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SUBSTITUTED HETEROCYCLIC CHALCONES: ELECTROCHEMICAL, SPECTROSCOPIC AND THEORETICAL STUDY

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ABSTRACT

We have studied the electronic and electrochemical properties of seven substituted heterocyclic chalcones (***CHL 1-6***) wich are functionalized with 2-thienyl groups. The phenyl ring of the chalcone scaffold has been substituted in *orto* or *para* position with electron donnor and acceptor groups (-F, -NO_2, -CH_3O). The electrochemical features were analyzed by cyclic voltammetry; irreversible processes were observed and attributed to the oxidation and reduction of the 2-thienyl group and the carbonyl group of the chalcone, respectively. DFT calculations were made to gain more in-depth understanding of their electronic properties. Relatively high HOMO level and low LUMO values were calculated, E_g values computed varies between 3.0-3.29 eV. These values enable us to postulate that these type of compounds are suitable building blocks to fabricate optoelectronic devices.

Keywords: *Chalcones, Cyclic Voltammetry, DFT calculations, HOMO-LUMO levels, optoelectronic materials*.

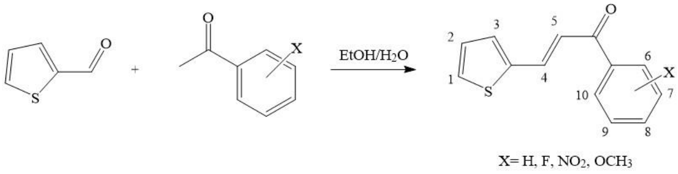
INTRODUCTION

Chalcones are α,β-unsaturated carbonylic compounds, they constitute one of the major classes of flavonoids and isoflavonoids, with a widespread distribution in fruits and vegetables. They present inherent and exceptional antibacterial, antifungal, antitumor and anti-inflammatory properties [1-7]. In addition, to its intrinsic biological importance, these compounds have conjugated π-systems, conferring interesting optical properties, including high extinction coefficients in the *UV* absorption region and a significant nonlinear optical response, thus they can be considered as: (1) promising candidates in the preparation of novel nonlinear optical (NLO) materials [8-12], (2) organic light emitting diodes (OLED) [13-17] and (3) electrochemical sensors [18-20]. Particularity, these type of compounds are attractive, due to the possibility of modulate their electronic properties by embedding electron donors or withdrawing groups into the aromatic ring.

In this work we analyze the effects of different substituents (-F, -NO_2, -OCH_3) in the ortho or para position of the benzene ring from different chalcones, according to scheme 1 (***CHL 1-6***), and how these different architectures influence over the electrochemical and electronic properties of these organic compounds.

EXPERIMENTAL

General synthetic procedure.



***Scheme 1**. Synthetic pathway for the substituted heterocyclic chalcones CHL 1-6.*

All the liquid chemical reagents used in this work were distillates under high vacuum although the solids reagents were used without further purification. Compounds ***CHL 1*** [21,22], ***CHL 2*** [22,23], ***CHL 3*** [24], ***CHL 4*** [22,23] and ***CHL 6*** [24] have been reported elsewhere. We describe herein a synthetic route, with minimal modifications including a fully assigned characterization by spectroscopic methods. The general procedure involves dissolving in a 100-mL flat-bottomed flask, the respective 2-or 4-substituted acetophenone in a 10% KOH ethanolic solution (1:1 ethanol-water), then 2-thiophenecarboxaldehyde was added dropwise and lefted overnight under stirring in an ice water bath (*Scheme 1*). The solution was neutralized with a few drops of HCl (1 M), the formed precipitated was filtered and washed with a cold ethanol-water solution. The solid products formed were recrystallized from a hot (1:1 ethanol-water) mixture and dried out under high vacuum.

