Molecular Structure and Vibrational Spectra of Alpha-Benzoinoxime by Density Functional Method[1]

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Abstract—In the present study, an exhaustive conformational search of the Alpha-benzoinoxime has been performed. The FT-IR spectrum of this compound was recorded in the region 4000–400 cm^{-1}. The FT-Raman spectrum was also recorded in the region 3500–50 cm^{-1}. Vibrational frequences of the title compound were calculated by B3LYP method using 6-311++G(d, p) basis set. The calculated vibrational frequences were analysed and compared with experimental results.

1. INTRODUCTION

As mentioned in our previous oxime studies [1–4], oximes and vic-dioximes are important compounds for coordination chemistry and their derivatives play significant roles as model systems especially in applied chemistry. They are used as biological model compounds (i.e., vitamin B12) and chemical building blocks for the synthesis of agrochemicals and pharmaceuticals. They are also used in photography, medicine, textiles, dye chemistry, and semiconductor manufacturing processes [5–9]. Several papers have been published on the structure of oximes and dioximes discussing the interesting property of forming complexes with transition metals [10–15]. In recent years, the findings of antitumor effects of coordination compounds in cancer research have increased the attention especially on vic-dioxime complexes [16].

Alpha-benzoinoxime (ABO) is one of the important oxime derivatives but, in the literature, we have found neither experimental data nor the calculation results on molecular structure of ABO. However, we performed a basic level conformational analysis for investigate possible model radials of gamma-irradiated ABO before [4]. It is known that, infrared and Raman spectroscopy is an efficient method to probe electronic and geometric structure of molecules, and has been widely used in studying the structural consequences. In recent years density functional theory (DFT) has become a powerful tool in the investigation of molecular structures and vibrational spectra, especially B3LYP method has been widely used [17–20].

To the best of our knowledge, neither detailed quantum chemical calculations nor the vibrational spectra of ABO have been reported.

In the present paper, an exhaustive conformational search of the ABO has been performed. Vibrational frequencies of the title compound have been calculated by B3LYP method using 6-31++G(d, p) basis set. The calculated geometric parameters and vibrational frequencies were analyzed and compared with obtained experimental data.

2. EXPERIMENTAL

The solid form of ABO was purchased from Merck. FT-IR spectrum of solid ABO was recorded in the range 4000–400 cm^{-1} on Brucker IFS 66/S with PIKE Gladi ATR (Diamond) spectrometer at room temperature with 2 cm^{-1} resolution. The FT-Raman spectrum was recorded on a Brucker FRA 106/S spectrometer using 1064 nm excitation from a Nd:YAG laser. The detector was a Ge-diode cooled to liquid nitrogen temperature. The upper limit for wavenumbers was 4000 cm^{-1} and the lower wavenumber is around 50 cm^{-1}. The measured FT-IR and FT-Raman spectra along with theoretical FT-IR spectrum are shown in Figs. 1 and 2.

3. COMPUTATIONAL DETAILS

In order to establish stable possible conformations, the conformational space of ABO was scanned with molecular mechanics method. This calculation was

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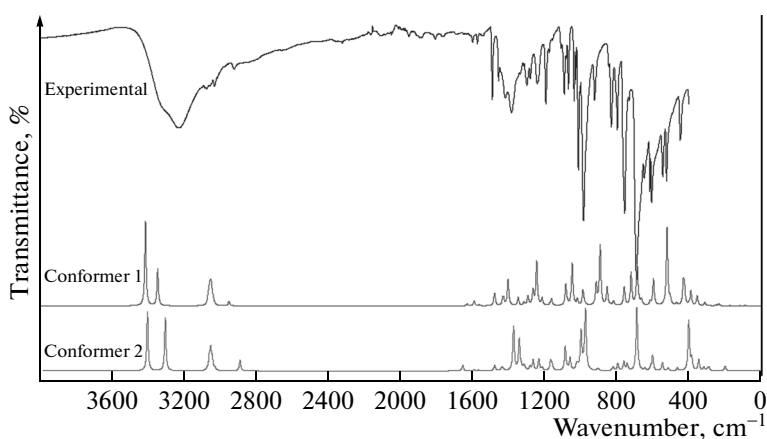[1] The article is published in the original.

