

Spectroscopic characterization (FT-IR, RAMAN and UV–VIS), thermogravimetric analysis, XPD and DFT calculations of highly stable hydroxy-functionalized chalcone: (2E)-1-(4-hidroxyphenyl)-3-(4-methoxyphenil)-prop-2-en-1-one

J.R.P.S. Souza^{a,b}, G.V.S. Mota^b, H.R. Bitencourt^b, S.G. Moreira^b, C.M.R. Remédios^{b,*}

^a Instituto Federal de Educação, Ciência e Tecnologia do Pará, Belem, 66093-020, Pará, Brazil

^b Institute of Exact and Natural Sciences, Federal University of Pará at Belém, 66075-110, Brazil

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ABSTRACT

(2E)-1-(4-hydroxyphenyl)-3-(4-methoxyphenyl)-prop-2-en-1-one, a hydroxy-functionalized chalcone has been characterized by FT-IR, RAMAN and UV–VIS spectroscopy, thermogravimetric analysis, X-ray powder diffraction, and DFT calculations. The detailed assignments of vibrational modes are compared with the literature and supported by theoretical calculations. The calculated energy gap at B3LYP/6–311++G(2d,2p) level shown values of 2.97 eV and 2.8 eV for experimental data. The intermolecular interaction in the solid state is responsible for the small differences between theoretical optimized geometry and experimental parameters. Thermogravimetric analysis shows very high thermal stability, and the spectroscopic UV–VIS shows that the compound under analysis has the potential for possible applications in organic LEDs.

1. Introduction

Organic materials often present easy flexibility for structural modifications and may exhibit very interesting physical or biological properties. Among these are chalcones and chalcone derivatives [1]. Chalcones are a group of plant-derived polyphenolic compounds belonging to the flavonoid family that are characterized by two aromatic rings linked by an α , β -unsaturated ketone system. They belong to the class of benzylideneacetophenones and serve as precursors in the biosynthesis of flavonoids and isoflavonoids [1]. Chalcone derivatives possess remarkable features, which are often attributed to the presence of the α , β -unsaturated moiety. By introducing different substituents into the two aryl rings, a valuable structure-activity relationship can be established. For instance, the incorporation of hydroxyl groups into either ring yields hydroxychalcone derivative compounds, which find diverse applications in pharmacology and industry.

Chalcones have been extensively investigated for various applications, including nonlinear optics (NLO) [2], as well as possessing a wide variety of cytoprotective and modulatory functions. Their biological activity may have therapeutic potential for multiple diseases, such as anti-cancer [3], antileishmanial [4], anti-tuberculosis [5], antimicrobial

[6,7], anti-malarial [8], antifungal [9], and anti-inflammatory [10–12]. Synthesizing new organic compound derivatives and advancing their pharmacological applications have been the focus of considerable effort, encompassing precise control over molecular synthesis, as well as a comprehensive understanding and description of their properties [13–18]. This effort includes the study of the vibrational properties through detailed spectroscopic assessments. For instance, previous studies have reported comprehensive surveys regarding the preparation, structural characterization, spectroscopic analysis, complemented by theoretical approaches, to investigate the molecular vibrations, boundary orbitals, and electronic transitions of four hydroxy-substituted chalcones. It was determined that the four synthesized chalcone derivatives are semiconducting materials and have potential for application in the development of OLEDs [19].

In previous work, X-ray diffraction studies have shown that the hydroxy-functionalized chalcone (2E)-1-(4-hydroxyphenyl)-3-(4-methoxyphenyl)-prop-2-en-1-one crystallizes as an orthorhombic structure, space group *Pbca* (61), with eight molecules per unit cell and lattice parameters: $a = 13.4563(16)$ Å, $b = 11.4986(14)$ Å, $c = 16.720(2)$ Å, $V = 2587.1(5)$ Å³ [20]. In this work, we present the results of a combined experimental and theoretical spectroscopic characterization

* Corresponding author.

E-mail address: remedios@ufpa.br (C.M.R. Remédios).

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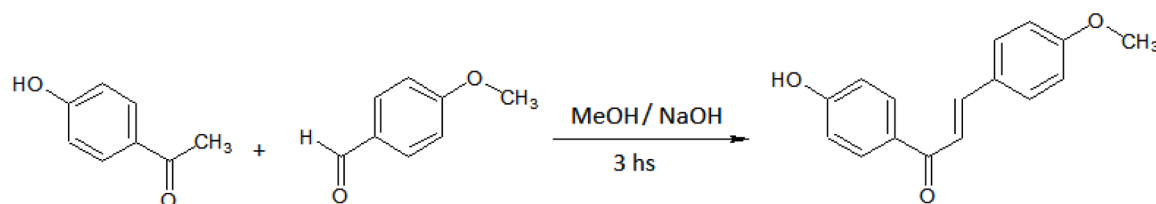


Fig. 1. Chemical reaction equation of the synthesis of the title compound.

(Raman, FT-IR absorption, and UV-VIS), thermogravimetric analysis, and DFT calculations of this compound. To the best of our knowledge, characterizations like these for this specific compound have not been reported before.

1.1. Experimental

The title compound was obtained in a flat-bottomed flask (250 mL). 10 mmol of 4-hydroxy acetophenone, 10 ml of sodium hydroxide solution (10 %), and 10 mmol of 4-anisaldehyde (Fig. 1) were stirred in 20 ml of methanol at room temperature during 3 h. After this period, the reaction solution was acidified with acetic acid (25 %), extracted with chloroform, washed with distilled water (3 times) and dried with anhydrous Na_2SO_4 . After filtration and evaporation, a liquid material was obtained from which a colorless crystalline solid material (74,36 %) precipitated.

Conventional X-ray powder diffraction was carried out on a Bruker D8 Advance diffractometer operating at 40 kV/40 mA and using Cu- K_α radiation ($\lambda = 1.54,056 \text{ \AA}$). The diffraction patterns were obtained in a counting time of 1 s/step with steps of 0.02° . The diffraction data was refined by Rietveld refinement using the General Structure Analysis System II (GSAS-II).

The Raman experiment was performed in the backscattering geometry, and the scattered light was analyzed by using a spectrometer iHR 320, Horiba; width resolution 0.06 nm and equipped with a charge-coupled-device (CCD) Synapse detector. The excitation source was a He-Ne laser emitting at 632.8 nm, and the slits of the spectrometer were set for a 2 cm^{-1} spectral resolution. A long-working distance plan achromatic objective ($f = 20.5 \text{ mm}$) was used to avoid the propagation of oblique phonons. The Raman spectra were obtained at room temperature in the $100\text{--}1800 \text{ cm}^{-1}$ spectral range. The band components were analyzed using the Peakfit software. The Lorentzian function was used to adjust bands in all spectra obtained. The vibrational assignments of the normal modes were made using the computed vibrational frequencies. In addition, the assignment of the modes was made by comparing the results with previous studies. The FT-IR spectra were measured using a BRUKER brand equipment, MODEL: VERTEX 70v.

Thermogravimetry (TGA) and differential thermal analysis (DTA) were performed on a Netzsch STA 449 F3 Jupiter thermal analyzer device for a temperature range to 303 K to 673 K with a heating rate of 10 K

min^{-1} .

