

Research Article

Ground State Hydrogen Conformations and Vibrational Analysis of Isomers of Dihydroxyanthraquinone by Density Functional Theory Calculation

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Keywords

- Dihydroxyquinone
- Hartree-fock
- Density functional theory
- Infrared
- Vibration

Abstract

The ground state hydrogen conformations of 1,2- (alizarin), 1,4- (quinizarin), 1,8- (danthron) and 2,6-(anthraflavic acid) dihydroxyanthraquinone have been investigated using density functional theory (B3LYP) method with 6-31 G (d,p) basis set. The calculations indicate that the compounds in the ground state exist with the doubly bonded O atom linked intra-molecularly by the two hydrogen bonds. The vibrational frequencies and optimized geometry parameters of all the possible conformers of alizarin isomer were given.

INTRODUCTION

Dihydroxyquinones have important applications as a prominent family of pharmaceutically active and biologically relevant chromophores, as an analytical tool for the determination of metals, and in many aspects of electrochemistry [1]. Alizarin, quinizarin, danthron and anthraflavic acid are isomers of dihydroxyquinone. 1,2-Dihydroxyanthraquinone (alizarin) is a red coloring mordant dye, and used as an acid-base indicator in the determination of fluorine. 1,4-Dihydroxyanthraquinone (quinizarin) and 1,8-dihydroxyanthraquinone (danthron) are the simplest molecules showing the chromophore framework peculiar to several compounds of biological and pharmaceutical interest. 2,6-Dihydroxyanthraquinone (anthraflavic acid) is an isomer of the well known alizarin dye and a compound used from commercial suppliers without further purification. Danthron is present in some antitumor drugs. The structure of quinizarin has been subject of numerous spectroscopic investigations, including fluorescence studies in Shpolskii matrices [2], resonance Raman and infrared spectroscopy [3,4], laser spectroscopy in supersonic expansion [5], and X-ray crystallographic investigations [6]. For danthron also, fluorescence studies in Shpolskii matrices [7,8], resonance Raman [9] and infrared spectroscopy [10] studies have been made.

After the development by Lee and co-workers, infrared spectroscopy combined with ab initio quantum theoretical calculations has become a powerful and general method to find the ground state conformations of molecular clusters. An ab initio study of 1,4-, 1,5- and 1,8-dihydroxyanthraquinone was conducted to identify the absolute minimum [11]. Electronic structure of alizarin, two of its isomers, with different transition metal complexes and five rare-earth complexes were studied by using density functional theory (DFT) [12]. Experimental (FT-IR and Raman) and theoretical (B3LYP and B3PW91) vibrational analysis of quinizarin were studied by Xuan and *et al* [13]. The interaction between quinizarin and metal ions was studied by UV-Visible and fluorescence spectroscopies in solution and, the complex structures were confirmed by time-dependent density functional theory calculations [14]. In the present study we have calculated the optimized molecular geometries and vibrational analysis of isomers of dihydroxyquinone molecule using density functional theory (B3LYP) method with 6-31G (d,p) basis set to find out their ground state hydrogen conformations.

COMPUTATIONAL METHOD

The optimized conformations and vibrational frequencies of dihydroxyquinones have been calculated by using DFT/B3LYP method at 6-31 G (d,p) basis set level. All the computations were

performed using Gaussian 03 program package on personal computer [15] and Gauss-View molecular visualization program [16]. The scale factor of 0.9613 was used for B3LYP with 6-31G (d,p) basis set [17]. The proposed vibrational assignments were made by inspection of each of the vibrational mode by Gauss-View molecular visualization program.