The FT-IR spectrum were recorded on a *Shimadzu IR-Prestige-21* using KBr pellets. ^{1}H-NMR was recorded on an *Avance 400 Digital Bruker NMR* spectrometer (chemical shifts references to residual solvent peaks, TMS = 0) using $CDCl_3$ as solvent. UV-Vis absorption spectrum were recorded in acetonitrile solutions on an *Agilent 8453 Diode-Array spectrometer* in the range of 225-500 nm. The melting points were measured using a *Kapur Scientific* automatic melting point apparatus and the values were not corrected.

(E)-1-phenyl-3-(thiophen-2-yl)prop-2-en-1-one (***CHL 1***).

0.570 g of acetophenone was dissolved in 5 mL of absolute ethanol and placed in a water-ice bath with stirring. 0.348 g of KOH was dissolved in 10 mL ethanol-water (1:1) mixture and then, it was added to acetophenone solution. 0.506 g of 2-thiophenecarboxaldehyde was dissolved in 5 mL of ethanol was then added dropwise to above mixture. After 2 hours of stirring a pale yellow solid precipitated. Yield 94%.

Melting point: 53°C. ^{1}H-RMN (ppm): δ_H 8.0085 (2H, d, J = 7.2 Hz, H_6, H_{10}); 7.9492 (1H, d, J = 15.3 Hz, H_4); 7.5840 (1H, t, J = 7.3, 7.2 Hz, H_8); 7.5043 (2H, t, J = 7.8, 7.2 Hz, H_7, H_9); 7.4239 (1H, d, J = 5 Hz, H_1); 7.3632 (1H, d, J = 4.2 Hz, H_3); 7.3386 (1H, d, J = 15.5 Hz, H_5); 7.0939 (1H; dd; J = 3.8, 3.7 Hz, H_2).

FT-IR (cm^{-1}): 3110 ν C-H thiophene (w); 3054, 3080 ν C-H aromatic (w); 1655 ν C=O (st); 1588 ν C=C (st); 1421, 1366, 1237 ring vibration (med); 975 $\delta_{\text{oop trans}}$ CH=CH (med); 840, 870 $\delta_{\text{oop thiophene}}$ C-H (med); 719, 775 $\delta_{\text{oop aromatic}}$ C-H (st).

(E)-1-(4-fluorophenyl)-3-(thiophen-2-yl) prop-2-en-1-one (***CHL 2***).

0.671 g of 4-fluoroacetophenone were dissolved in 5 mL of absolute ethanol and it was placed in an ice-water bath with stirring. 0.378 g of KOH were dissolved in 10 mL ethanol-water (1:1) mixture, which it was added to the above mixture. 0.503 of 2-thiophenecarboxaldehyde were dissolved in 5 mL of ethanol was added dropwise to above solution. After 45 min a pale yellow solid appeared. Yield 96%. Melting Point 88°C. ^{1}H-RMN **(**ppm**)**: δ_H 8.0268 (2H, dd, J = 5.6, 5.6 Hz, H_6, H_{10}); 7.9337 (1H, d, J = 15.3 Hz, H_4); 7.4108 (1H, d, J = 5 Hz, H_1); 7.3473 (1H, d, J = 3.6 Hz, H_3); 7.2853 (1H, d, J = 15.3 Hz, H_5); 7.1522 (2H, t, J = 8.4, 8.7 Hz, H_7, H_9); 7.0759 (1H, t, J = 4.6, 4.1 Hz, H_2).

FT-IR (cm^{-1}): 3110 ν C-H thiophene (w); 3073, 3088 ν C-H aromatic (w); 1657 ν C=O (st); 1584 ν C=C (st); 1419, 1369 ring vibration (med); 1213 δ C-F (st); 975 $\delta_{\text{oop trans}}$ CH=CH (med); 840, 872 $\delta_{\text{oop thiophene}}$ C-H (med); 709, 741 $\delta_{\text{oop aromatic}}$ C-H (st).

(E)-1-(2-nitrophenyl)-3-(thiophen-2-yl) prop-2-en-1-one (***CHL 3***).

0.782 g of 2-nitroacetophenone were dissolved in 5 mL of ethanol and it is placed in an ice-water bath with stirring. 0.359 g of KOH dissolved in 15 mL of ethanol-water solution (2:1) were added to above mixture with stirring.