The UV-VIS optical absorption spectroscopy was performed in ethanol solution by a xenon lamp with a power of 1000 W and an optical spectrophotometer, model USB2000. For the acquisition of emission spectra, a monochromator was used to select the excitation wavelengths. To select a specific wavelength, the samples were excited, using an Acton monochromator, model 300i, at 365 nm, in which the emission reaches high intensity. The time-resolved fluorescence signal was acquired using a Delta Flex Delayed Count Photon Count system developed by Horiba (27 ps temporal resolution), which is equipped with a pulsed LED (8 MHz repetition rate) as an excitation source (wavelength of excitation at the 352 nm).

1.2. Theoretical calculations

All quantum chemical computational were performed using DFT method at the triple-zeta 6-311++G(2d,2p) split valence-shell basis set, which was augmented by *d* and *p* polarization functions on all atoms as well as diffuse functions [21]. The initial geometry for the optimization was obtained from CIF file of the single crystal X-ray diffraction [20] (<https://www.ccdc.cam.ac.uk> (ID: CCDC- 1,842,374) and the Becke's gradient-corrected hybrid exchange-correlation (B3LYP) density functional [22,23] was used.

The optimization was performed in gas phase for four molecules due to the conformational configuration of the chalcone in the crystal (shown in Fig. 1), and then a single point calculation was used to minimize the energy of the system. In addition, the ethanol solvent effect was studied by means of the self-consistent reaction-field (SCRF) method based on PCM method by Tomasi and coworkers [24] in UV-VIS calculation. The calculated infrared vibrational frequencies were scaled with 0.9671 [25]. Raman spectra were used to identify the main contribution to the experimental spectra. UV-Vis spectral parameters were calculated using time dependent DFT [26] with B3LYP functional at the same basis set to obtain excitation energy and compare with the experimental UV-vis absorption spectra. All Quantum-chemical calculations were performed using the Gaussian 09 W package.

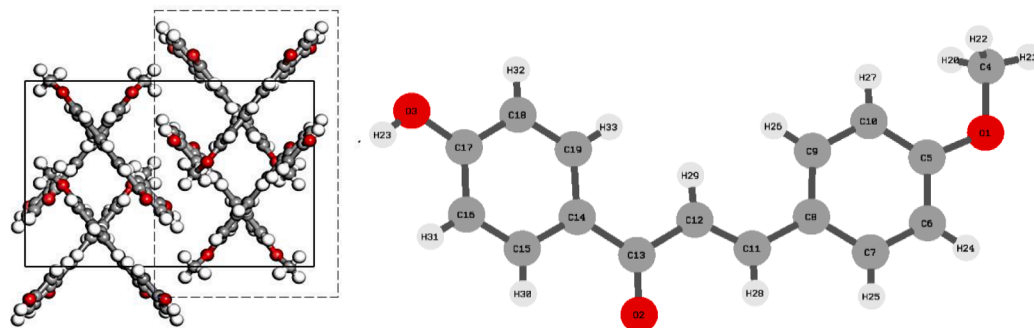


Fig. 2. Optimized structure (left) was performed at the B3LYP/6-311++G(2d,2p) level (dashed line) for the (2E)-1-(4-hydroxyphenyl)-3-(4-methoxyphenyl)prop-2-en-1-one chalcone. Molecular geometry (right) with respective atom position in each unit which compound the cell.

Table 1

Calculated and experimental geometric parameters (in Å and degree) of (2E)-1-(4-hydroxyphenyl)-3-(4-methoxyphenyl) prop-2-en-1-one chalcone.

Geometric parameters	Theoretical	Experimental [20]	% Error
O1 – C4	1.4309	1.424 (2)	0.48
O2 – C13	1.2345	1.234 (2)	0.04
C6 – C7	1.3860	1.378 (2)	0.58
C16 – C17	1.3945	1.387 (2)	0.54
C4 – O1 – C5	118.69	118.32 (12)	0.31
C6 – C7 – C8	121.68	122.35 (13)	0.55
O3 – C17 – C18	122.54	122.84 (12)	0.24
C4 – O1 – C5 – C6	179.99	175.62 (14)	2.43
O2 – C13 – C14 – C15	–179.99	–179.63 (13)	0.20
C15 – C14 – C19 – C18	0.0	–0.5 (2)	–

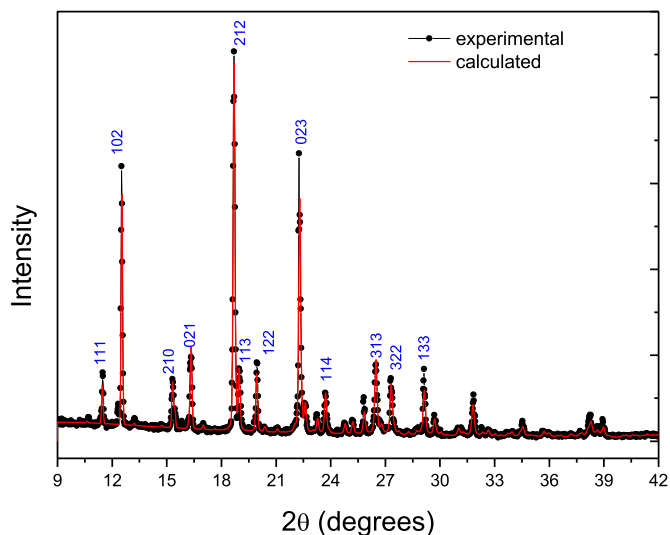


Fig. 3. Results of Rietveld profile refinement of the powder X-ray diffraction pattern of (2E)-1-(4-hydroxyphenyl)-3-(4-methoxyphenyl)prop-2-en-1-one.

2. Result and discussion

2.1. Structural analysis

The optimized molecular structure of (2E)-1-(4-hydroxyphenyl)-3-(4-methoxyphenyl) prop-2-en-1-one is shown in Fig. 2. The calculated bond lengths are present and compared with geometric parameters obtained by Yesilyurt et al. [20]. The crystal packing shows two relevant intermolecular hydrogen bonds, O3-H23::O2 and C11-H28::O1.

The structural parameters obtained with the B3LYP/6-311++G (2d,2p) level in the gas phase is listed in Table 1. The differences between the experimental and calculated data are due to intermolecular interactions, electron correlation effects, the anharmonicity negligence, and basis set deficiencies in the solid phase were ignored in the theoretical computations.

The calculated molecular geometry was compared with the experimental data and showed a good agreement with structures predicted in Ref. [20].

The percent error in the dihedral angle (C4 – O1 – C5 – C6) can be explained by that B3LYP does not include long-range dispersion corrections leading in some cases to errors in the molecular geometries. Furthermore, the effect of the electronegativity of the oxygen atom can, in some cases, affect the geometry due to the basis set superposition error (BSSE) [27]. However, the popular B3LYP functional is still capable of producing computational results in good agreement in describing molecular geometries obtained experimentally.