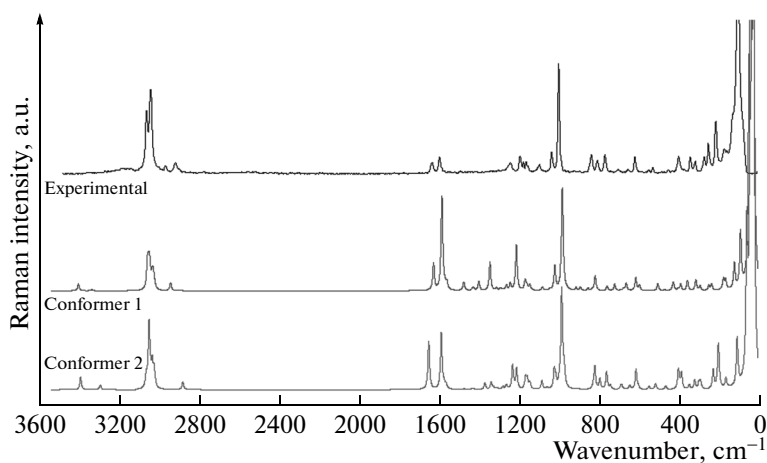**Fig. 1.** Experimental and theoretical FT-IR spectra of ABO.

Fig. 2. Experimental and theoretical Raman spectra of ABO.

performed with the Spartan 08 program [21]. In the second step, geometry optimizations of the obtained possible conformations were performed with B3LYP method using the standard 6-311++G(d, p) basis set. After the most stable conformer of the title compound determined, geometry optimizations and frequency calculations of this conformer have been performed by B3LYP method with 6-311++G(d, p) basis set. The optimized structural parameters were used in the vibrational frequency calculations at the same level to characterize all stationary points as minima. In this step, all the calculations were performed using Gaussian 03 program package [22] with the default convergence criteria without any constraint on the geometry [23]. The theoretical vibrational spectra of the title compound were interpreted by means of TEDs using the SQM program [24]. It should be noted that Gaussian 03 package does not calculate the Raman intensities. The Raman activities were transformed in to Raman intensities by using Raint program [25].

4. RESULTS AND DISCUSSION

4.1. Conformational Stability and Molecular Structure

The different conformational structures of a compound are correlated with many of the physical and chemical properties and hence their investigation is important for drug designs and to understand several medical effects. To found stable conformers, a meticulous conformational analysis was carried out for the title compound. Rotating 10° each degree intervals around the free rotation bonds, conformational space of the title compound was scanned by molecular mechanic calculation. The geometry optimizations of the obtained conformers were performed by B3LYP/6-311++G(d, p) method. Results of conformational analysis were indicated that the title compound has nine conformers as shown in Fig. 3. Ground state energies, zero point corrected energies (E_{elect} + ZPE), relative energies of conformers and dipole moments, were presented in Table 1. From the