Then 0.505 g of 2-thiophenecarboxaldehyde were dissolved in 5 mL of ethanol and it were added dropwise to above mixture. The reaction mixture becomes caramel red and after 1 h a brown precipitate appears. Yield 90%. Melting point 82 °C.

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^{1}H-RMN **(**ppm**):** δ_H 8.1762 (1H, dd, *J* = 0.9, 0.8 Hz, H_7); 7.7584 (1H, ddd, *J* = 1, 1, 1.2, Hz, H_9); 7.6517 (1H, ddd, *J* = 1.4, 1.3, 1.4 Hz, H_8); 7.4991 (1H; dd, *J* = 1.4, 1.3 Hz, H_3); 7.4539 (1H, d, *J* = 5.1 Hz, H_1); 7.4006 (1H, d, *J* = 15.7 Hz, H_4); 7.2560 (1H, d, *J* = 3.3 Hz, H_{10}); 7.0638 (1H, dd, *J* = 3.6, 3.7 Hz, H_2); 6.7986 (1H, d, *J* = 15.9 Hz, H_5).

FT-IR (cm^{-1}): 3101 ν C-H thiophene (w); 3035, 3088 ν C-H aromatic (w); 1656 ν C=O (st); 1608 ν C=C (st); 1529 ν_{as} Ar-NO_2 (st); 1419, 1247 ring vibration (med); 1339 ν_s Ar-NO_2 (st); 973 $\delta_{oop\ trans}$ CH=CH (med); 855 ν C-N (Ar-NO_2) 833 $\delta_{oop\ thiophene}$ C-H (med); 723, 790 $\delta_{oop\ aromatic}$ C-H (st).

(E)-1-(4-nitrophenyl)-3-(thiophen-2-yl) prop-2-en-1-one (***CHL 4***).

0.779 g of 4-nitroacetophenone were dissolved in 5 mL of ethanol. 0.360 g of KOH dissolved in 5 mL water-ethanol mixture (2:1) and it were added to previous solution. The mixture was placed in a water-ice bath with stirring. 0.490 g of 2-thiophenecarboxaldehyde were dissolved in 5 ml of ethanol are added dropwise to above solution. A few minutes later, a reddish precipitate appears. Yield 51%. Melting point 153°C. ^{1}H-RMN (ppm): δ_H 8.3522 (2H, d, *J* = 8.9 Hz, H_9, H_7); 8.1352 (2H, d, *J* = 8.8 Hz, H_{10}, H_6); 7.9933 (1H, *J* = 15 Hz, H_4); 7.4945 (1H, d, *J* = 5 Hz, H_1); 7.4214 (1H, d, *J* = 3.6 Hz, H_3); 7.2782 (1H, d, *J* = 15.6 Hz, H_5); 7.1293 (1H, dd, *J* = 3.6, 3.8 Hz, H_2).

FT-IR (cm^{-1}): 3105 ν C-H thiophene (w); 3080 ν C-H aromatic (w); 1650 ν C=O (st); 1595 ν C=C (st); 1518 ν_{as} Ar-NO_2 (st); 1419, 1247 ring vibration (med); 1345 ν_s Ar-NO_2 (st); 970 $\delta_{oop\ trans}$ CH=CH (med); 858 ν C-N (Ar-NO_2) 823, 860 $\delta_{oop\ thiophene}$ C-H (med); 712, 790 $\delta_{oop\ aromatic}$ C-H (st).

(E)-1-(2-methoxyphenyl)-3-(thiophen-2-yl) prop-2-en-1-one (***CHL 5***).