2.2. X-ray diffraction analysis

Powder X-ray diffraction measurements of the grown (2E)-1-(4-hydroxyphenyl)-3-(4-methoxyphenyl)prop-2-en-1-one crystal and the analysis by Rietveld refinement of obtained patterns were performed to check if the compound crystallized in the same symmetry and space group reported in the literature. The final values of the R factors were $R_p = 6.1\%$ and $R_{wp} = 8.4\%$. The diffraction pattern is shown in Fig. 3. This figure contains the observed data (black dots) and calculated (red

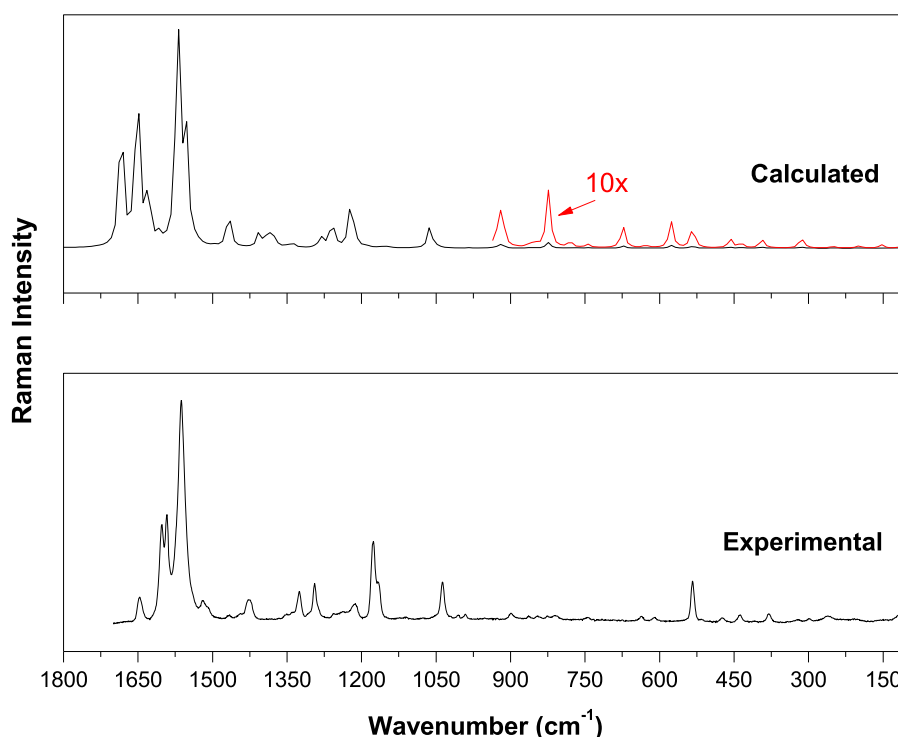


Fig. 4. Experimental and simulated Raman spectra of (2E)-1-(4-hydroxyphenyl)-3-(4-methoxyphenyl) prop-2-en-1-one.

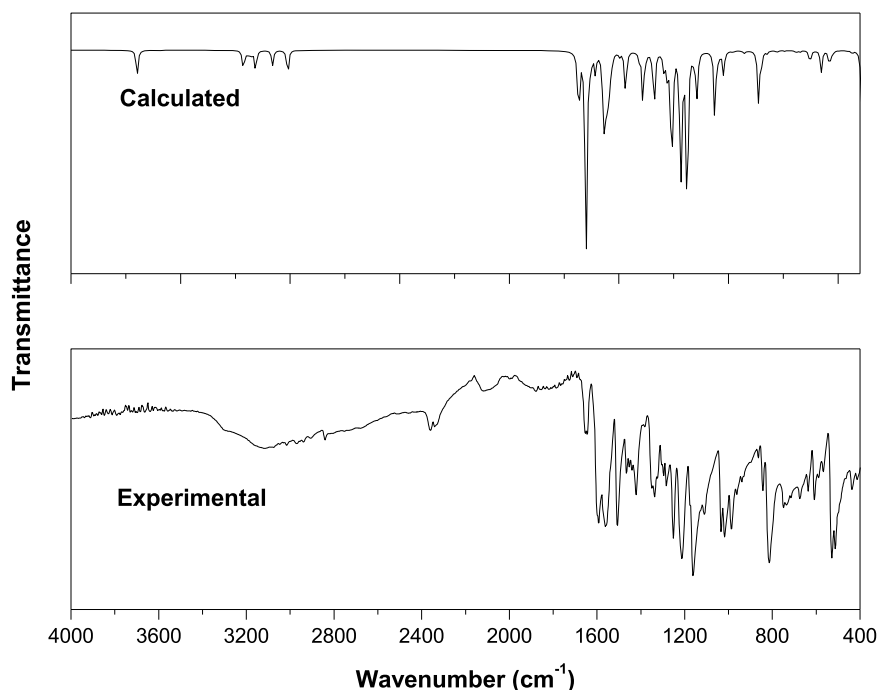


Fig. 5. Experimental and simulated IR spectra of (2E)-1-(4-hydroxyphenyl)-3-(4-methoxyphenyl) prop-2-en-1-one.

line). The starting point for the Rietveld refinement was the well-known structure of $C_{16}H_{14}O_3$ at room temperature [20]. The diffraction pattern confirms that the sample has crystallized as expected with known structure of $C_{16}H_{14}O_3$ at room temperature belongs to the Orthorhombic system, space group $Pbca$ (no 61), with $Z = 8$ [20]. The lattice parameters obtained from the adjustment of the crystal diffraction patterns via Rietveld refinement are: $a = 13.37901(14)$ Å, $b = 11.46496(12)$ Å and $c = 16.60996(15)$ Å,

2.3. Vibrational analysis

The room temperature Raman and FT-IR spectra of the (2E)-1-(4-hydroxyphenyl)-3-(4-methoxyphenyl)prop-2-en-1-one are shown in Figs. 4 and 5, respectively. The theoretical spectra are also shown for comparison. The FT-IR spectrum was recorded in the range of $4000\text{--}400\text{ cm}^{-1}$, while the Raman spectrum was recorded in the range of $1700\text{--}100\text{ cm}^{-1}$.

The vibrational assignments of the normal modes were made using the computed vibrational frequencies. In addition, the discussion of the vibrational assignments of the chalcone is also carried out based on literature survey of previous studies [19,28–33].

For low wavenumbers, the DFT calculations often exhibit larger errors, which correspond to long-range oscillations that are challenging to compute within the limited size of simulated unit cells. These low wavenumber modes, with wavelengths in the micrometer range, can be influenced by long-range features such as defects, dislocations, and grain boundaries. Unfortunately, simulations of perfectly periodic, single crystal structures fail to capture these complex features. Therefore, these errors can influence both the simulated values of frequencies and intensities for a crystal [34].

Table 2 presents the experimental and simulated IR and Raman data for (2E)-1-(4-hydroxyphenyl)-3-(4-methoxyphenyl) prop-2-en-1-one. The vibrational parameters, including wavenumbers, IR intensities, and Raman scattering activities, were calculated using the B3LYP/6-311++G(2d,2p) level in the gas phase and assigned to their respective vibrations.

Bands observed in the region of $40\text{--}200\text{ cm}^{-1}$ contain the lattice modes as well as ring deformation vibrations [29]. In the region between

250 and 1000 cm^{-1} , molecular vibrations associated with deformations of the rings are observed.

Aromatic stretching is based in two types on the nature of the carbon bond: unsaturation and aromatic chain. It is observed a dominant C—C stretching in the range of 1036 up to 1675 cm^{-1} in the plane in Raman and IR. However, the hydrogen (methyl group) and C=O (unsaturation chain) show wagging characteristic around 1233.5 cm^{-1} and stretching characteristic around 1641.5 cm^{-1} .

The bending modes are the main contribution in the vibrational mode of the molecule, with bands assigned at 570 , 389 and 685 with 52% , 52% and 56% contribution of the PED, respectively. The calculate vibrations in the regions of $149\text{--}384\text{ cm}^{-1}$ reveal torsions and out-of-plane bending bands in the carbon ring and the hydroxyl group, contributing 79% and 93% to the PED, respectively. The experimental wavelength assignments are consistent with Ref. [30].