Conformer 1   Conformer 2   Conformer 3

Conformer 4   Conformer 5   Conformer 6

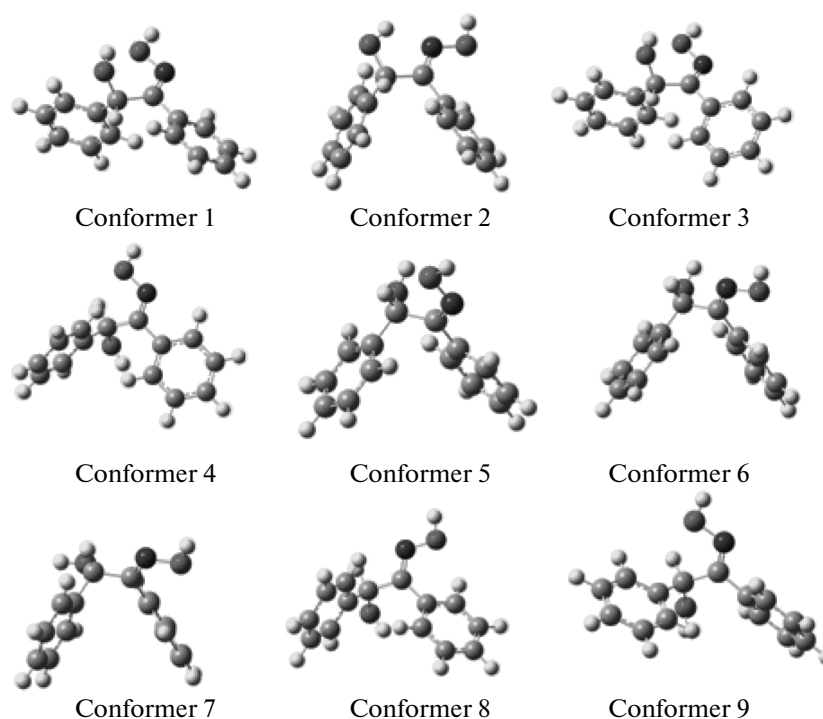Conformer 7   Conformer 8   Conformer 9

Fig. 3. Stable conformers of ABO.

calculated energies of nine conformers, given in Table 1, the conformer 1 is the most stable. Zero point corrections have caused changes in the stability order of conformer 1 and conformer 2. According to the zero point corrected energies, conformer 2 is more stable than conformer 1. The difference between the total energies of the most stable conformer1 and conformer 2 is 0.04 kcal/mol. This difference is 0.61 kcal/mol for zero point corrected energies. The only difference between molecular structures of these two conformers is in the orientation of oxime group and dihedrals of rings. So, both form was used in the future calcula-

tions. But it is seen in Figs. 1, 2 and the Table 2 that both calculated frequencies and intensity distributions of the conformer 2 are more compatible with the experimental counterparts than those of conformer 1. The optimized geometric parameters (bond lengths, bond angles and dihedral angles) of the conformer 1 and conformer 2 were given in Table 3. The atom numbering scheme adopted in this study is given in Fig. 4. In the literature, we have found neither experimental data nor the calculation results on molecular structure of ABO, therefore the molecular structure of the title compound is given for the first time in this study.

Table 1. Energetics of the conformers calculated at the B3LYP/6-311++G(d,p) level

Conf.	E (Hartree)	ΔE, kcal/mol	E_0 (Hartree)	ΔE_0, kcal/mol	Dip. Mom. (D)
1	−746.659893	0.00	−746.4185970	0.61	2.2615
2	−746.659824	0.04	−746.419261	0.00	2.858
3	−746.657859	1.28	−746.418438	0.79	1.0966
4	−746.657072	1.77	−746.418174	0.83	1.4296
5	−746.657018	1.80	−746.417469	0.95	0.8168
6	−746.656972	1.83	−746.417273	1.39	0.7727
7	−746.656569	2.09	−746.417205	1.56	1.6405
8	−746.655626	2.68	−746.416914	1.66	1.5647
9	−746.655026	3.05	−746.415954	2.08	1.4255

E_0—Zero point corrected energy.

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Table 2. Comparison of the observed and calculated vibrational spectra of ABO