0.711 g of 2-methoxyacetophenone were dissolved in 5 mL of ethanol, then 0.356 g of KOH dissolved in 15 mL of a water-ethanol (2:1) mixture and they were added to previous solution and then it was placed in an ice-water bath with stirring. 0.495 g of 2-thiophenecarboxaldehyde was dissolved in 5 mL of ethanol and it was added dropwise to above mixture. A few minutes later, a brown precipitate appears. Yield 72 %. Melting point: 94°C. ^{1}H-RMN (ppm): δ_H 7.764 (1H, d, *J* = 15.2 Hz, H_4); 7.6425 (1H, dd, *J* = 1.6, 1.6 Hz, H_{10}); 7.494 (1H, ddd, *J* = 2, 0.8, 0.2 Hz, H_8); 7.4085 (1H, *J* = 5.2 Hz, H_1); 7.321 (1H, d, *J* = 3.2 Hz, H_3); 7.2205 (1H, d, *J* = 15.6 Hz, H_5); 7.089 (1H, dd, *J* = 3.6, 3.6 Hz, H_2); 7.0445 (1H, dd, J = 1.2, 0.8 Hz, H_9); 7.0185 (1H, d, *J* = 8.4 Hz, H_7); 3.9046 (3H, s, -OCH_3).

FT-IR (cm^{-1}): 3096 ν C-H $_{thiophene}$ (w); 3071, 3005 ν C-H $_{aromatic}$ (w); 2840, 2954 ν C-H $_{aliphatic}$ (w); 1657 ν C=O (st); 1589 ν C=C (st); 1434, 1317 ring vibration (med); 1247 ν_{as} C-O-C (st); 1019 ν_s C-O-C (med); 964 $\delta_{oop\ trans}$ CH=CH (med); 845, 858 ν $\delta_{oop\ thiophene}$ C-H (med); 701, 745 $\delta_{oop\ aromatic}$ C-H (st) cm^{-1}

(E)-1-(4-methoxyphenyl)-3-(thiophen-2-yl) prop-2-en-1-one (***CHL 6***).

0.702 g of 4-methoxyacetophenone were dissolved in 5 mL of ethanol and 0.366 g of KOH dissolved in a 5 mL water-ethanol (2:1) mixture were added. The above mixture was placed in an ice-water bath with stirring. 0.498 g of 2-thiophenecarboxaldehyde were added dropwise to the above mixture. After a few minutes a pale yellow solid appears. Yield 70%. Melting point 102°C. ^{1}H-RMN (ppm): δ_H 8.0265 (2H, d, *J* = 7.2 Hz, H_{10}, H_6); 7.9336 (1H, d, *J* = 15.3 Hz, H_4); 7.4026 (1H, d, *J* = 5.1 Hz, H_1); 7.3467 (1H, d, *J* = 15.3 Hz, H_5); 7.3456 (1H, d, *J* = 3.5 Hz, H_3); 7.0849 (1H, dd, J = 3.6, 3.6 Hz, H_2); 6.9811 (2H, d, *J* = 8.9 Hz, H_9, H_7), 3.8877 (3H, s, -OCH_3).

FT-IR (cm^{-1}): 3105 ν C-H $_{thiophene}$ (w); 3080, 3012 ν C-H $_{aromatic}$ (w); 2970, 2830 ν C-H $_{aliphatic}$ (w); 1650 ν C=O (st); 1589 ν C=C (st); 1255 ν_{as} C-O-C (st); 1019 ν_s C-O-C (med); 964 $\delta_{oop\ trans}$ CH=CH (med); 827 ν $\delta_{oop\ thiophene}$ C-H (med); 712 $\delta_{oop\ aromatic}$ C-H (st) cm^{-1}

Electrochemical setup

The experimental setup to perform cyclic voltammetry (CV) and chronoamperometry (CA) experiments have been described previously [25]. The electrochemical experiments were performed in a DY2311 Potentiostat (*Digi-Ivy Inc*, Austin-Texas USA): a glassy carbon electrode (GCE) (*Bioanalytical System Inc*, *BASi*) was used as working electrode. The reference electrode used was a Ag/AgCl in tetraethylammonium chloride solution and its potential was adjusted with respect to the saturated calomel electrode (SCE). As auxiliary electrode a platinum coil was used, in a separated compartment of electrolytic cell from the working electrode. To avoid the gradual deactivation of GCE, the procedure described by Kuwana *et al* [26,27] was followed to activate it again. Prior to each experiment the GCE was rinsed with abundant ionized water and then with anhydrous acetonitrile.