2.3.1. C=O vibrations

The carbonyl group exhibits bands at 1595 cm^{-1} , which can be attributed to stretching modes with a 47% contribution to the PED. The experimental wavelength assignments are consistent with Refs. [28] and [29]. These stretching modes are significant in both Raman and IR spectra according to theoretical calculations. Stretching modes of the carbonyl group occur in the $1850\text{--}1600\text{ cm}^{-1}$ region displaying strong absorption due to $\pi\text{--}\pi$ bonding and its highly polar nature

Several factors, including inductive and mesomeric effects, cause the carbonyl stretching frequencies to shift towards functional groups found in aldehydes and ketones [19]. It is crucial to emphasize that the biological activities of chalcones are attributed to the presence of a double bond conjugated with the carbonyl group [29], which is of significant interest in scientific research. Moreover, vibrations of the carbonyl group generate distinctive bands in spectra, appearing as thin and pronounced bands, which is why their bands are extensively studied [31–33].

2.3.2. Hydroxyphenyl vibration (C—OH bond)

The torsion mode in the is exclusively observed at 431 cm^{-1} , with large contribution of the PED in the hydroxyphenyl group. However, it does not exhibit significant IR intensity or Raman activity in the

Table 2

The experimental and calculated vibrational assignments (in cm^{-1}) and their attributions of (2E)-1-(4-hydroxyphenyl)-3-(4-methoxyphenyl)prop-2-en-1-one (chalcone) were obtained using the B3LYP/6-311++G(2d,2p) level of theory.

Exp. Freq. (cm^{-1})					The calculated vibrational wavenumbers (cm^{-1})
Raman	IR	I_{IR}	S_{Raman}	Freq. (scaled)	Assignments [PED%]
		1	1	44	$\delta_s[\text{C8-C12-C13-C14}][77]$
		1	1	58	$\gamma[\text{C8-C11-C12-C13}][38] + \gamma[\text{C}_{ring}][38] + \tau[\text{H29-C12-C11-H28}][12] + \gamma[\text{C4-O1-C5-C6}][13]$
		1	0.00	94	$\tau[\text{C14-C13-C12-C11}][13] + \gamma[\text{C}_{ring}][13]$
		1	1	107	$\gamma[\text{C4-O1-C5-C6}][59]$
		1	1	145	$\gamma[\text{C8-C11-C12-C13}][13] + \gamma[\text{C}_{ring}][13] + \tau[\text{C14-C13-C12-C11}][50] + \gamma[\text{C}_{ring}][50]$
156		1	1	151	$\delta_s[\text{C7-C8-C11}][54] + \delta[\text{C12-C13-C14}][54] + \delta[\text{C13-C14-C19} + \text{C8-C11-C12} + \text{C7-C8-C11} + \text{C11-C12-C13}][10]$
		1	1	190	$\nu_{sym}[\text{C12-C13} + \text{C14-C15}][10] + \nu[\text{C8-C11}][13] + \delta_s[\text{C11-C12-C13} + \text{C8-C11-C12} + \text{C6-C5-C10}][25]$
208		1	1	192	$\tau[\text{C}_{methyl}\text{-O1}][18] + \tau[\text{H29-C12-C11-H28}][24] + \gamma[\text{C4-O1-C5-C6}][13]$
228		1	1	240	$\tau[\text{C}_{methyl}\text{-O1}][21] + \tau[\text{H29-C12-C11-H28}][20]$
260		1	1	244	$\delta[\text{C4-O1-C5} + \text{C10-C5-O1} + \text{C13-C14-C19}][70]$
299		3	1	303	$\delta[\text{C7-C8-C11} + \text{C13-C14-C19} + \text{C12-C13-O2} + \text{C15-C16-C17} + \text{C10-C5-O1}][50]$
320		1	1	310	$t[\text{C}_{ring}][79] + \gamma[\text{O3-C17-C18-C19}][79]$
380		30	1	384	$\gamma[\text{H23-O3-C17-C16}][93]$
		1	1	385	$\gamma[\text{C}_{ring}][68] + \delta[\text{H23-O3-C17}][68]$
		2	1	389	$\nu[\text{C13-C14}][11] + \delta_s[\text{C7-C8-C11}][11] + \delta[\text{C12-C13-C14}][11] + \delta_s[\text{C18-C17-O3} + \text{C15-C16-C17} + \text{C12-C13-O2}][52]$
410		1	1	428	$\delta[\text{C18-C17-O3} + \text{C16-C17-C18} + \text{C7-C8-C11} + \text{C17-C18-C19} + \text{C13-C14-C19} + \text{C10-C5-O1}][55]$
438		1	0.00	431	$\tau[\text{C}_{ring}][70]$
		1	0.00	437	$\gamma[\text{H26-C9-C10-C5} + \text{H27-C10-C9-C8} + \text{H25-C7-C8-C9}][14] + \tau[\text{C}_{ring}][53]$
473		1	1	451	$\delta_s[\text{C4-O1-C5} + \text{C10-C5-O1} + \text{C6-C5-C10}][63]$
516		1	0.00	515	$\gamma[\text{H32-C18-C19-C14} + \text{H33-C19-C18-C17} + \text{H31-C16-C17-C18}][57] + t[\text{H24-C}_{ring}\text{-H27}][11] + \gamma[\text{O2-C13-C12-C11}][11]$
532	522	4	1	526	$\delta[\text{C13-C14-C19} + \text{C8-C11-C12} + \text{C7-C8-C11} + \text{C11-C12-C13}][42]$
534	532	5	1	535	$\tau[\text{C}_{ring}\text{-CH3}][16] + w[\text{H}_{ring}][16] + \tau[\text{C}_{ring}\text{-OH}][44]$
		11	1	570	$\rho[\text{C6-C7-C8}][12] + \delta_s[\text{C4-O1-C5} + \text{C8-C11-C12} + \text{C12-C13-C2} + \text{C5-C10-C9} + \text{C6-C5-C10} + \text{C10-C5-O1} + \text{C16-C17-C18}][52]$
609	609	7	1	615	$\nu[\text{C13-C14}][11] + t[\text{C16-C17-C18} + \text{C6-C5-C10} + \text{C5-C10-C9}][51] + \delta[\text{C12-C13-O2}][51]$

Table 2 (continued)