RESULTS AND DISCUSSION

Dihydroxyquinones are molecules having 26 atoms, and belong to the point group C_s . The three Cartesian displacements of the 26 atoms provide 78 internal modes, namely;

$$\Gamma_{\text{inter.}} = 52A' + 26A''$$

From the character table for the C_s point group, since

$$\Gamma_{\text{trans.}} = 2A' + A'' \text{ and } \Gamma_{\text{rot.}} = 2A' + A''$$

we get

$$\Gamma_{\text{vib.}} = \Gamma_{39} - \Gamma_{\text{trans.}} - \Gamma_{\text{rot.}} = 49A' + 23A''$$

normal modes of vibration. All the vibrations are active both in infrared (IR) and Raman (R). For an N-atomic molecule, 2N-3 of all vibrations is in plane and N-3 is out of plane [18]. Thus, for dihydroxyquinone molecules, 49 of all the 72 vibrations are in plane and 23 out of plane. Since the molecules belong to the C_s

group all the vibrations being anti-symmetric through the mirror plane of symmetry σ_h will belong to the species A'' and the others being symmetric through σ_h belong to the species A' . Thus, since the compounds are planer all the vibrations of the A' species will be in plane and those of the A'' species will be out of plane.

The ab initio optimized structures of all the possible hydrogen conformers of the isomers of dihydroxyquinone are illustrated in (Table 1-4). The tables also show the correlation factors for the experimental and calculated geometrical parameters (bond lengths and bond angles) and vibrational frequencies. The experimental vibration values of the compounds are taken from the web page of Rio-Db Spectral Database for Organic Compounds [19], and the experimental parameters from the literature [20-24]. The correlation graphic at DFT 6-31G (d,p) level for alizarin are drawn in (Figure 1). In (Table 1- 4) are also given the sum of electronic and zero-point energies. As seen from these tables the correlation factors for the conformers with minimum energy of all the isomers are almost best. So, for all the compounds the preferential conformer in the ground state is the conformer with the doubly bonded O atom linked intramolecularly by the two hydrogen bonds. The tables also show the relative energies and the mean vibrational deviations ($|\Delta\nu|_{\text{ave}}$) between the calculated

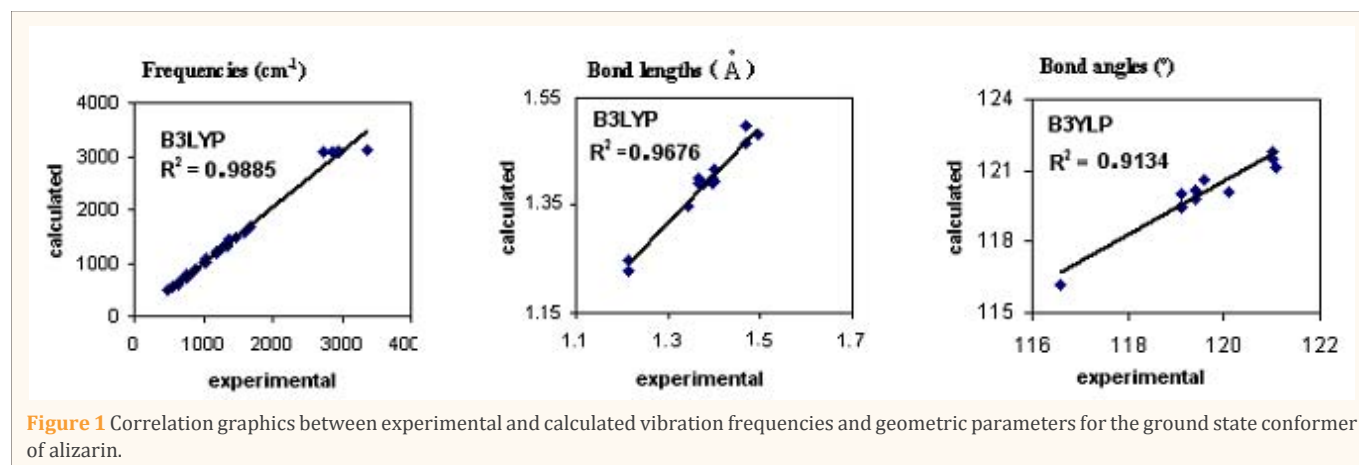


Figure 1 Correlation graphics between experimental and calculated vibration frequencies and geometric parameters for the ground state conformer of alizarin.

