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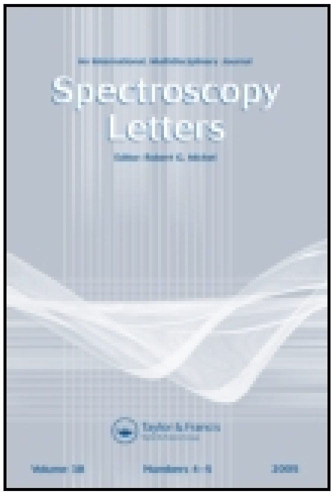

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A Comprehensive Study on Infrared Spectra of 2-Hydroxyxanthone

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A Comprehensive Study on Infrared Spectra of 2-Hydroxyxanthone

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ABSTRACT A study on the IR spectra of 2-hydroxyxanthone that was both experimental and theoretical was carried out in this work. The optimized structure and related spectral parameters were obtained by using the Becke-3-Lee-Yang-Parr (B3LYP) method with the 6-31G* and 6-311G** basis sets. The corresponding geometrical parameters were compared with each other. Detailed assignments of the vibration frequencies were performed. The agreement between the scaled theoretical frequencies and the observed frequencies was found to be quite good. Also, the calculation accuracies of the two basis sets are close.

KEYWORDS 2-hydroxyxanthone, B3LYP, IR

INTRODUCTION

Xanthones, 9H-xanthen-9-ones, are heterocyclic compounds with the dibenzo-γ-pyrone framework. The parent compound itself does not exist in the natural world, but its derivatives are widely distributed in nature. Naturally occurring xanthones are often separated from various parts of plants, such as Rheedia acuminata bark,[1] Cratoxylum cochinchinense,[2] Gentianuceae, Guttiferae, Anacardiaceae, and metabolic products of some lower fungi, for example, marine-derived fungi[3] and Penicillium raistrickii.[4] Early pharmacological studies have shown that xanthones have a very wide range of pharmacological activities and considerable bioactivity, including antibacterial, analgesic,[5] cytotoxic,[6] febrifuge,[7] antimalaria,[8] and antituberculosis[9] bioactivity. Due to their pronounced toxicity, they are classified as mycotoxins.[10]

Research on xanthone derivatives began in the 1960s. Synthesis and modification of natural xanthones not only form an important supplement to natural xanthones but also are very helpful to the development of new chemical entities. Also, studies on their vibration spectra might be useful for the design of novel drugs. However, to the best of our knowledge, the number of articles about the theoretical spectra of xanthones has been limited over the past few years. Therefore, an attempt was made in this work to comprehensively study the theoretical and experimental IR vibrational spectra of a xanthone derivative named "2-hydroxyxanthone." Vibrational spectroscopy has proven to be effective in the refinement of chemical structures as well as in researches on reaction kinetics of organic compounds.

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Also, this work can be of great help to understand spectral properties of its analogues.

In the current article, optimized geometrical parameters and IR vibrational frequencies are computed by DFT/B3LYP method with 6-31G* and 6-311G** basis sets. We choose the density functional theory (DFT) method rather than the Hartree-Fock (HF) method for the following two points. First, the DFT method requires relatively few computational resources.[11] Second, comparisons between the frequencies calculated with the two methods and the experimental values reveal that the DFT method predicts more accurately for the molecular structure and vibrational spectra. Furthermore, the observed vibrational spectrum is assigned and compared with the theoretical ones.

MATERIALS AND METHODS

General

Treatment of acetylsalicylic acid with thionyl chloride gave the acid chloride, which readily reacted with *p*-dimethoxy-benzene under the Friedel-Crafts conditions to form the benzophenone derivative. The precursor 2-methoxy-xanthone was synthesized via the reaction of the benzophenone derivative with potassium hydroxide and ethanol under reflux for 72 hr. Further treatment of 2-methoxy-xanthone with hydrobromic acid under reflux over nitrogen gave the crude product 2-hydroxyxanthone.

The infrared absorption spectra of 2-hydroxyxanthone diluted in the KBr pellets was recorded using a Nexus 470 FT-IR spectrophotometer (Thermo Nicolet Co., USA) at room temperature.