Exp. Freq. (cm^{-1})					The calculated vibrational wavenumbers (cm^{-1})
Raman	IR	I_{IR}	S_{Raman}	Freq. (scaled)	Assignments [PED%]
636	631	1	1	637	$t[\text{C17-C18-C19} + \text{C5-C10-C9} + \text{C5-C6-C7}][55] + \rho[\text{C6-C7-C8}][10]$
		1	1	668	$\rho[\text{C17-C18-C19} + \text{C5-C6-C7} + \text{C5-C10-C9} + \text{C15-C16-C17}][66]$
		1	0.00	685	$\gamma[\text{H32-C18-C19-C14} + \text{H33-C19-C18-C17} + \text{H31-C16-C17-C18}][57] + \tau[\text{H24-C}_{ring}\text{-H27}][12] + \gamma[\text{O2-C13-C12-C11}][56] + \tau[\text{C}_{ring}\text{-OH}][56]$
		1	0.00	731	$\tau[\text{C}_{ring}\text{-OH}][67] + t[\text{H33-H32} + \text{H25+H24}][12] + \tau[\text{C}_{ring}\text{-CH3}][51]$
742	743	1	1	739	$\nu[\text{O1-C5}][21] + \nu[\text{C8-C11}][11] + \rho[\text{C6-C7-C8}][16]$
		1	1	773	$\gamma[\text{H33-C19-C18-C17} + \text{H32-C18-C19-C14} + \text{H26-C9-C10-C5} + \text{H25-C7-C8-C9} + \text{H27-C10-C9-C8}][15] + \tau[\text{C}_{ring}\text{-CH3}][55]$
810		1	2	817	$\nu_{sym}[\text{C18-C19} + \text{O3-C17}][10] + \nu[\text{C5-C10}][10] + t[\text{C16-C17-C18} + \text{C6-C5-C10} + \text{C5-C10-C9}][14] + \delta[\text{C12-C13-O2}][14]$
825	827	2	1	842	$\tau[\text{C}_{ring}][85] + w[\text{H30-31} + \text{H32+H33}][85]$
842		2	1	844	$\tau[\text{C}_{ring}][71] + w[\text{H26-H27} + \text{H24-H25}][71]$
847	849	4	1	847	$\nu[\text{O3-C17}][10] + \nu[\text{C18-C17}][16] + \nu_{sym}[\text{C18-C19} + \text{O3-C17}][19]$
865		25	1	857	$\tau[\text{C}_{ring}\text{-OH}][67] + w[\text{H}_{ring}][67]$
		0.00	0.00	870	$\gamma[\text{H32-C18-C19-C14} + \text{H33-C19-C18-C17} + \text{H31-C16-C17-C18}][57] + \tau[\text{C}_{ring}\text{-CH3}][57] + \tau[\text{C}_{ring}\text{-OH}][18] + \gamma[\text{O2-C13-C12-C11}][18]$
900		1	2	911	$\delta_s[\text{C11-C12-C13} + \text{C8-C11-C12} + \text{C6-C5-C10}][37]$
		1	1	923	$\gamma[\text{H29-C12-C13-C14}][69]$
		1	0.00	975	$\tau[\text{C}_{ring}\text{-OH}][67] + t[\text{H33-H32} + \text{H25+H24}][56] + \tau[\text{C}_{ring}\text{-CH3}][18]$
		1	1	978	$\gamma[\text{H33-C19-C18-C17} + \text{H32-C18-C19-C14} + \text{H26-C9-C10-C5} + \text{H25-C7-C8-C9} + \text{H27-C10-C9-C8}][62] + \tau[\text{C}_{ring}\text{-CH3}][11]$
994	988	0	1	993	$\gamma[\text{H26-C9-C10-C5} + \text{H27-C10-C9-C8} + \text{H25-C7-C8-C9}][69] + \tau[\text{C}_{ring}\text{-OH}][10] + w[\text{H26-H27} + \text{H24-H25}][10]$
1006		13	1	1016	$\nu[\text{O1-C4}][73] + \nu[\text{C5-C10}][10]$
		1	1	1021	$\tau[\text{H30-C15-C16-C17} + \text{H31-C16-C17-C18}][71] + \tau[\text{C}_{ring}\text{-OH}][10]$
1006		1	1	1037	$\rho[\text{C5-C6-C7} + \text{C5-C10-C9} + \text{C6-C5-C10}][79]$
1008	1008	3	1	1039	$\rho[\text{C15-C16-C17} + \text{C17+C18-C19} + \text{C16-C17-C18}][71]$
1037	1035	30	9	1056	$\nu_{as}[\text{C12-C13} + \text{C14-C15}][59] + \nu_{sym}[\text{C6-C7} + \text{O1-C5}][59]$
	1110	5	1	1057	$\tau[\text{H28-C11-C12-C13}][83]$
1165	1163	22	1	1138	$\delta[\text{H23-O3-C17}][11] + \delta[\text{H29-C12-C13} + \text{H30-C15-C16}][11] + \delta[\text{H32-C18-C19}][11] + \delta[\text{H29-C12-C13} + \text{H33-C19-C18}][13]$

(continued on next page)

Table 2 (continued)

Exp. Freq. (cm ⁻¹)					The calculated vibrational wavenumbers (cm ⁻¹)
Raman	IR	I _{IR}	S _{Raman}	Freq. (scaled)	Assignments [PED%]
1174		6	1	1149	$\nu_{as}[\text{C9-C10} + \text{C7-C8}][12] + \delta[\text{H26-C9-C10}][15] + \delta[\text{H27-C10-C9}][20]$
1177	1171	1	1	1160	$\delta[\text{H21-C4-O1}][24] + \tau[\text{H20-C4-H22}][24] + \tau[\text{CH3-O1}][38]$
1180		93	1	1183	$\nu[\text{C18-C17}][15] + \delta[\text{H23-O3-C17}][44] + \delta[\text{H32-C18-C19}][19]$
		1	1	1201	$\delta[\text{H20-C4-H22} + \text{H20-C4-H21}][19] + \delta_s[\text{H22-C4-H20}][64]$
1212	1213	56	6	1210	$\nu_{as}[\text{C16-C17} + \text{C18-C19}][10] + \delta[\text{H30-C15-C16} + \text{H33-C19-C18}][25] + \delta[\text{H32-C18-C19}][10] + \delta[\text{H31-C16-C17}][13]$
1218		14	15	1218	$\delta[\text{H24-C6-C7}][17] + \delta[\text{H27-C10-C9}][11] + \delta[\text{H25-C7-C8}][12]$
		39	7	1251	$\nu[\text{C8-C11}][20] + \nu[\text{C13-C14}][16]$
1237		25	5	1259	$\nu[\text{O1-C5}][10] + \nu_{sym}[\text{C5-C6} + \text{C7-C8}][10] + \delta[\text{H25-C7-C8}][10] + \delta[\text{H28-C11-C12}][15]$
1254		12	4	1276	$\nu[\text{O1-C5}][35]$
1287	1284	8	1	1290	$\nu[\text{O3-C17}][42] + \nu_{sym}[\text{C18-C19} + \text{O3-C17}][10] + \delta[\text{H30-C15-C16} + \text{H33-C19-C18}][15]$
1293		30	1	1333	$\nu[\text{C5-C6}][10] + \nu_{sym}[\text{C5-C6} + \text{C7-C8}][19]$
1308		3	1	1343	$\nu_{as}[\text{C14-C15-C16}][13] + \delta[\text{H29-C12-C13} + \text{H33-C19-C18}][23]$
1326		1	1	1361	$\delta[\text{H26-C9-C10}][19] + \delta[\text{H27-C10-C9}][11] + \delta[\text{H25-C7-C8}][15]$
1340		5	7	1375	$\nu_{as}[\text{C14-C15-C16}][19] + \delta[\text{H29-C12-C13} + \text{H33-C19-C18}][21]$
1352		24	3	1386	$\nu_{sym}[\text{C5-C6} + \text{C7-C8}][12] + \delta[\text{H28-C11-C12}][32]$
1423		4	6	1401	$\delta[\text{H29-C12-C13} + \text{H30-C15-C16}][44]$
1430		4	15	1462	$\nu_{as}[\text{C9-C10} + \text{C7-C8}][10]$
1447	1421	18	1	1465	$\delta[\text{H32-C18-C19}][12]$
1466		2	1	1493	$\delta[\text{H21-C4-O1}][88] + \tau[\text{H20-C4-H22}][88]$
1510		2	1	1526	$\delta[\text{H21-C4-O1}][75] + \tau[\text{H20-C4-H22}][75] + \tau[\text{CH3-O1}][17]$
1520	1510	19	2	1536	$\delta[\text{H20-C4-H22} + \text{H20-C4-H21}][72] + \delta_s[\text{H22-C4-H20}][21]$
		24	48	1549	$\nu[\text{O2-H13}][14] + \rho[\text{H30-C15-C16} + \text{H33-C19-C18}][19]$
		18	6	1556	$\delta[\text{H24-C6-C7}][14] + \delta[\text{H26-C9-C10}][14] + \delta[\text{H27-C10-C9}][12] + \delta[\text{H25-C7-C8}][13]$
1563	1563	38	100	1595	$\nu[\text{O2-C13}][47]$
1572	1593	10	4	1602	$\nu[\text{C5-C6}][39] + \rho[\text{C6-C7-C8}][11]$
1593		6	24	1624	$\nu_{as}[\text{C16-C17} + \text{C18-C19}][39] + \delta[\text{C16-C15-C14}]\text{ring}[18]$
1646	1647	100	50	1644	$\nu_{as}[\text{C9-C10} + \text{C7-C8}][26]$
1651	1653	12	21	1652	$\nu_{as}[\text{C9-C10} + \text{C7-C8}][11] + \nu_{as}[\text{C14-C15-C16}][13] + \nu[\text{C18-C17}][10]$