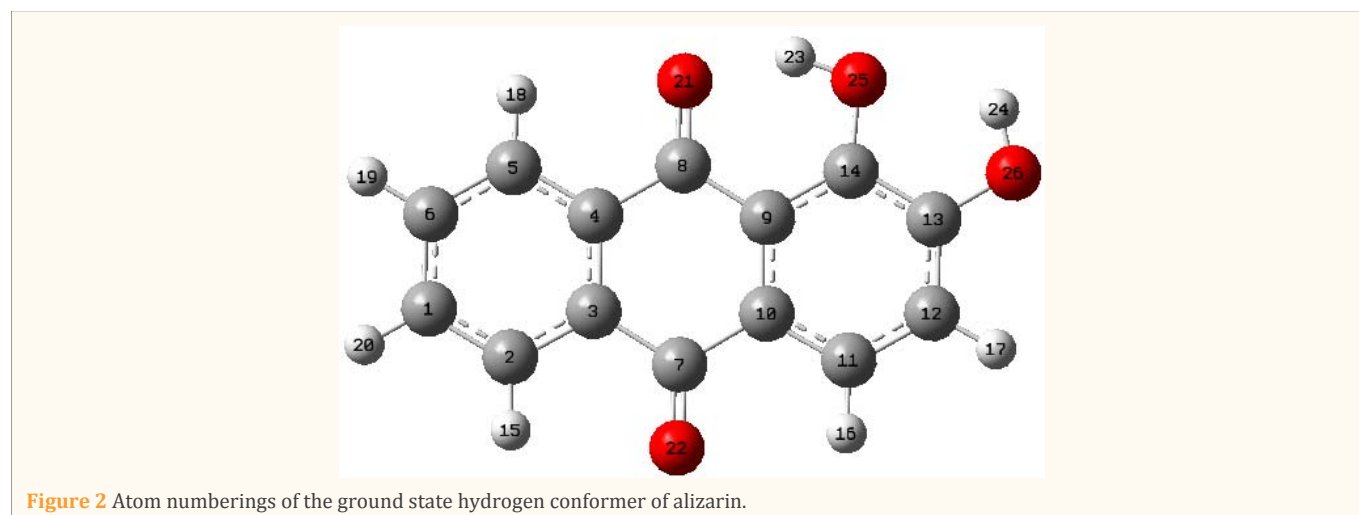


Figure 2 Atom numberings of the ground state hydrogen conformer of alizarin.

Table 1: Sum of electronic and zero point energies, relative energies and correlation factors for the possible conformations of alizarin, calculated at B3LYP [6-31G (d,p)].

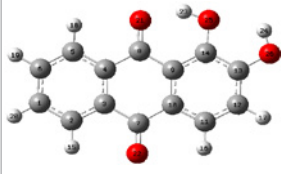
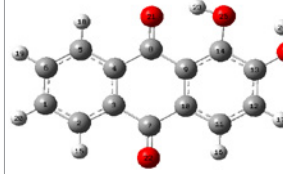
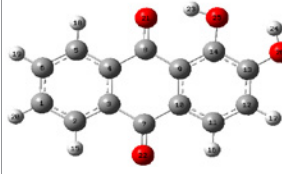
Conformation				
	I	II	III	
Sum of electronic and zero point energy (Hartree/particle)	-839.061304	-839.052911	-839.038278	
Relative energy (kcal/mol)	0.0	5.26	14.44	
Vibrational deviation $ \Delta v _{ave}$	0.0	7.46	24.93	
Correlation factor	Frequencies	0.9885	0.9899	0.9976
	Bond lengths	0.9676	0.9652	0.9803
	Bond angles	0.9134	0.5047	0.4558

Table 2: Sum of electronic and zero point energies, relative energies and correlation factors for the possible conformers of quinizarin, calculated at B3LYP [6-31G (d,p)].