Mode nos.	Experimental					Theoretical			
	Conformer 1					Conformer 2			
	IR	Raman	Scaled Freq.[a]	I_{IR}^{b}	I_{Raman}^{c}	Scaled Freq.[a]	I_{IR}^{b}	I_{Raman}^{c}	TED,[d] %
ν_1	3332		3417	100	2	3406	100	3	100υ OH
ν_2	3234		3349	43	0	3307	89	1	100υ OH
ν_3	3076	3073	3071	2	4	3076	2	3	88υ CH
ν_4		3055	3069	5	5	3063	12	6	86υ CH
ν_5			3064	9	5	3062	11	7	84υ CH
ν_6	3034		3060	12	6	3055	17	1	93υ CH
ν_7			3056	14	2	3054	16	1	92υ CH
ν_8			3051	15	1	3046	12	2	95υ CH
ν_9			3046	4	3	3045	5	3	90υ CH
ν_{10}			3041	4	4	3038	0	1	94υ CH
ν_{11}			3038	1	1	3037	1	3	93υ CH
ν_{12}		2983	3033	1	1	3031	3	1	89υ CH
ν_{13}	2925	2930	2954	5	3	2892	18	2	99υ CH
ν_{14}	1652	1640	1632	2	9	1656	10	10	80υ NC
ν_{15}	1600	1601	1592	5	4	1593	2	4	64υ C=C + 17 δHCC, Ring A
ν_{16}			1589	0	28	1593	0	8	62υ C=C + 19 δHCC, Ring A
ν_{17}	1588		1574	0	1	1578	1	1	71υ C=C+ 11 δHCC, Ring B
ν_{18}	1575	1576	1564	1	2	1569	1	1	64υ C=C + 11 δHCC, Ring A
ν_{19}	1491	1495	1480	7	2	1479	4	0	53 δHCC+ 20 δCCC, Ring A
ν_{20}			1478	8	0	1478	6	0	63 δHCC+ 11 δCCC , Ring B
ν_{21}	1446		1434	7	1	1439	5	0	58 δHCC + 19 υ CC, Ring B
ν_{22}	1428		1429	6	0	1431	3	0	62 δHCC + 13 υ CC, Ring A
ν_{23}	1385		1404	31	3	1374	75	1	59 δHOC + 16 δHCO
ν_{24}	1337		1348	9	9	1342	54	2	74 δHON
ν_{25}			1316	3	1	1330	5	0	73 δHCO
ν_{26}	1316		1315	0	0	1316	9	0	73 δHCC + 11 υ CC, Ring A
ν_{27}	1300		1294	11	1	1308	2	0	54 υ C=C + 26 δHCO + 10 δHCC, Ring B
ν_{28}	1281		1284	1	0	1282	7	1	65 υ C=C, Ring A
ν_{29}	1251		1265	17	2	1265	19	1	44 δHCO + 13 δHOC + 11 υ CC
ν_{30}	1241	1246	1246	52	2	1233	20	5	36 υ CC
ν_{31}	1193	1196	1215	8	15	1214	6	4	58 δHCC + 11 υ CC
ν_{32}			1172	1	2	1171	1	1	73 δHCC , Ring A
ν_{33}	1176	1179	1170	0	1	1168	16	2	49 δHCC , Ring B
ν_{34}	1155	1155	1163	7	2	1160	10	2	59 δHCC + 18 υ CC, Ring B
ν_{35}			1148	0	1	1149	0	1	79 δHCC + 12 υ CC, Ring A
ν_{36}			1146	0	1	1146	0	1	75 δHCC , Ring B
ν_{37}	1092	1098	1084	24	1	1087	40	2	48 δHCC, Ring A−B
ν_{38}			1073	2	0	1073	3	0	71 δHCC, Ring A−B
ν_{39}	1069		1048	50	0	1060	21	0	71 δHCC, Ring A−B
ν_{40}	1028	1038	1022	1	7	1024	9	4	50 δCCC + 12 υ CC, Ring A−B
ν_{41}	1013	1002	1019	6	1	1017	7	2	66 δCCC + 12 δHCC Ring B
ν_{42}	998	993	989	16	0	999	65	1	53 δCCC, Ring A
ν_{43}			986	0	8	987	6	15	70 δCCC, Ring B
ν_{44}			983	5	26	986	3	5	79 δCCC, Ring A
ν_{45}			976	0	0	976	24	1	71 Γ HCCH, Ring A + 14 υ ON

Table 2. (Contd.)