Note: ν , stretching; δ , in-plane bending; τ , torsion; γ , out-of-plane bending; δ_s , scissoring; ρ , rocking; t , twisting; w , wagging; I_{IR} , IR intensity (km/mol); S_{Raman} , Raman scattering activity; PED, potential energy distribution.

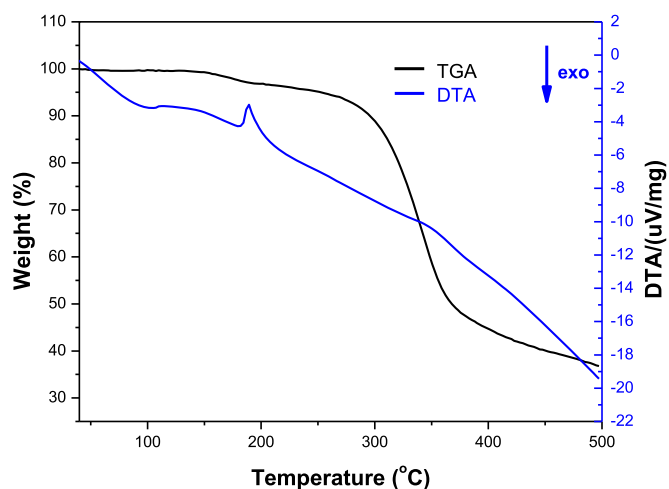


Fig. 6. TGA and DTA curves of the C₁₆H₁₄O₃ chalcones showing the response to increasing temperature from 40 to 500 °C in N₂ atmosphere.

Table 3

Identification and assignment for absorption spectra in the UV-visible region by the TD-DFT method performed B3LYP/6-311++G(d,p) level in methanol of the (2E)-1-(4-hydroxyphenyl)-3-(4-methoxyphenyl)prop-2-en-1-one chalcone.

Wavelength, nm	Oscillator Strength	Major Contribution	Assignment
437.7	0.20	HOMO-1 → LUMO+2 (28 %) HOMO-1 → LUMO+7 (14 %) HOMO-14 → LUMO+12 (11 %)	$\pi \rightarrow \pi^*$ transition
436.9	0.22	HOMO → LUMO+3 (22 %) HOMO-2 → LUMO (12 %) HOMO → LUMO+10 (11 %)	$\pi \rightarrow \pi^*$ transition
435.5	0.25	HOMO-3 → LUMO+1 (28 %)	$\pi \rightarrow \pi^*$ transition
435.3	0.23	HOMO-2 → LUMO (22 %) HOMO-2 → LUMO+4 (11 %)	$\pi \rightarrow \pi^*$ transition

simulated spectrum. Out-of-plane bending modes are observed at 310, 384 and 385 cm⁻¹, with strong IR intensity observed at 384 cm⁻¹ and PED contribution of 79 %, 93 % and 68 %, respectively. A strong IR intensity and low Raman activity is observed at 857 cm⁻¹ in the hydroxyphenyl group due to torsion mode, contributing 67 % to the PED.

2.3.3. Methoxyphenyl vibration (O—CH₃ bond)

On the other hand, the methoxyphenyl group present vibrational modes at 570 (scissor), 773 (torsion), 884 (torsion), 1016 (stretching), 1526 (bending), and 1536 (bending) cm⁻¹, with contribution of the 52, 55, 71, 73, 75, and 72 % to the PED.

The phase deformation of the CH₃ group is intimately dependent on the electronegativity of the adjacent atom, that is, the more electronegative the atom, the higher the frequency with a range within the range of 1470–1250 cm⁻¹ [30]. In the IR calculation is observed a strong contribution to the PED of 88 % at 1493 cm⁻¹ in this study.

2.4. Thermogravimetric analysis

Thermograms for the Chalcone sample were obtained to study its thermal stability. The temperature ranged from room temperature to 500 °C in N₂ atmosphere. Fig. 6 shows the TGA and DTA curves of

