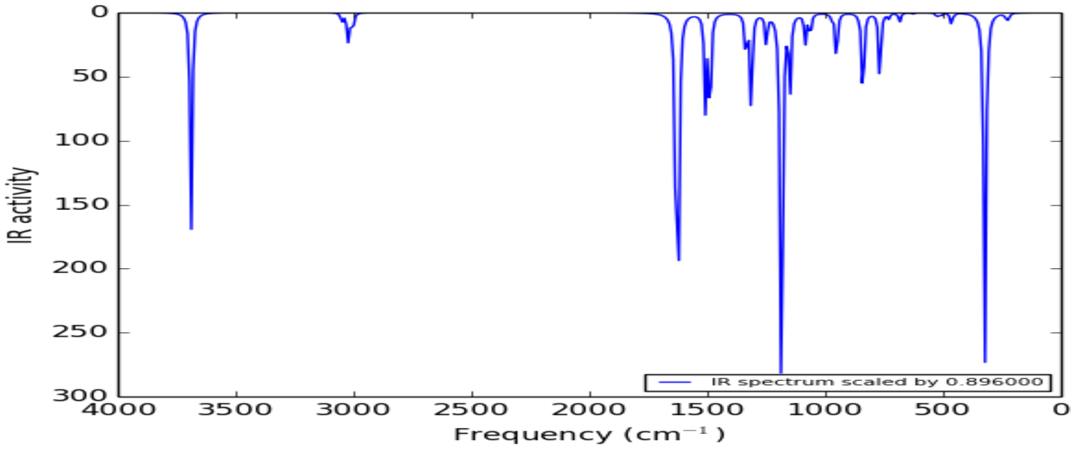
In vibrational spectra, the strength of hydrogen bond determines the position of O–H band. Generally stretching appears at high frequency ranging from 3600–3400 cm^{-1} [30] because of lower reduced mass. In this study, Resorcinol showed very strong absorption peaks a 3207cm^{-1}, which is due to the O–H stretching vibration. The observed frequency range is different from experimental one and probably this is due to the low scattering factor for hydrogen and also the intermolecular interaction occurring in the molecule which overestimates the stretching modes. The various bending vibrations of the hydroxyl groups are also found to be in good agreement with the observed spectra and literature [31].

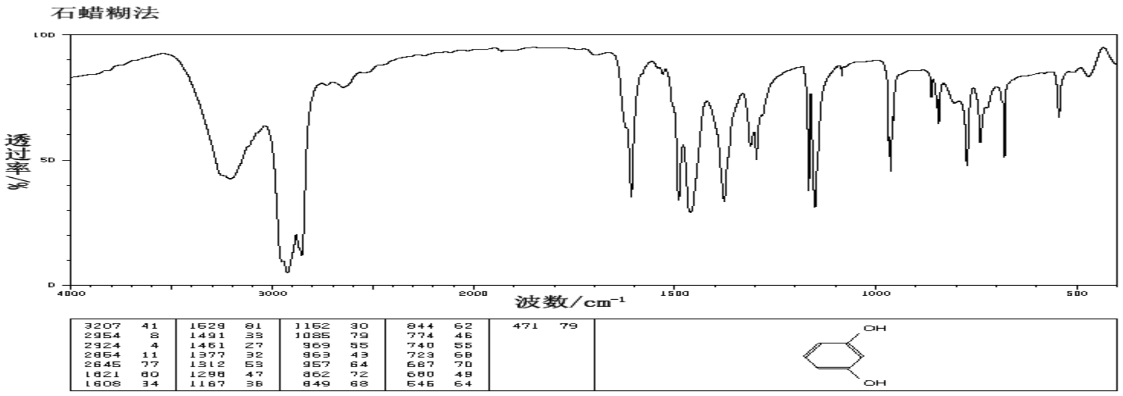
C-C Vibration

The C–C aromatic stretch known as semi-circle stretching, is calculated at in 1821 cm^{-1} etc. respectively, and is supported by the literature [31]. The theoretically calculated C–C–C bending modes have also been found to be consistent with the recorded spectral values and the literature [31].