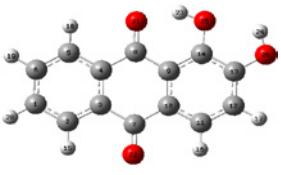
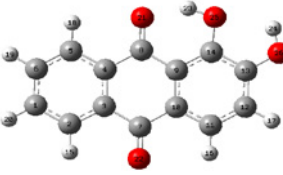
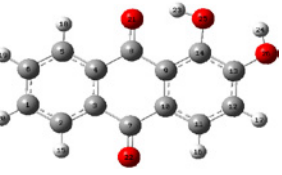
Conformation				
	I	II	III	
Sum of electronic and zero point energy (Hartree/particle)	-839.069404	-839.046979	-839.02363	
Relative energy (kcal/mol)	0	14.06	28.70	
Vibrational deviation $ \Delta v _{ave}$	0	21.38	21.85	
Correlation factor	Frequencies	0.9878	0.9996	0.9995
	Bond lengths	0.9733	0.9682	0.9737
	Bond angles	0.8300	0.7420	0.6499

Table 3: Sum of electronic and zero point energies, relative energies and correlation factors for the possible conformers of dantron, calculated at B3LYP [6-31G (d,p)].


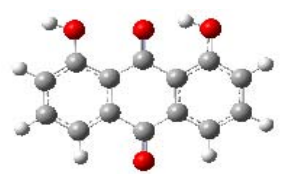
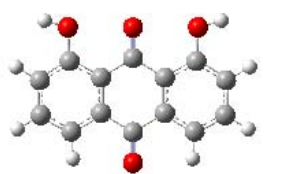
Conformation				
	I	II	III	
Sum of electronic and zero point energy (Hartree/particle)	-839.068724	-839.049242	-839.026133	
Relative energy (kcal/mol)	0	12.22	26.71	
Vibrational deviation $ \Delta v _{ave}$	0	19.11	36.04	
Correlation factor	Frequencies	0.9846	0.9976	0.9975
	Bond lengths	0.9878	0.9817	0.9681
	Bond angles	0.9175	0.8652	0.7630

Table 4: Sum of electronic and zero point energies, relative energies and correlation factors for the possible conformers of anthraflavic acid, calculated at B3LYP [6-31G (d,p)].




Conformation				
	I	II	III	
Sum of electronic and zero point energy (Hartree/particle)	-839.048803	-839.047633	-839.046533	
Relative energy (kcal/mol)	0	0.734	1.423	
Vibrational deviation $ \Delta v _{ave}$	0	3.04	5.88	
Correlation factor	Frequencies	0.9803	0.9818	0.9816
	Bond lengths	0.9817	0.9813	0.9814
	Bond angles	0.8886	0.8684	0.8459

Table 5: Experimental and calculated vibration frequencies of the possible conformers of alizarin.

Sym.	Assignments	Exp.* freq.(cm ⁻¹) IR	B3LYP 6-31G (d,p)		
			I	II	III
			A'	v(OH)	3602
A'	v(CH)	3371	3104	3129	3609
A'	v(CH)		3100	3104	3105
A'	v(CH)		3194	3101	3099
A'	v(CH) + v(OH)	2955	3089	3098	3096
σ_h	v(OH) + v(CH)	2925	3083	3081	3078
A'	v(CH) + v(OH)	2864	3081	3067	3064
A'	v(CH)	2731	3068	3048	3052
$ \Delta v _{ave}$	v(C=O)	1664	1677	1676	1686
A'	v(C=O) + δ (OH) + v(C-OH)	1633	1629	1633	1675
A'	v(ring) + δ (CH) + δ (OH)	1588	1585	1585	1585
A'	v(ring) + δ (CH) + δ (OH)		1580	1579	1582
A'	v(ring) + δ (CH) + δ (OH)		1577	1569	1574
A'	v(ring) + δ (CH)		1560	1561	1566
A'	v(ring) + δ (CH) + δ (OH) + v(C=O)	1462	1468	1468	1471
A'	δ (CH) + v(ring) + δ (OH)		1457	1462	1461
A'	δ (OH) + v(ring) + δ (CH)		1450	4561	1447
A'	v(ring) + δ (CH)		1437	1436	1434
A'	v(ring) + δ (OH) + δ (CH)	1377	1396	1374	1361
A'	v(ring) + δ (CH) + δ (OH)	1350	1346	1350	1324
A'	v(ring) + δ (CH) + δ (OH)	1331	1324	1327	1296