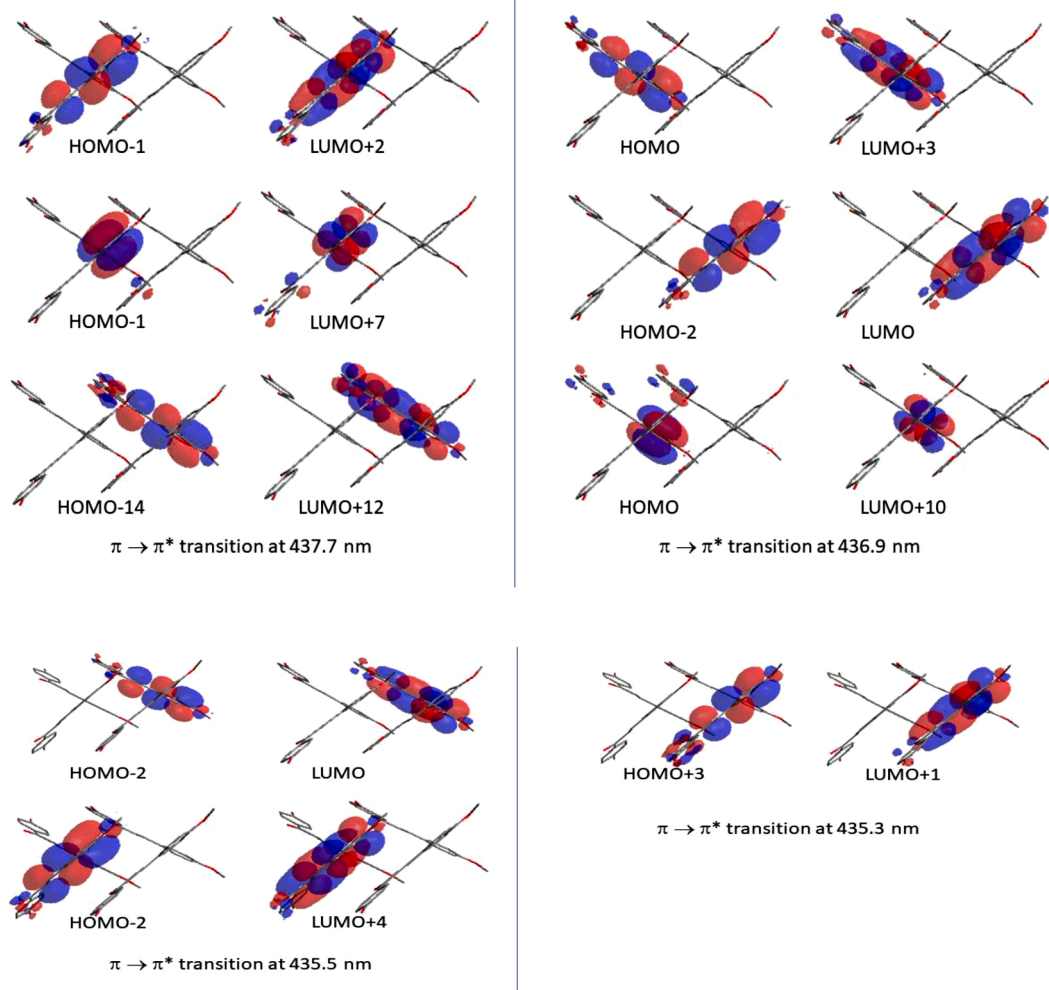


Fig. 7. HOMOs and LUMOs plots calculated for the main contribution in the absorption process in the chalcone molecule. A contour of 0.002 was used for the electron density difference plot.

chalcone (2E)-1-(4-hydroxy-phenyl)-3-(4-methoxy-phenyl)-prop-2-en-1-one. The peak of endothermic curve represents the temperature at which the melting process ends, pointing to a melting point of 189 °C. After the $T = 308.7$ °C (onset temperature) a very sharp drop in the TGA curve is observed that was associated with the decomposition of the sample. In addition, the relatively high melting point value favors several technological applications for the compound, when materials with good thermal stability are required. It is evident from Fig. 6 that no phase transition occurs before the melting temperature (189 °C).

2.5. UV-visible absorption analysis

Time-dependent density functional theory (TD-DFT) study was performed B3LYP/6-311++G(d,p) level in methanol and the absorbance calculated (λ) are summarized in Table 3. The electron density depletion (in red) for molecule are localized on the unsaturated rings and chains for chalcone molecules with compound the unit cell. The electron density increases (in blue) are mainly on the unsaturated rings and chains for chalcone molecules. There is just one type of excitation level in the compound with assignment of π and π^* characteristic between 700 and 500 nm, which is commonly the region used in experimental survey in the laboratories and covers from red to green region. TD-DFT showed that absorption occurs around 437 nm with $\pi \rightarrow \pi^*$ transition in methanol. In TD-DFT calculations it does not consider the crystal size, it only considers a small unit (unit cell). The bandwidth of the DFT calculations

presents contributions only from the geometry used, which results in the sharp shape of the theoretical spectrum in relation the experimental spectrum.

In general, TD-DFT calculation provides a similar spatial distribution of electron for the molecular orbitals on the chalcone molecule. The molecular orbitals are centered on the unsaturated ring and chain at 437.7 and 436.9 nm, with highest populational contribution for HOMO-1 $\rightarrow$ LUMO+2 and HOMO $\rightarrow$ LUMO+3, respectively. The same contributions for the molecular orbitals were found at 435.3 and 435.5 nm (highest populational contribution), however there were the contribution of the oxygens on the hydroxyl and -C=O groups.

The major contributions are related to the transition between HOMO-1 $\rightarrow$ LUMO+2 and corresponds approximately 28 % in the transitions at 437.7 nm, HOMO $\rightarrow$ LUMO+3 and HOMO-2 $\rightarrow$ LUMO+2 correspond approximately 22 % and 12 % in the transitions at 436.9 nm, respectively; HOMO-3 $\rightarrow$ LUMO+1 corresponds approximately 28 % in the transitions at 435.5 nm, and HOMO-2 $\rightarrow$ LUMO and HOMO-2 $\rightarrow$ LUMO+4 correspond approximately 22 % and 11 % in the transitions at 435.3 nm, respectively, therefore, the unsaturated ring. The structure of the unsaturated ring and chain will be responsible for the most of pi transitions in the chalcone molecule, related to absorption, emission and charge transfer [35].

An important role in chemical reactions are the highest occupied molecular orbitals (HOMOs) and the lowest unoccupied molecular orbitals (LUMOs). They can be employed to estimate donor and acceptor

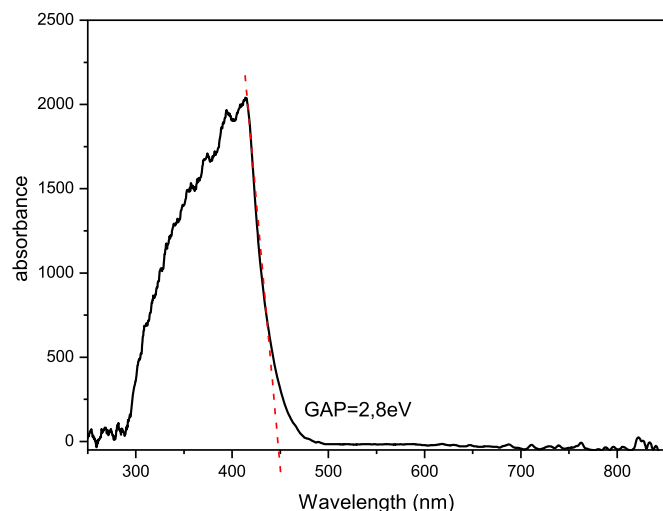


Fig. 8. Chalcone absorption spectrum (2E)-1-(4-hydroxy-phenyl)-3-(4-methoxy-phenyl)-prop-2-en-1-one.

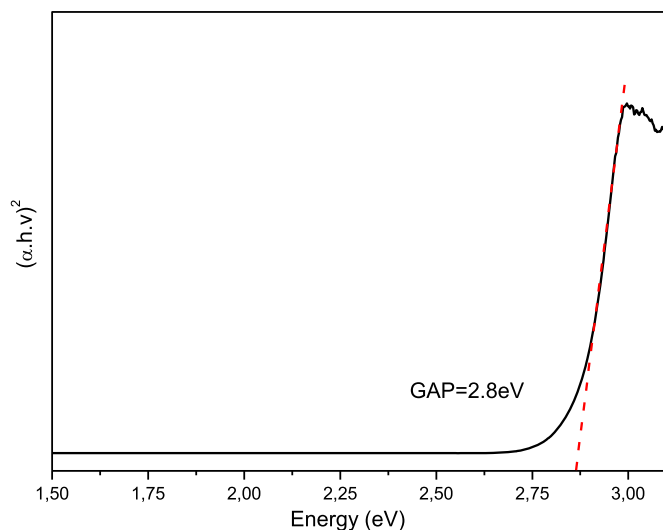


Fig. 9. Gap determination of chalcone (2E)-1-(4-hydroxy-phenyl)-3-(4-methoxy-phenyl)-prop-2-en-1-one, via Tauc's theory.

properties of the molecule; also, they can be evaluating the charge transfers to/from the molecule. The small order contribution cannot produce a significant contribution in the absorption spectrum calculated by DFT because presented oscillator strength was very low.

The band gap difference is determined by subtracting the energy of the highest occupied molecular orbital (HOMO) from the energy of the lowest unoccupied molecular orbital (LUMO). In the case of chalcones with atom substituents, a calculated band gap of 2.97 eV was obtained, consistent with the findings reported in Ref. [36]. These theoretical calculations align with the experimental results obtained in this work, further supporting the accuracy and validity of the calculated band gap value. The absorption of (2E)-1-(4-hydroxyphenyl)-3-(4-methoxyphenyl)prop-2-en-1-one is attributed to perturbations in the crystal symmetry induced by the vibrations of the bonds in the unsaturated bond system. The vibrations of the unsaturated bonds in the crystal lattice, alter the electronic environment and facilitate the energy transfer necessary for the electronic transition.