Method of Calculation

The structural geometry was optimized using B3LYP method at 6-31G* and 6-311G** levels of theories with the Gaussian 03 program.[12] Based on the Gaussian output files, IR vibration frequencies were obtained. Aided by the Gaussview program,[13] we made the vibrational assignments with a high degree of accuracy. In order to offset the errors resulting from electron correlation effects and basis-set deficiencies, the scaling factors were introduced to scale down the theoretical wave numbers.

RESULTS AND DISCUSSION

Molecular Geometry

The optimized structure and atomic numbering of the title compound is illustrated in Fig. 1. Note that rings of C1C2C3C4C5C6, C4C5C10C9C8O7, and C9C8C11C12C13C14 are defined as R1, R2, and R3, respectively. The absence of negative frequencies indicates that the molecule is at stationary point on the potential energy surface. The global minimum energy at B3LYP/6-31G* and B3LYP/6-311G** level is −725.880220 a.u. and −726.064465 a.u., respectively. In this study, geometry optimization parameters were obtained without symmetry constraints. The selected structural parameters, including bond lengths, bond angles, and dihedral angles, are reported in Table 1. Clearly, bond lengths calculated at the 6-31G* level are slightly larger than those obtained at the 6-311G** level. The largest deviation is in the O16-H24 bond, the value of which is only 0.008 Å. For bond angles, the situation is different. The values of C1C2C3 angle, C4C5C6 angle, and C4O7C8 angle computed at the two levels are equal. The bond angle values of C5C10O15 and H24O16C13 calculated with the small basis set are slightly smaller. However, a contrary trend was observed in cases of angles C5C10C9, C9C8C11, and C12C13C14. With regard to dihedral angles, the corresponding values are almost identical to each other. These values confirm the planar conformation of the molecule.

Vibrational Analysis

It is of interest to study the spectral features in IR spectra, which strongly correlate to those of vibrational structures. This enables us to identify chemical structures and to carry out researches on

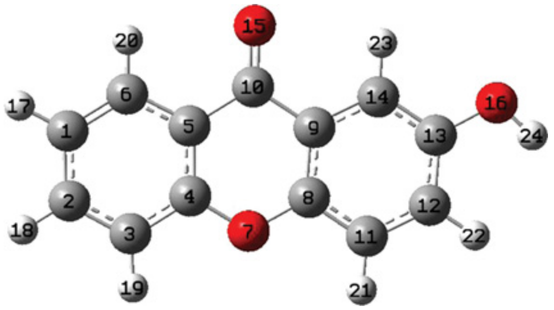

FIGURE 1 The optimized geometric structure and atom numbering of 2-hydroxyxanthone. (color figure available online.)

TABLE 1 Comparison of Selected Bond Lengths, Bond Angles, Dihedral Angles of 2-Hydroxyxanthone Computed Using DFT/B3LYP Method with Two Different Basis Sets

Parameters	B3LYP/6-31G*	B3LYP/6-311G**	O16-H24	0.970	0.962
Bond length (Å)					
C1-C2	1.406	1.403	C14-H23	1.084	1.082
C2-C3	1.388	1.385	C10 = O15	1.228	1.222
C3-C4	1.400	1.398	Bond angle (°)		
C4-C5	1.404	1.402	C1-C2-C3	120.8	120.8
C5-C6	1.406	1.405	C4-C5-C6	118.6	118.6
C4-O7	1.366	1.364	C4-O7-C8	119.5	119.5
O7-C8	1.371	1.370	C5-C10-C9	114.3	114.2
C8-C9	1.404	1.401	C9-C8-C11	120.6	120.5
C5-C10	1.477	1.477	C5-C10-O15	122.9	123.0
C9-C10	1.480	1.480	C12-C13-C14	119.7	119.6
C8-C11	1.397	1.395	H24-O16-C13	109.2	109.5
C9-C14	1.402	1.400	Dihedral angle (°)		
C11-C12	1.388	1.385	H19-C3-C4-O7	0.0	0.0
C12-C13	1.407	1.405	C6-C5-C10-O15	0.0	0.0
C13-C14	1.389	1.386	O15-C10-C9-C14	0.0	0.0
C13-O16	1.367	1.366	H24-O16-C13-C14	180.0	180.0

reaction kinetics. For instance, IR spectroscopy has been used in the structural elucidation of 1-phenylacridones.[14] The experimental frequencies with general mode assignments are summarized in Table 2. The observed IR spectrum is shown in Fig. 2. The detailed vibrational assignments of 2-hydroxyxanthone are briefly discussed in the following paragraphs.