A'	$\nu(\text{C-OH}) + \delta(\text{OH}) + \delta(\text{CH}) + \delta(\text{ring})$		1316	1324	1294
A'	$\nu(\text{C-OH}) + \delta(\text{CH}) + \delta(\text{ring}) + \delta(\text{OH})$	1298	1286	1282	1269
A'	$\delta(\text{CH}) + \delta(\text{OH}) + \nu(\text{ring})$	1271	1271	1277	1261
A'	$\delta(\text{OH}) + \delta(\text{CH})$		1245	1246	1235
A'	$\delta(\text{OH}) + \delta(\text{CH})$	1199	1209	1204	1178
A'	$\delta(\text{CH}) + \delta(\text{OH})$	1185	1177	1173	1164
A'	$\delta(\text{CH}) + \delta(\text{OH})$		1165	1148	1139
A'	$\delta(\text{CH})$		1140	1139	1131
A'	$\delta(\text{CH})$		1130	1135	1123
A'	$\delta(\text{CH}) + \delta(\text{ring})$	1047	1073	1074	1074
A'	$\delta(\text{CH})$	1033	1031	1029	1026
A'	$\delta(\text{CH}) + \delta(\text{ring})$	1013	1014	1016	1001
A'	$\delta(\text{CH}) + \delta(\text{ring}) + \delta(\text{C-OH})$		996	998	989
A''	$\gamma(\text{CH})$		979	978	977
A''	$\gamma(\text{CH})$		958	958	959
A''	$\gamma(\text{CH})$		938	921	923
A''	$\gamma(\text{CH})$		888	887	887
A'	$\delta(\text{ring}) + \delta(\text{C=O})$	896	873	875	873
A''	$\gamma(\text{CH}) + \gamma(\text{OH})$	848	832	826	806
A'	$\delta(\text{ring}) + \gamma(\text{C=O})$	829	818	813	802
A''	$\gamma(\text{OH}) + \gamma(\text{CH})$		812	809	783

Table 5: Continued.

A''	$\gamma(\text{CH}) + \gamma(\text{OH}) + \gamma(\text{ring})$	763	780	779	769
A''	$\gamma(\text{CH}) + \gamma(\text{ring})$	757	759	760	733
A'	$\delta(\text{ring})$	749	737	736	711
A''	$\gamma(\text{CH}) + \gamma(\text{ring})$	714	706	707	686
A''	$\gamma(\text{ring})$	676	676	686	668
A'	$\delta(\text{ring}) + \delta(\text{C=O}) + \delta(\text{C-OH})$	661	670	668	648
A''	$\gamma(\text{ring})$		649	656	646
A'	$\delta(\text{ring})$		647	647	601
A'	$\delta(\text{ring}) + \delta(\text{C-OH})$	621	604	603	560
A'	$\delta(\text{ring})$	582	562	559	559
A''	$\gamma(\text{ring})$		557	559	492
A''	$\gamma(\text{OH})$	487	495	484	481
A''	$\gamma(\text{OH}) + \gamma(\text{ring})$		474	473	467
A'	$\delta(\text{ring}) + \delta(\text{OH})$		469	457	447
A'	$\delta(\text{ring}) + \delta(\text{C-OH})$		458	441	436

A''	$\gamma(\text{ring})$		439	414	412
A''	$\gamma(\text{ring})$		412	411	381
A'	$\delta(\text{C=O}) + \delta(\text{ring})$		410	380	371
A'	$\delta(\text{ring}) + \delta(\text{C-OH})$		381	380	341
A'	$\delta(\text{C-OH}) + \delta(\text{C=O})$		335	336	328
A''	$\gamma(\text{ring}) + \gamma(\text{C-OH})$		327	325	313
A'	$\delta(\text{ring})$		316	316	279
A'	$\rho(\text{OH}) + \rho(\text{C=O}) + \rho(\text{ring})$ in the plane		278	284	264
A''	$w(\text{ring}) + w(\text{OH})$		248	245	233
A'	$\rho(\text{ring})$ in the plane		187	191	184
A''	$w(\text{ring}) + w(\text{C=O}) + w(\text{C-OH})$		177	173	172
A''	$\rho(\text{ring})$ out of plane + $w(\text{C-OH}) + w(\text{C=O})$		140	138	121
A''	$\rho(\text{ring}) + w(\text{C-OH}) + w(\text{C=O})$		122	121	114
A''	$\rho(\text{ring})$ out of plane		92	91	73
A''	$w(\text{ring})$		48	46	35

v: stretching; δ : bending; γ : out of plane bending; ρ : rocking; w: wagging.
 *Taken from Ref. [15].