3.7 Some other modes of vibration

Out of plane bending as well inplane bending are obtained at lower side spectra. A less intense mode corresponding to ring Torsion lies at 345 cm^{-1} while some significant intense polarized corresponding twisting in C-H bond is shown in 309, 455, 669cm^{-1}. Ring breeding mode are also lies on lower region of this band. Due to mixing of band at lower region intensity as well other properties not well defined in this region. The lower region vibration has unique characteristics which is fingerprint of title molecule so this region is also called fingerprint region.





3207	41	1629	81	1162	30	844	62	471	79
2954	8	1491	33	1085	79	774	46		
2924	4	1461	27	969	55	740	55		
2864	11	1377	32	963	43	723	68		
2645	77	1312	53	957	64	687	70		
1821	80	1298	47	862	72	680	49		
1608	34	1167	36	849	68	646	64		

Fig.3: Calculated and Experimental IR spectra of Title Molecule NBO analysis.

NBO Examination NBO analysis play important role of intermolecular contact in the complexes. This can carried out all possible interface between empty acceptor and filled donor. This can appraised on the basis of their energetic position by second-order perturbation theory. For each donor NBO (i) and acceptor NBO (j), the steadying energy $E^{(2)}$ related with electron delocalization between donor and acceptor .

NBO analysis offers an efficient method for studying intra and intermolecular attachment and communication among bonds, and also delivers a suitable basis for investigation of charge transfer or conjugative connections in molecular system. Some electron donor orbital, acceptor orbital and the interacting steadying energy resulting from the second order micro-disturbance theory are reported [32, 33]. The larger the $E^{(2)}$ value, the more intensive is the interaction between electron donors and the greater the extent of conjugation of the whole system. Delocalization of electron density between unavailable Lewis type (bond or lone pair) NBO orbitals and formally unoccupied (antibonding or Rydberg) non Lewis NBO orbital's resemble to a stabling donor acceptor interaction. The π–conjugation and resonance due to π–electron delocalization in pyridine ring is due to the $\pi\rightarrow\pi^*$ interactions. The primary hyperconjugative exchanges causes ($\sigma \rightarrow\pi^*$, $\pi\rightarrow \sigma^*$, $n\rightarrow \sigma^*$) due to the various types of orbital overlaps and secondary hyperconjugative connections due to the $\sigma \rightarrow \sigma^*$ orbital overlap .Second–order perturbation theory analysis of the Fock matrix in NBO basis is calculated in this study . The hyper conjugative interaction formed by orbital overlap between π(C3—C5) → π*(C3- C4), π*(C3-O11) and π* (C3—C5) → π*(C3-C4) which results in intermolecular charge handover producing the stabilization of the ring by stabilization energy 53.69, 43.95, and 402.94kcal/mol respectively.

4. Conclusions

Equilibrium geometries and harmonic frequencies of title were determined by DFT theory using 6-31G (d) basis set. The vibrational frequency calculations proved that the structure is stables (no imaginary frequencies). The difference between the observed and scaled wavenumbers values of most of the fundamentals is very small. Any discrepancy noted between the observed and the calculated frequencies may be due to the fact that the calculations have been actually done on a single molecule in the gaseous state contrary to the experimental values recorded in the presence of intermolecular interactions.

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Table-1

Calculated Band Length and bond angle (A) of Resorcinol

S. NO.	CALCULATED BOND LENGTH	VALUE
1	R(C1-C2)	1.38
2	R(C1-C6)	1.38
3	R(C1- H7)	1.07
4	R(C2-C3)	1.38
5	R(C2-O13)	1.34
6	R(C3-C4)	1.38
7	R(C 3-H8)	1.07
8	R(C4-C5)	1.39
9	R(C4-O11)	1.34
10	R(C5-C6)	1.37
11	R(C5-H9)	1.07
12	R(C6-H10)	1.07
13	R(O11-H12)	0.94
14	R(O13-H14)	0.94
BOND ANGLE		
15	A(C_2-C_1-C_6)	118.7
16	A(C_2-C_1-H_7)	120.5
17	A(C_6-C_1-H_7)	120.6
18	A(C_1-C_2-C_3)	120.7
19	A(C_1-C_2-O_{13})	122.5
20	A(C_3-C_2-O_{13})	116.7
21	A(C_2-C_3-C_4)	119.4
22	A(C_2-C_3-H_8)	119.0
23	A(C_4-C_3-H_8)	121.5
24	A(C_3-C_4-C_5)	120.8
25	A(C_3-C_4-O_{11})	121.8