Anhydrous acetonitrile (*Aldrich Chemical Co*) was used as solvent and it was manipulated with a syringe. The supporting electrolyte was tetrabutylammonium hexafluorophosphate, (TBAPF$_6$) (*Aldrich Chemical Co*) and it was dried under vacuum at 40°C for 24 h and stored in a vacuum desiccator.

The electrolytic solution was gasified with argon during 15 min after each experiment, and before an inert atmosphere was kept during electrochemical perturbation.

Computational calculations

DFT calculations were performed using the Gaussian 09 suite of programs [28]. The geometries of organic molecules were optimized without symmetry restrictions using the B3LYP/LanL2DZ basis set [29-31]. In all calculations, the effect of the solvent (acetonitrile) was considered employing a self-consistent reaction field (SCRF) using the SMD implicit solvation model [32].

RESULTS

Electrochemical behavior of chalcones.

The electrochemical behavior of chalcones are shown in the Figure 1. In the anodic scan, one oxidation peak could be observed in the range of 1.87 V and - 2.08 V (I), but in the case of 2- or 4-methoxy derivatives the anodic scan shows two successive oxidation peaks were observed between 1.77-1.86 V (I) and 2.05-2.19 V (II) respectively. Both peaks seem to be irreversible, since in the return sweep no reduction peak was observed until at least 0.01 V. A closer inspection of the CV experiments reveals a similar feature to those found with other chalcones in aprotic medium [33]. In the case of cathodic voltammograms (Figure 1), one well defined reduction peak was observed between -1.28 V and - 1.41 V, the reduction peak can be attributed to carbonyl group reduction [34-36] but in the case of 2- and 4- nitro derivatives two additional peaks could be observed between -1.0 V and -1.01 V and -1.47 V and 1.56 V respectively. The first peak can be attributed to monoelectronic reduction of nitro group and the second one to the carbonyl group.

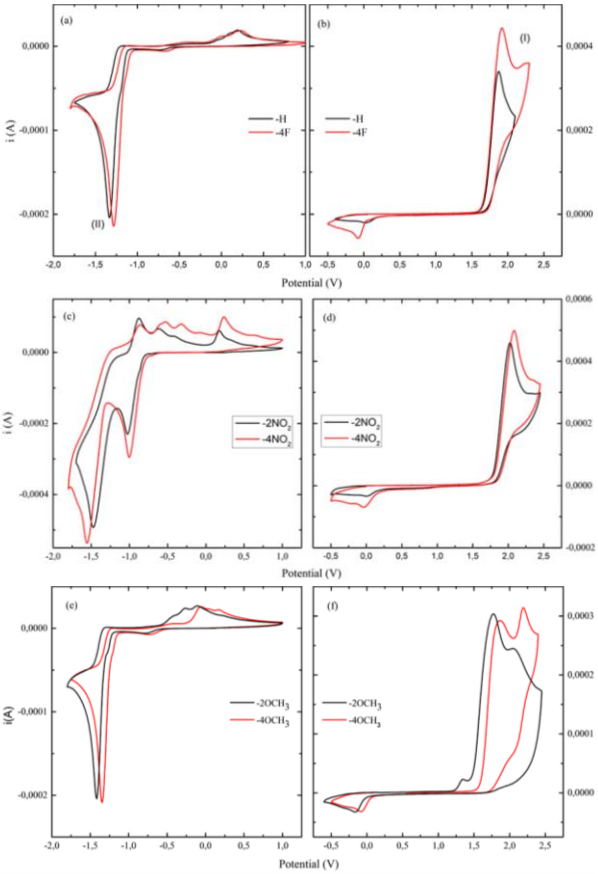

Figure 1. CVs of chalcones on GCE in acetonitrile solution with TBAPF$_6$ 0.1 M, scan rate 100 mV/s. (a), (c), I and (g) cathodic scans; (b), (d), (f) and (h) anodic scans.