Table 6: Experimental and calculated bond lengths of the possible conformers of alizarin.

Bond lengths (Å)	Exp.*	B3LYP 6-31G (d,p)		
		I	II	III
C1-C2	1.399	1.416	1.423	1.415
C1-O1	1.343	1.347	1.334	1.349
O1-H1		0.998	0.995	0.971
C1-C11		1.403	1.411	1.407
C2-O2		1.352	1.356	1.371
O2-H2		0.972	0.967	0.965
C2-C3	1.397	1.390	1.390	1.387
C3-H3		1.085	1.088	1.088
C3-C4	1.365	1.399	1.399	1.394
C4-H4		1.084	1.084	1.084
C4-C12	1.379	1.392	1.388	1.393
C12-C11		1.421	1.422	1.422
C12-C10	1.495	1.481	1.483	1.490
C10-O10	1.214	1.228	1.228	1.228
C10-C14	1.469	1.497	1.494	1.487
C14-C13		1.410	1.409	1.406
C14-C5		1.398	1.398	1.400
C5-H5		1.085	1.085	1.085
C5-C6	1.399	1.393	1.393	1.391
C6-H6		1.086	1.066	1.086
C6-C7	1.397	1.399	1.400	1.400
C7-H7		1.086	1.086	1.086
C7-C8	1.365	1.392	1.392	1.392

C8-H8		1.084	1.084	1.085
C8-C13		1.400	1.400	1.400
C13-C9	1.495	1.481	1.484	1.499
C9-O9	1.214	1.248	1.247	1.224
C9-C11	1.469	1.465	1.466	1.491

*Taken from Ref. [16].

Table 7: Experimental and calculated bond angles of the possible conformers of alizarin.

Bond angles (°)	Exp.*	B3LYP 6-31G(d,p)		
		I	II	III
C1-O1-H1		105.7	105.8	107.3
O1-C1-C11		123.8	123.3	122.3
C2-C1-C11	120.1	120.1	119.0	119.3
C2-C1-O1		116.1	117.7	118.3
C1-C2-C3	119.4	119.8	119.8	121.5
C1-C2-O2		119.2	116.2	114.4
C2-O2-H2		107.3	109.2	110.3
O2-C2-C3		120.9	124.0	124.4
C2-C3-C4		120.2	121.0	119.4
C2-C3-H3		118.6	119.1	119.9
C4-C3-H3		121.2	119.9	120.7
C3-C4-C12		120.8	120.3	120.4
C3-C4-H4		120.8	121.1	121.3
C12-C4-H4		118.3	118.6	118.3
C4-C12-C10		119.8	119.1	117.3
C4-C12-C11		119.6	119.7	121.0
C10-C12-C11	119.6	120.6	121.1	121.8
C12-C10-C14		117.3	117.3	117.7
C12-C10-O10		122.0	121.8	121.2
C14-C10-O10		120.7	120.9	121.1
C10-C14-C13	121.0	121.5	121.2	120.8
C10-C14-C5		119.0	119.1	119.2
C5-C14-C13	119.1	119.5	119.6	120.0
C14-C5-C6		120.2	120.2	120.1
C14-C5-H5		118.1	118.1	118.2
C6-C5-H5		121.7	121.7	121.7
C5-C6-C7	119.4	120.2	120.2	120.0
C5-C6-H6		119.8	119.9	120.0
C7-C6-H6		119.9	119.9	120.0
C6-C7-C8		120.1	120.1	120.2
C6-C7-H7		120.0	120.0	119.9
C8-C7-H7		119.9	119.9	119.9
C7-C8-C13	119.1	120.0	120.0	120.2
C7-C8-H8		121.5	121.5	121.7
C13-C8-H8		118.5	118.5	118.1
C8-C13-C9		119.4	119.3	118.4
C8-C13-C14		120.0	119.9	119.5
C9-C13-C14	119.6	120.6	120.9	122.0