Mode nos.	Experimental					Theoretical			
	Conformer 1					Conformer 2			
	IR	Raman	Scaled Freq.[a]	I_{IR}^b	I_{Raman}^c	Scaled Freq.[a]	I_{IR}^b	I_{Raman}^c	TED,[d] %
ν_{46}	984		974	0	0	974	75	3	43 υ ON + 22Γ HCCH
ν_{47}			960	0	0	971	9	0	80 Γ HCCH, Ring B
ν_{48}			959	0	0	956	1	0	88 Γ HCCH, Ring A
ν_{49}			915	24	1	953	0	0	89 Γ HCCC, Ring B
ν_{50}	924		908	1	0	907	3	0	81 Γ HCCC, Ring A
ν_{51}			893	71	1	901	2	0	85 Γ HCCC, Ring B
ν_{52}			854	21	1	830	0	0	89 Γ HCCC, Ring A
ν_{53}			834	0	0	827	0	0	85 Γ HCCC, Ring B
ν_{54}	830	837	830	0	0	821	6	5	37 δCCC
ν_{55}	796	807	819	5	5	795	12	2	32 Γ HCCC, Ring A−B
ν_{56}	756	769	759	22	2	761	16	3	45 Γ HCCC, Ring A
ν_{57}	733		721	38	2	742	12	1	45 Γ HCCC, Ring B
ν_{58}	690	703	690	17	0	690	86	1	48 Γ HCCC, Ring A−B
ν_{59}			687	35	0	688	22	0	74 Γ HCCC, Ring A−B
ν_{60}			676	3	0	684	4	1	43Γ CCCC +14 Γ HCCC, Ring A−B
ν_{61}	648	652	663	7	2	645	4	1	45 δCCO
ν_{62}	617	619	616	4	2	614	2	2	80 δCCC, Ring A−B
ν_{63}			614	1	3	612	4	2	81 δCCC, Ring A−B
ν_{64}	606	612	597	31	2	602	26	1	52 δCCC, Ring A−B
ν_{65}	545	550	522	92	0	548	14	1	47 δCCO
ν_{66}	524	528	503	7	2	515	5	1	44 Γ CCCC Ring B
ν_{67}	448	451	469	3	0	464	5	1	47 Γ CCCC Ring A
ν_{68}	400	398	431	24	0	401	60	2	66 Γ HONC
ν_{69}			425	19	3	400	24	1	81 Γ CCCC Ring B
ν_{70}			401	1	0	397	0	1	88 Γ CCCC Ring A
ν_{71}			401	1	0	385	20	3	35 Γ HONC
ν_{72}		339	389	17	2	346	19	1	70 Γ HOCC
ν_{73}		315	355	11	3	318	6	2	44 δCCC
ν_{74}			313	4	4	297	4	1	40 δCCO
ν_{75}		270	291	1	1	289	6	2	55 Γ CCNO
ν_{76}		250	247	1	2	225	0	4	36 δCCC
ν_{77}		212	234	2	2	200	5	6	36 δCCC
ν_{78}			174	0	4	198	3	4	71 δCCN
ν_{79}		170	163	0	3	161	0	2	50 Γ CCCO
ν_{80}		102	119	0	8	105	1	10	76 Γ CCCC
ν_{81}			88	1	18	56	1	29	36 Γ CCCC +29 δCCC
ν_{82}			45	0	64	39	0	67	78 Γ CCCC
ν_{83}			32	0	75	29	0	37	81 Γ CCCC
ν_{84}			21	0	100	23	0	100	92 Γ CCCC

ν − stretching, a − antisymmetric, s − symmetric, δ − in-plane bending, Γ- out-of-plane bending.

[a] Obtained from the wave numbers calculated at B3LYP/6-311++G(d, p) using Arjunan's scale factors, performed for oximes, of 0.89 for O−H and N−H stretching, 0.96 for C−H stretching and 0.97 for all other vibrational modes.

[b] Relative absorption intensities normalized with highest peak absorption equal to 100.

[c] Relative Raman intensities normalized with highest peak absorption equal to 100.

[d] Total energy distribution calculated B3LYP/6-311++G(d, p) level of theory. Only contributions ≥10% are listed.