Table - 2

Polarizability & Hyper Polarizability Resorcinol

Polarizability	
αxx	42.03
αxy	5.83
αyy	-39.83
αyz	-0.00
αzz	-49.9
αzx	-0.00
A	2.68
βxxx	40.37
βxxy	1.33
βxyy	0.00
βyyy	-11.05
βzzz	-0.00
βxxz	0.00

βxzz	-0.00
βyzz	0.01
βyyz	-17.65
βxyz	-5.05
βtotal	7.62

Table – 3

HOMO-LUMO Gap and Dipole moment Resorcinol

PARAMETERS	VALUE
Total energy E(a.u.)	-380.4147
Dipole moment (Debye)	1.4504
LUMO	-0.30526
HOMO	0.15003
Frontier Orbital Energy Gap (ev)	0.45529

Table -4

Mulliken Atomic Charges of (Resorcinol)

S. No	Atoms	Atomic Charge
1	C	-0.31
2	C	0.43
3	C	-0.34
4	C	0.44
5	C	-0.27
6	C	-0.16
7	H	0.18
13	O	-0.75
11	O	-0.75

Table - 5

Thermodynamic properties of Resorcinol

Parameter	E (Thermal) Kcal/Mol	Cv Cal/Mol-Kelvin	S Cal/Mol-Kelvin
Total	77.378	24.534	78.628
Electronic	0.000	0.000	0.000
Translational	0.889	2.981	40.003
Rotational	8.889	2.981	27.981
Vibrational	75.600	18.573	10.644

Table-6

Comparison between Calculated and Experimental IR and Raman Intensity of Resorcinol

S. No.	Calculated Frequency	Scale Frequency	Experimental Frequency	I R	Raman Activity	Modes of Vibration
1	248	213		5.82	1.56	β(in whole ring)
2	261	225		2.75	2.83	in (O-H)
3	345	297		14.38	3.43	γ in (O-H)
4	359	309		273.04	1.24	β in (O-H)
5	360	309		13.59	0.48	γ in (C-H)
6	507	436		1.87	0.11	β in (C-H)
7	519	446		7.90	0.14	β in (O-H)
8	567	488	471	2.49	3.94	β(in whole ring)
9	585	503		3.57	5.90	μ in (C-C)
10	699	601	680	0.89	0.03	β in (C-C)
11	762	655	687	7.41	0.03	γ in (C-H)
12	813	700	729	4.12	16.17	μ in (C-C)
13	856	736	774	59.29	1.96	γ in (C-H)
14	935	804	849	78.11	1.93	β in (C3-H3)
15	953	820	862	2.02	1.62	γ in (C-H)
16	1061	913		42.60	1.01	β(in whole ring)
17	1083	931	957	3.51	20.97	μ in (C-H)
18	1095	942	969	0.53	0.50	γ in (C-H)
19	1185	1019		18.90	3.84	μ in (C-H)
20	1209	1040	1085	23.82	2.56	μ in (C-C)
21	1281	1101	1167	59.85	3.30	γ in (C-H)
22	1321	1136	1298	366.98	2.18	β in (O-H)
23	1332	1146	1312	12.25	1.38	β(in whole ring)
24	1393	1198	1377	25.80	1.68	β in (C-H)
25	1465	1260	1461	85.66	7.07	β(in whole ring)
26	1490	1282	1491	35.43	0.27	β in (O4-H4)
27	1660	1427	1621	93.15	1.23	μ in (C-C)
28	1682	1446	1629	73.75	0.49	μ in (C-C)
29	1808	1555		168.92	11.12	μ in (C-C)
30	1821	1566	1821	189.38	13.79	μ in (C-C)
31	3351	2881	2854	13.96	70.41	μ in (C1-H7)
32	3369	2897		11.40	63.26	μ in (C3-H8)
33	3380	2902	2924	16.86	118.15	μ in (C6-H10)
34	3402	2926	2954	7.63	129.52	μ in (C5-H9)
35	4115	3539	3207	91.34	71.97	μ in (O11-H12)
36	4117	3540		82.20	83.48	μ in (C13-H14)
ABBREVIATION-μ-stretching , γ-out of plane banding, β-in plane banding						