TABLE 2 Experimental and Calculated Frequencies (cm^{-1}) and General Mode Assignments for 2-Hydroxyxanthone

		B3LYP/6-31G*				B3LYP/6-311G**		
		Freq.						
No.	Experimental Freq.^{a}	Unscaled	Scaled^b	IR intensity	Reduced mass	Unscaled	Scaled^c	Vibrational Assignments^d
1	–	326	313	119.7	1.1	311	301	γ O-H
2	562 w	569	547	11.8	3.3	569	551	γ C-H R3
3	622 m	641	616	17.9	7.2	642	622	δ-R1, δ-R3
4	753 ms	793	762	50.8	7.1	792	767	β C-O R2, δ-R3
5	826 m	822	790	31.4	1.7	830	804	γ C-H R3
6	872 w	900	865	2.5	7.0	895	867	trigonal ring breathing
7	1108 m	1170	1125	50.2	1.4	1158	1121	β C-H
8	1147 ms	1215	1168	123.8	1.5	1204	1166	β O-H
9	1230 s	1355	1303	391.1	2.6	1342	1299	v_{as} C-C
10	1305 m	1396	1342	83.7	5.2	1378	1334	v_{as} C-O R2, v C=C R3
11	1342 ms	1500	1442	100.1	3.0	1484	1437	v C=C R1, v C=C R3
12	1465 vs	1519	1460	187.9	3.0	1502	1454	v C=C R1, β O-H
13	1582 ms	1540	1480	185.5	3.1	1522	1474	v C=C R3
14	1620 s	1686	1621	45.7	6.7	1670	1617	v C=C R3
15	1655 s	1748	1680	223.7	12.4	1730	1675	v C=O
16	3196 s	3223	3088	4.6	1.1	3201	3067	v C-H
17	3314 s	3756	3598	59.0	1.1	3836	3675	v O-H

[a] vs: very strong; s: strong; ms: medium strong; m: medium; w: weak.

[b] With the scale factor of 0.958 for calculated wave numbers greater than 3000 cm^{-1} and the scale factor of 0.9613 for lower wave numbers.

[c] With the scale factor of 0.958 for calculated wave numbers greater than 3000 cm^{-1} and the scale factor of 0.9682 for lower wave numbers.

[d] v: stretching; v_{as}: asym. Stretching; β: in-plane bending; γ: out-of-plane bending; δ: deformation.

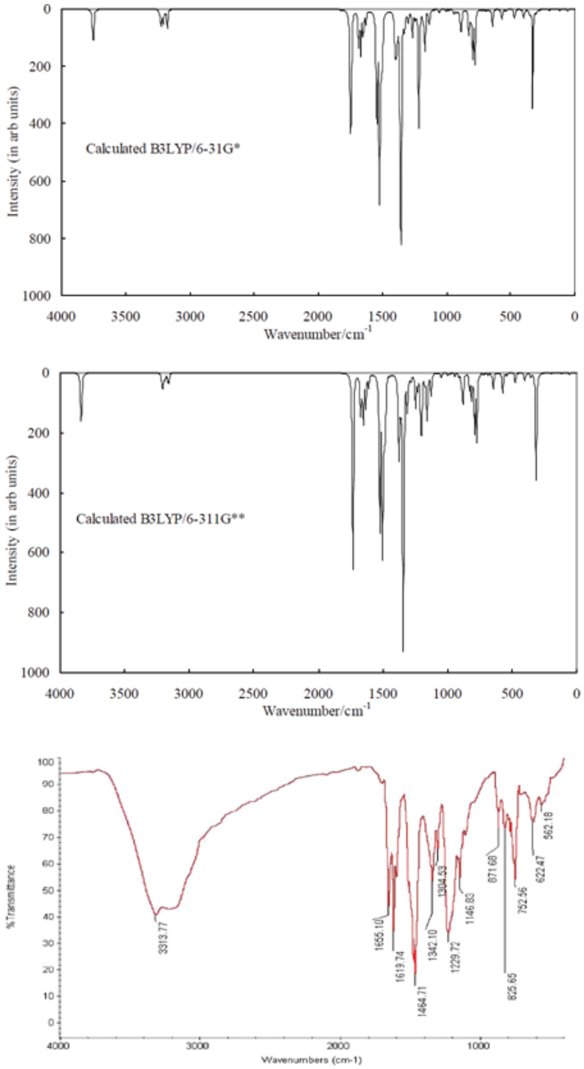

FIGURE 2 **The theoretical and experimental IR spectra of 2-hydroxyxanthone. (color figure available online.)**