Table 3. The geometric parameters of two conformers calculated by B3LYP/6-311++G(d, p) method, bond lengths in angstrom (Å) and angles in degrees (°)

| Parameters	Calculated		Parameters	Calculated	
	Conformer 1	Conformer 2		Conformer 1	Conformer 2
Bond lengths (Å)			Bond angles (°)		
C_1-C_2	1.533	1.532	$C_{20}-C_{23}-C_{24}$	120.595	120.622
C_1-N_4	1.282	1.277	$C_{21}-C_{24}-C_{23}$	120.244	120.003
C_1-C_9	1.486	1.485	$C_{21}-C_{25}-C_{22}$	120.337	120.211
C_2-O_7	1.421	1.415	Selected dihedral angles (°)		
C_2-C_{20}	1.534	1.527	$N_4-C_1-C_2-O_7$	54.322	11.456
C_4-O_5	1.413	1.401	$N_4-C_1-C_2-C_{20}$	74.429	112.965
C_9-C_{11}	1.404	1.401	$C_9-C_1-C_2-O_7$	125.419	169.013
C_9-C_{12}	1.402	1.401	$C_9-C_1-C_2-C_{20}$	105.830	66.567
$C_{10}-C_{13}$	1.393	1.395	$C_2-C_1-N_4-O_5$	2.180	179.856
$C_{10}-C_{14}$	1.395	1.393	$C_9-C_1-N_4-O_5$	178.067	0.366
$C_{11}-C_{14}$	1.390	1.393	$C_2-C_1-C_9-C_{11}$	145.486	54.040
$C_{12}-C_{13}$	1.393	1.391	$C_2-C_1-C_9-C_{12}$	35.434	125.282
$C_{20}-C_{22}$	1.397	1.398	$N_4-C_1-C_9-C_{11}$	34.752	126.492
$C_{20}-C_{23}$	1.398	1.395	$N_4-C_1-C_9-C_{12}$	144.328	54.186
$C_{21}-C_{24}$	1.394	1.392	$C_1-C_2-C_{20}-C_{22}$	148.574	74.805
$C_{21}-C_{25}$	1.393	1.396	$C_1-C_2-C_{20}-C_{23}$	34.923	105.315
$C_{22}-C_{25}$	1.394	1.392	$O_7-C_2-C_{20}-C_{22}$	20.808	50.077
$C_{23}-C_{24}$	1.394	1.395	$O_7-C_2-C_{20}-C_{23}$	162.689	129.803
Bond angles (°)			$C_1-C_9-C_{11}-C_{14}$	179.134	179.683
$C_2-C_1-N_4$	123.932	114.221	$C_{12}-C_9-C_{11}-C_{14}$	0.032	0.348
$C_2-C_1-C_9$	120.495	119.182	$C_1-C_9-C_{12}-C_{13}$	178.794	178.854
$N_4-C_1-C_9$	115.573	126.595	$C_{11}-C_9-C_{12}-C_{13}$	0.300	0.475
$C_1-C_2-O_7$	111.538	111.922	$C_{14}-C_{10}-C_{13}-C_{12}$	0.379	0.270
$C_1-C_2-C_{20}$	112.503	110.523	$C_{19}-C_{10}-C_{13}-C_{12}$	179.516	179.634
$O_7-C_2-C_{20}$	113.415	111.114	$C_{13}-C_{10}-C_{14}-C_{11}$	0.048	0.552
$C_1-N_4-O_5$	112.218	114.746	$C_9-C_{11}-C_{14}-C_{10}$	0.157	0.863
$C_1-C_9-C_{11}$	120.207	119.990	$C_9-C_{12}-C_{13}-C_{10}$	0.508	0.786
$C_1-C_9-C_{12}$	121.121	120.951	$C_2-C_{20}-C_{22}-C_{25}$	177.301	179.872
$C_{11}-C_9-C_{12}$	118.667	119.056	$C_{23}-C_{20}-C_{22}-C_{25}$	0.708	0.247
$C_{13}-C_{10}-C_{14}$	119.616	119.753	$C_2-C_{20}-C_{23}-C_{24}$	177.052	179.752
$C_9-C_{11}-C_{14}$	120.606	120.493	$C_{22}-C_{20}-C_{23}-C_{24}$	0.524	0.367
$C_9-C_{12}-C_{13}$	120.586	120.317	$C_{25}-C_{21}-C_{24}-C_{23}$	0.285	0.121
$C_{10}-C_{13}-C_{12}$	120.257	120.300	$C_{30}-C_{21}-C_{24}-C_{23}$	179.785	179.732
$C_{10}-C_{14}-C_{11}$	120.267	120.073	$C_{24}-C_{21}-C_{25}-C_{22}$	0.102	0.240
$C_2-C_{20}-C_{22}$	119.599	120.197	$C_{30}-C_{21}-C_{25}-C_{22}$	179.969	179.851
$C_2-C_{20}-C_{23}$	121.445	120.725	$C_{20}-C_{22}-C_{25}-C_{21}$	0.401	0.055
$C_{22}-C_{20}-C_{23}$	118.866	119.078	$C_{26}-C_{22}-C_{25}-C_{21}$	179.691	179.108
$C_{24}-C_{21}-C_{25}$	119.430	119.658	$C_{20}-C_{23}-C_{24}-C_{21}$	0.031	0.185
$C_{20}-C_{22}-C_{25}$	120.524	120.427	$C_{27}-C_{23}-C_{24}-C_{21}$	179.813	179.523
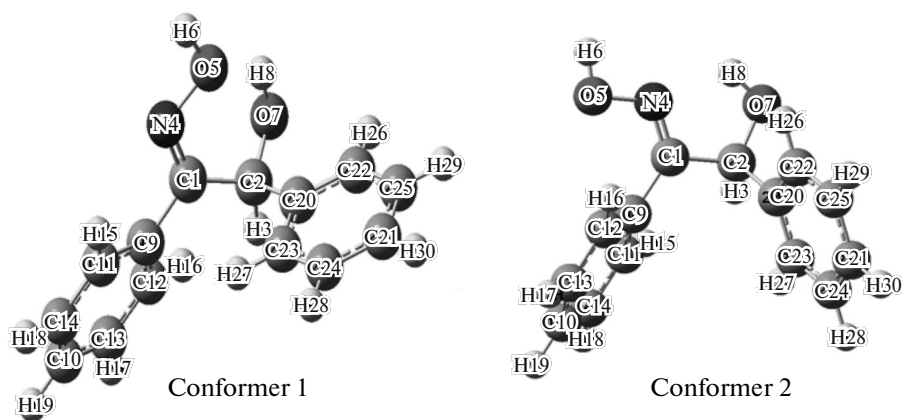
Fig. 4. Atom numbering scheme adopted in this study.