C13-C9-C11	116.6	116.2	118.4	117.3
C13-C9-O9		120.7	120.2	119.9
C11-C9-O9	121.1	121.1	120.4	122.7
C9-C11-C12	121.0	121.8	121.1	120.4
C9-C11-C1		118.8	118.8	121.1
C1-C11-C12	119.1	119.4	120.1	118.5

* Taken from Ref. [16].

vibrational frequency values of the conformers. The relative energy values and vibrational deviations are respect to the conformer with minimum energy. As seen, the mean vibrational deviation increases while the relative energy increases. This is an expected result since the more different the molecular structure of the conformer is the higher the relative energy is between them, and so a bigger mean vibrational deviation occurs. This comment has also been given for pyridine carboxaldehyde and difluorobenzaldehyde molecules in our previous studies [25,26].

The resulting vibrational frequencies and proposed vibrational assignments for all the possible conformers of alizarin are given in (Table 5). The table also shows the experimental vibrations of the compounds. The proposed vibrational assignments in the table well correspond to the assignments given in [27]. The calculated vibrations are scaled and their symmetry species are written in the first column of the table. As we said before, the vibrations in plane belong to the A' species and the ones out of plane to the A'' species. This was corrected by means of the visual inspection of all the vibrations.

Table 6, 7 shows the calculated optimized structure parameters (bond lengths and bond angles, respectively) for all the possible conformers of alizarin isomer of the title molecule, in corresponding to the atom numberings in (Figure 2). As seen the parameters in the tables are close to their corresponding experimental values.

CONCLUSION

In this study the ground state hydrogen conformers of the isomers of dihydroxyquinone were investigated using density functional theory (B3LYP) method with 6-31G (d,p) basis set. As expected for the conformers with minimum energy of all the isomers the best correlation factors between the experimental and calculated geometrical parameters (bond lengths and bond angles) and vibrational frequencies were obtained. It was concluded that all the isomers exist with the doubly bonded O atom linked intramolecularly by the two hydrogen bonds in the ground state. The vibrational analysis of the conformers of all the isomers of the compound was made. The proposed vibrational assignments and their symmetry species and optimized geometry parameters for all the possible conformers of alizarin were written. It was also seen that the mean vibrational deviation between the calculated vibrational frequency values of all the conformers of the isomers increases while the relative energy increases. Therefore it was emphasized that the more different the molecular structure of the conformers is the higher the relative energy is between them, and so, a bigger mean vibrational deviation arises.