O–H Vibrations

It is known that hydrogen bonding easily affects the O–H stretching vibrations. A free or non-hydrogen–bonded hydroxyl group absorbs strongly in the range of 3550–3700 cm^{-1}. The O–H stretching band would shift to the region 3200–3550 cm^{-1} if hydrogen bonding is present in a 5- or 6-membered ring system.[15] The strong band observed at 3314 cm^{-1} is assigned to O–H stretching vibration, showing that 2-hydroxyxanthone is hydrogen bonded. The O–H in-plane bending vibration appears as a medium-strength band at 1147 cm^{-1}, corresponding to the scaled frequencies at 1168 cm^{-1} on 6-31G* level and 1166 cm^{-1} on 6-311G** level. The calculated bands at 313 cm^{-1} for 6-31G* and 301 cm^{-1} for 6-311G** are ascribed to the O–H out-of-plane bending. However, this band is not observed in the IR spectrum.

C–H Vibrations

The band of C–H stretching vibration in the title compound was observed at 3196 cm^{-1} in the IR spectrum. For aromatic structures, the C–H in-plane bending modes usually arise in the region 1000–1300 cm^{-1}[16] In the present study, the C–H in-plane bending vibration showed as a medium band at 1108 cm^{-1}, which corresponds to the theoretical frequencies at 1125 cm^{-1} on 6-31G* level and 1121 cm^{-1} on 6-311G** level. A medium IR band observed at 826 cm^{-1}, in reasonable agreement with the computed data 790 cm^{-1} (6-31G*) and 804 cm^{-1} (6-311G**), is assigned to C–H out-of-plane bending vibration in R3. Another weak IR band at 562 cm^{-1} is assigned to this mode, too. The calculated bands at 547 cm^{-1} for 6-31G* and 551 cm^{-1} for 6-311G** well match the experimental result.

C=O and C–O Vibrations in Ring R2

The stretching frequency of the carbonyl group has been most extensively studied by infrared spectroscopy. Since the electronegativity of carbon and oxygen is different, the bonding electrons are not equally distributed along the two atoms. The lone pairs of electrons on oxygen also have influence on the nature of the carbonyl group. This highly polar group usually gives rise to an intense infrared absorption band. For the title molecule, the strong C=O stretching vibration is observed at 1655 cm^{-1} in IR spectra, which agrees well with the scaled values at 1680 cm^{-1} (6-31G*) and 1675 cm^{-1} (6-311G**).

The theoretical frequencies at 1342 cm^{-1} on 6-31G* level and 1334 cm^{-1} on 6-311G** level with medium intensity are both in reasonable agreement with the experimental data (1305 cm^{-1} in IR spectrum). The observation from the Gaussview program reveals that the vibration mainly results from the combination of the C-O asymmetric stretching and the R3 C=C aromatic semicircle stretching vibration. The band appeared at 753 cm^{-1}, which corresponds to 762 cm^{-1} on 6-31G* level and 767 cm^{-1} on 6-311G** level, and is assigned to C-O in-plane bending vibration interacting with deformation of R3.

Ring Vibrations

The peak observed at 622 cm^{-1}, which corresponds to the theoretical data at 616 cm^{-1} on 6-31G* level and 622 cm^{-1} on 6-311G** level, results from the coupling of the ring deformation vibrations of R1 and R3. The trigonal ring breathing vibration is observed at 872 cm^{-1}. And the calculated bands at 865 cm^{-1} for 6-31G* and 867 cm^{-1} for 6-311G** well match the observation. The medium strong IR band at 1342 cm^{-1}, corresponding to the calculated values at 1442 cm^{-1} on 6-31G* level and 1437 cm^{-1} on 6-311G** level, is mainly due to the C=C stretching vibrations of the two phenyl rings. The R1 ring stretching vibration appears at 1465 cm^{-1} in the IR spectrum, which shows excellent agreement with the scaled frequencies at 1460 cm^{-1} for 6-31G* and 1454 cm^{-1} for 6-311G**. This band is coupled with in-plane bending of OH. The R3 C=C stretching vibrations showed as two absorptions, the medium strong band at 1582 cm^{-1} and the strong band at 1620 cm^{-1}. Both of the experimental frequencies are consistent with the corresponding theoretical values.