Fig. 7 presents HOMOs and LUMOs plots calculated for the main contribution in the absorption process and Fig. 8 presents the absorption spectrum of the chalcone under study. This spectrum gives us, via

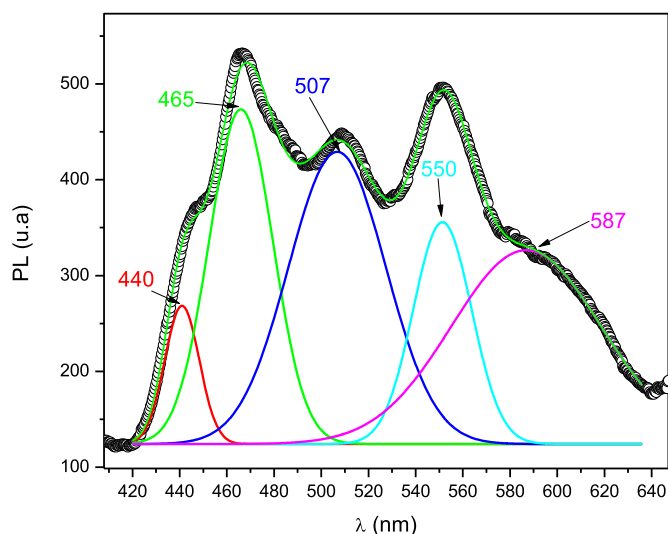


Fig. 10. Fluorescence spectrum of the compound (2E)-1-(4-hydroxy-)-3-(4-methoxy-phenyl)-prop-2-en-1-one excited by a 250 nm wavelength radiation wave.

extrapolation of the linear part of the absorbance curve, the wavelength related to the Gap energy, according to Fig. 7, which was substituted in the Planck equation ($E=hc/\lambda$) to calculate the Gap value of 2.8 eV. For the same purpose, concepts from Tauc's theory [36,37] were used to plot $(\alpha \cdot h \cdot \nu)^2 \times h\nu$, which also provided us, by extrapolation of the linear part, and satisfactorily the same value of 2.8 eV, as shown in Fig. 9. It is worth noting here that the Gap energy value found for (2E)-1-(4-hydroxy-phenyl)-3-(4-methoxy-phenyl)-prop-2-en-1-one is within the range for semiconductors (between 0.5 and 4.0 eV), indicating probable applications in the manufacture of new electronic devices.

2.5.1. Fluorescence spectra

The fluorescence emission spectrum of compound (2E)-1-(4-hydroxy-phenyl)-3-(4-methoxy-phenyl)-prop-2-en-1-one is shown in Fig. 10. The excitation was performed with 5 nm increments, from 250 to 415 nm. We can observe emissions over a long range of wavelengths. With the sample excited by a 250 nm source, we can observe, for example, a strong emission band limited approximately between 650 and 400 nm, which covers a large visible region, starting still in violet, going to the initial part of red. In this broad band there are five emission maxima, at 440, 465, 507, 550 and 587 nm, obtained by curve fitting. It is opportune to observe the evolution of the emission spectra by excitation wavelength, Fig. 11, in this way the photoluminescence is well characterized.

The compound under analysis has potential for possible applications in organic LEDs, due to its broad emission spectrum covering almost the entire visible region of the electromagnetic spectrum.

3. Conclusion

In conclusion, various spectroscopic techniques have been employed to examine the compound 1-(2'-hydroxyphenyl)-3-hydroxy-3-(4-methoxyphenyl)-propan-1-one. Its broad emission bands position it as a promising candidate for application in organic light-emitting diodes. Its semiconductor nature is evidenced by its bandgap, calculated from absorption spectra, within the range of 0.5–4.0 eV, well-suited for semiconductor materials employed in electronic devices. Furthermore, the thermal stability exhibited by the compound in the thermogravimetric analysis serves to emphasize its suitability for these applications. This is due to the absence of any noticeable phase transition before the melting temperature of 189 °C. Additionally, the experimental Raman,

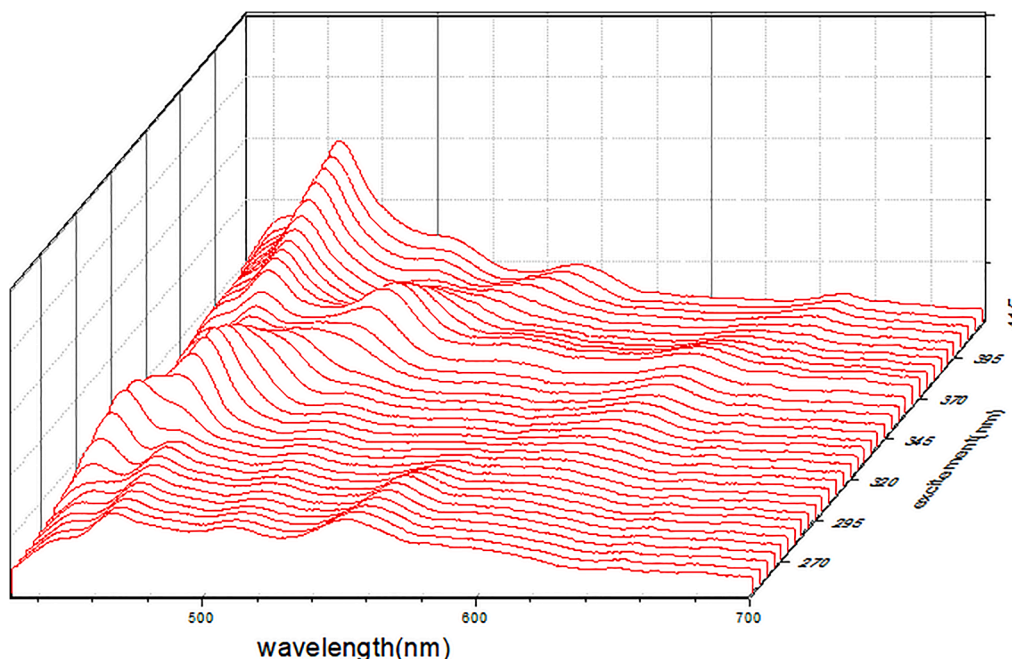


Fig. 11. Fluorescence spectrum of compound (2E)-1-(4-hydroxy-phenyl)-3-(4-methoxy-phenyl)-prop-2-en-1-one, with excitation from 250 to 415 nm.

FT-IR absorption, and UV-VIS spectra were successfully compared and interpreted in relation to the theoretical calculation providing a validation in the theoretical model.

CRediT authorship contribution statement

J.R.P.S. Souza: Conceptualization, Formal analysis, Investigation, Data curation, Writing – original draft. **G.V.S. Mota:** Conceptualization, Writing – review & editing. **H.R. Bitencourt:** Writing – review & editing. **S.G. Moreira:** Conceptualization, Formal analysis, Writing – review & editing, Investigation. **C.M.R. Remédios:** Conceptualization, Formal analysis, Investigation, Resources, Writing – original draft, Writing – review & editing, Visualization, Supervision, Project administration, Funding acquisition.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

No data was used for the research described in the article.

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