4.2. Vibrational Assignments

The ABO molecule has 30 atoms, which possess 84 normal modes of vibrations. All the vibrations are active in the infrared and Raman spectra. Usually the calculated harmonic vibrational wavenumbers are higher than the experimental ones, because of the anharmonicity of the incomplete treatment of electron correlation and of the use of finite one-particle basis set. The harmonic frequencies were calculated by B3LYP method using 6-311++G(d, p) basis set and then scaled by Arjunan's scale factors, performed for oximes, of 0.89 for O−H and N−H stretching, 0.96 for C−H stretching and 0.97 for all other vibrational modes [26]. Experimentally observed and theoretically calculated harmonic vibrational frequencies and their correlations were gathered in Table 3. From the calculations, the computed values are in good agreement with the observed values. The vibrational bands assignments have been made by using the animation option of Gauss View 3.0 graphical interface for Gaussian programs [27] along with available related molecules and also by means of TEDs using the SQM program [24].

4.3. Oxime Group Vibrations

The O−H stretching of oximes absorbs IR radiation strongly in the range of 3300−3100 cm^{-1} as a very broad band, but it contributes weak or no Raman scattering [28]. In this study, the shoulder observed at 3332 cm^{-1} was assigned as O−H streching vibration of oxime group. The calculated values of this band are 3417 cm^{-1} for conformer 1 and 3406 cm^{-1} for conformer 2. The difference between experimental and calculated values shows the presence of strong intramomecular and intermolecular hydrogen bonding in our sample [29], similar to studied oximes in literature [26, 30]. Their frequencies in the 1300 and 900 cm^{-1} region are attributed to the O−H deformation and N−O stretching modes in oximes [26]. According to the

TED given in the Table 2, these vibrations were observed at 1337 and 984 cm^{-1} in our FT-IR spectrum. The computations were predicted these bands as 1348 and 974 cm^{-1} for conformer 1 and as 1342 and 974 cm^{-1} for conformer 2. The Raman band observed at 398 cm^{-1} was assigned as O−H out-of-plane bending vibration. Due to intermolecular hydrogen bonding effects, this band observed higher wavenumber than 300 cm^{-1} [30]. As it is seen in Table 2, the calculated value of this band for conformer 2 show good agreement with recorded spectral data.