REFERENCES

1. Thomson RH. Naturally Occurring Quinones. Academic Press, New York, 1971.
2. Carter TP, Gillisple GD, Connolly A. Intramolecular hydrogen bonding probed by laser-induced fluorescence. 1. 1,4-Dihydroxyanthraquinone (Quinizarin). J Phys Chem. 1982; 86: 192-196.
3. Smulevich G, Angeloni L, Giovannardi S, Marzocchi MP. Resonance Raman and polarized light infrared spectra of 1,4-dihydroxyanthraquinone. Vibrational studies of the ground and excited states. Chem. Phys. 1982; 65: 313-322.
4. Dutta PK, Lee BS. Optical spectroscopic studies of the polymorphic forms of 1,4 dihydroxy anthraquinone. J. Raman Spectrosc. 1988; 19: 175-178.
5. Smulevich G, Amirav A, Even U, Jortner J. Electronic-vibrational excitations of a hydrogen-bonded molecule in supersonic expansions: 1,4-dihydroxyanthraquinone and its deuterated derivatives. J Chem Phys. 1982; 73: 1-18.
6. Nigam GD, Deppisch BZ. Redetermination of the structure of 1,4-dihydroxyanthraquinone (C14H8O4). Kristallogr. 1980; 151: 185-191.
7. Smulevich G, Foggi P, Feis A, Marzocchi MP. Fluorescence excitation and emission spectra of 1,8-dihydroxyanthraquinone-d0 and -d2 in n.octane at 10 K. J Chem Phys. 1987; 87: 5664-5669.
8. Gillispie GD, Balakrishnan N, Vangsness M. Intramolecular hydrogen bonding. X. Comparison of free jet and Shpol'skii matrix electronic spectra of 1,8-dihydroxyanthraquinone. Chem Phys. 1989; 136: 259-269.
9. Smulevich G, Marzocchi MP. Raman excitation profiles of 1,8-dihydroxyanthraquinone at 8K. Chem Phys. 1986; 105: 159-171.
10. Smulevich G, Marzocchi MP. Single crystal and polarized infrared spectra of two forms of 1,8- dihydroxyanthraquinone. Vibrational assignment and crystal structures. Chem Phys. 1985; 94: 99-108.
11. Ferreira ML, Rodriguez-Otero J. Ab initio studies of the intramolecular proton transfer in dihydroxyanthraquinones. J Mol Struct. (Theochem). 2001; 542: 63-77.
12. Komiha N, Kabbaj OK, Chraibi M. A density functional study of alizarin two of its isomers and its transition metals and rare-earth complexes. J Mol Struct. (Theochem). 2002; 594: 135-145.
13. Xuan X, Wang X, Wang N. Theoretical study of molecular structure and vibrational spectra of 1,4-dihydroxyanthraquinone. Spectrochim Acta. 2011; 79: 1091-1098.
14. Yin C, Zhang J, Huo F. Combined spectral, experiment and theoretical calculation to study the interaction of 1,4-dihydroxyanthraquinone for metal ions in solution. Spectrochim Acta. 2013; 115A: 772-777.
15. Frisch MJ, et al. GAUSSIAN 03, Revision C.02, Gaussian Inc., Pittsburgh, PA, 2003.
16. Frish A, Nielsen AB, Holder AJ. Gauss View User Manual, Gaussian Inc.

- Pittsburg, PA, 2001.
17. Young DC. Computational Chemistry: A Practical Guide for Applying Techniques to Real-World Problems, (Electronics), John Wiley & Sons, Inc., New York 2001.
18. Wilson EB, Decius JC, Cross PC. Molecular Vibrations, Dover Pub. Inc., New York 1980.
19. Rio-Db Spectral Database for Organic Compounds, Web Page, Japan 2001.
20. Hall D, Nobbs CL. The crystal and molecular structure of 1,5-dihydroxyanthraquinone. Acta Cryst. 1966; 21: 927-934.
21. Johnson O, Jones DW, Hazell RG, Sheldrick B. Structure of 1,4-dihydroxy-2-(1-hydroxy-2,3:4,5-di-O-isopropylidene-D-arabinityl)-9,10-anthraquinone. Acta Cryst. 1989; 45: 123-126.
22. Marasinghe PAB, Gillispie GD. Structure of 1,5-dihydroxyanthraquinone: a redetermination. Acta Cryst. 1993; 49: 113-114.
23. Zain SM, Ng SW. 1,8-Dihydroxyanthraquinone. Acta Cryst. 2005; E61: 2921-2923.
24. Adaboh RK, Kashino S. Disordered structure of 2-methylanthraquinone. Acta Cryst. 1995; 51: 2094-2096.
25. Sağlam A, Ucun F, Güçlü V. Molecular structures and vibrational frequencies of 2-, 3- and 4-pyridine carboxaldehydes by ab initio Hartree-Fock and density functional theory calculations. Spectrochim. Acta 2007; 67A: 465-471.
26. Sağlam A, Ucun F. Conformational and vibrational analysis of 2-, 4-, 5- and 6-difluorobenzaldehydes by ab initio Hartree-Fock and density functional theory calculations. Z Naturforsch. 2008; 61: 175-182.
27. Fabriciova G, Garcia-Ramos JV, Miskovsky P, Sanchez-Cortes S. Adsorption and acidic behavior of anthraquinone drugs quinizarin and danthron on Ag nanoparticles studied by Raman spectroscopy. Vib Spect. 2004; 34: 273-281.

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