Comparisons of the Experimental and Theoretical Frequencies

Due to the combination of vibrational anharmonicity and basis-set incompleteness, the DFT/B3LYP method tends to overestimate the fundamental frequencies. It is necessary to scale down the calculated vibrational frequencies so that they can fit with the experimental ones. The work done by Palafox et al. describes the interest and necessity of scaling to correct the deficiencies in the calculation of the harmonic vibrational wave numbers.[17] The vibrational frequencies greater than 3000 cm^{-1} are uniformly scaled by 0.958, and the lower wave numbers are scaled by 0.9613 at the 6-31G* level and 0.9682 for the 6-311G** basis set.[18] The unscaled and scaled wave numbers are also reported in Table 2. It can be seen from Table 2 that after application of the scaling factors, the theoretical calculations agree well with the experimental data. Comparison between the calculated and observed vibrational spectra helps us to further understand the vibrational modes. The calculated IR spectrum is also shown in Fig. 2 for visual comparisons. In addition, a correlation graph between the scaled and observed frequencies is adopted to judge the prediction agreement with experiment (Fig. 3).

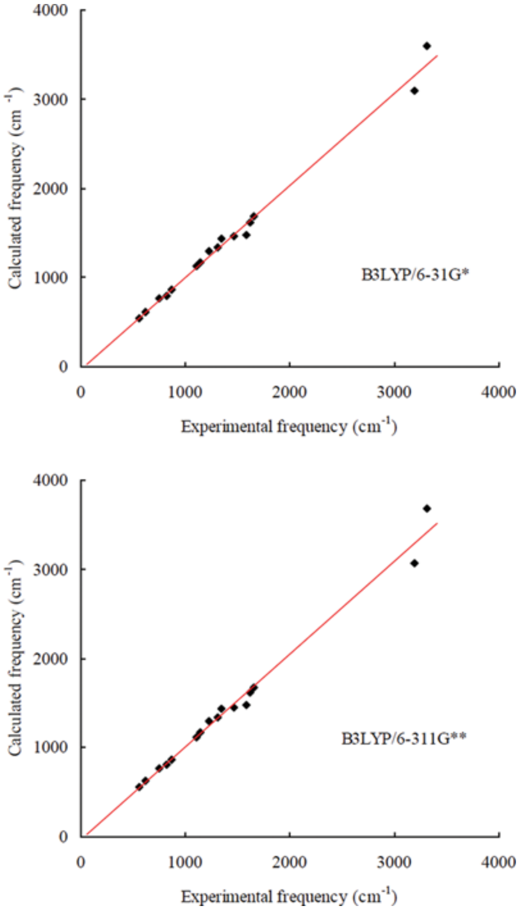

FIGURE 3 Correlation graph between the scaled and the observed frequencies at different level of theories. (color figure available online.)

Using the least squares method, the correlation equation between the theoretical values calculated at the B3LYP/6-31G* level and the experimental frequencies is obtained as follows:

$$\begin{aligned} y &= 1.0353\,x - 31.853 \\ r^2 &= 0.9898 \end{aligned} \tag{1}$$

Also, the correlation equation between the calculated frequencies at the B3LYP/6-311G** level and the experimental data is as follows:

$$\begin{aligned} y &= 1.0446\,x - 42.244 \\ r^2 &= 0.9859 \end{aligned} \tag{2}$$

Obviously, for the two correlation equations, the slopes are almost equal to 1.00, the intercepts are relatively small, and the squared correlation coefficients r^2 are larger than 0.98, indicating that good linearity relationships exist between the scaled and experimental frequencies.

CONCLUSION

A relatively comprehensive study on the vibrational spectrum of 2-hydroxyxanthone was carried out. The molecular geometry was optimized by B3LYP method with 6-31G* and 6-311G** basis sets. The vibrational frequencies were then calculated using the same method and compared with the experimental values. In general, the scaled theoretical vibration frequencies are consistent with the observations. The small basis set 6-31G* gives the best match to the observed spectra, and also this method provides the best linearity between calculated and experimental wave numbers (with a correlation coefficient of 0.9898). The larger squared correlation coefficients ($r^2 > 0.98$) indicate that the computed values may reproduce the observed frequencies. Furthermore, vibrational modes were assigned with a high degree of accuracy by employing the Gaussview program.

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