An oxime exhibits the C=N stretching band observed between 1650−1630 cm^{-1} [28]. The corresponding band is observed at 1652 cm^{-1} in FT-IR and at 1640 cm^{-1} in FT- Raman spectra, respectively. The computations predicted this band as 1632 cm^{-1} for conformer 1 and as 1656 for conformer 2.

4.4. O−H Group Vibrations

The bands observed at 3234 and 1251 cm^{-1} in FT-IR spectrum were assignet to O−H stretching and deformation vibrations. The calculated values of these bands are 3349 and 1265 cm^{-1} for conformer 1 and 3307 and 1265 cm^{-1} for conformer 2. Because of strong intramomecular and intermolecular hydrogen bonding interactions in our sample, experimental and calculated values of O−H stretching band is quite different [26, 30]. The O−H out-of-plane bending vibration was observed at 339 cm^{-1} in FT-Raman spectrum. For conformer1, the calculated value this band is 398 cm^{-1}, while 346 cm^{-1} for conformer 2.

4.5. C−H Vibrations

The heteroaromatic structure shows the presence of C−H stretching vibration in the region 3100−3000 cm^{-1}, which is the characteristic region for the ready identification of C−H stretching vibration [31,

32]. In this region, the bands are not affected appreciably by the nature of the substituent. Hence in our present work, the FT-IR band observed at 3076 cm^{-1} was assigned to C2−H3 stretching vibration The FT-Raman conterpart of this band was observed at 3073 cm^{-1}. The calculated values of this band for conformer 1 and conformer 2 are 3071 and 3076 cm^{-1}, respectively. The very weak FT-IR bands observed at 3034 and 2925 cm^{-1} and FT-Raman bands observed at 2983 and 2930 cm^{-1} were assigned to aromatic C−H stretching vibrations. For ABO, the C−H stretching vibrations were predicted between 3071 and 2892 cm^{-1} frequency range for both of the conformers.

The aromatic C−H in-plane bending vibration occurs in the region 1500−1100 cm^{-1}, the bands are sharp but have weak-to-medium intensity [32]. The C−H in-plane bending vibrations observed at 1491, 1446, 1428, 1316, 1251, 1193, 1176, 1155, 1092 and 1069 cm^{-1} in the FT-IR spectrum and at 1495, 1196, 1179, 1155 and 1098 cm^{-1} in the FT-Raman spectrum. The out-of-plane bending vibrations occur in the wavenumber range 800−1000 cm^{-1} [32]. The bands observed at 924, 796, 756, 733, and 690 cm^{-1} in the FT-IR spectrum and the bans observed at 807, 769, and 703 cm^{-1} were assigned to C−H out-of-plane bending vibrations. For both of the conformers, the calculated wavenumbers of in-plane and out-of-plane CH bands well reproduced the experimental ones in the infrared and Raman spectrum.

4.6. C=C Vibrations

In the present work, the frequencies observed in the FT-IR spectrum at 1600, 1588, 1575, 1300 and 1281 cm^{-1} and the bands observed at 1601 and 1576 cm^{-1} in the FT-Raman spectrum were assigned to C−C stretching vibrations. The C−C−C bending vibrations were observed at 1028, 1013, 998, 617 and 606 cm^{-1} in FT-IR spectrum and at 1038, 1002, 993, 619 and 612 cm^{-1} in FT-Raman spectrum. The theoretically computed C−C stretching and C−C−C out-of-plane and in-plane bending vibrational modes have been found to be consistent with recorded spectral values for both of the conformers.

5. CONCLUSIONS

The FT-IR and FT-Raman spectra of ABO were studied. The equilibrium geometries, harmonic wavenumbers, ground state energy, and dipole moment were calculated for the first time. The calculated vibrational values are in good agreement when they are compared with IR and Raman experimental data. Ab initio programs were used to find the most stable conformer of ABO.

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