In order to establish the nature (irreversible or quasirreversible) of the oxidation and reduction peaks, cyclic voltammetry experiments were performed at different scan rate. The logarithmic relation between anodic (I_{ap}) and cathodic (I_{cp}) peak current were proportional to logarithmic scan rate v (R = 0.99) (Figure 2, Table 1), which is consistent with the diffusion as the rate-limiting step [37] during oxidation and reduction process.

In both processes, there is a linear dependence between I_p and $v^{1/2}$, however, in a quasirreversible process there is no such proportionality. The slopes founds vary between 0.4-0.54 (Table 1). Further, the relation E_p *vs* log v was not linear, so the nature of both peaks seems not to be irreversible. Even more, from the difference between $|E_p\text{-}E_{p/2}|$ at different scan rates, makes it possible to calculate the value of transfer coefficient α. The values of α varies between (0.15-0.5) when the scan rate decreases, as this value was not constant, it is possible to confirm that the nature of both processes were quasirreversible.

Table 1. Values of slope log i_p *vs* log v .

Compound	Anodic slope log i_{pa} *vs* log v	R	Cathodic slope log i_{pc} *vs* log v	R
CHL 1 (-H)	0.41	0.999	0.49	0.997
CHL 2 (4-F)	0.40	0.999	0.45	0.999
CHL 3 (2-NO_2)	0.54	0.958	0.42	0.999
CHL 4 (4-NO_2)	0.45	0.999	0.42	0.999
CHL 5 (2-OCH_3)	0.46	0.998	0.51	0.990
CHL 6 (4-OCH_3)	0.46	0.999	0.48	0.995

For a better understanding of the effect of the substituent on the electrochemical properties of the compounds (***CHL 1-6***), the reduction and oxidation peaks were correlated with Hammett substituent constants [38] using single regression analysis. From the plots of potentials peaks *vs* Hammet substituent constant values for each substituent in *p*-position (Figure 2), a linear relationships were found for both processes. As it is known, there are not valid values for *ortho* substituens due to anomalous (mainly sterics) effects. The oxidation potential increased with the electrowithrawing properties of the group attached. For the reduction of the ketone group, an opposite trend was observed, where a lower potential was found with a substituent with a lower Hammet constant value [39]. Similar trends have been found in others chalcone systems [40].

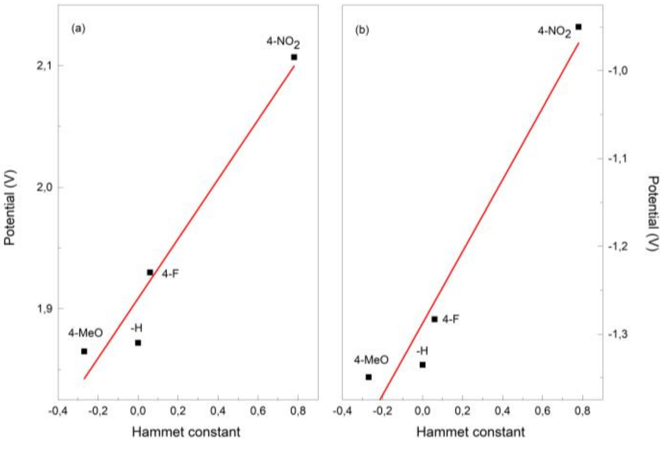

Figure 2. Plots of oxidation potential (a) and reduction potential (b) potentials *vs* Hammet constant value.

The correlation shown the effect of the different groups in the redox potentials and how the redox potentials can be finely tuned. Also give the possibility of predicting the values if other other substituents are used, by using the Hammet parameters.

Frontier molecular orbital (FMO) and UV–Vis absorption

FMO analysis provides insight into electronic as well as optical properties of organic compounds [41]. In this work, the FMO analysis showed that the HOMO levels are mainly concentrated on the thienyl vinylic moiety while the LUMO levels are mainly delocalized over whole molecule. These features were also described in other heterocyclic chalcone [33] (Figure 3).

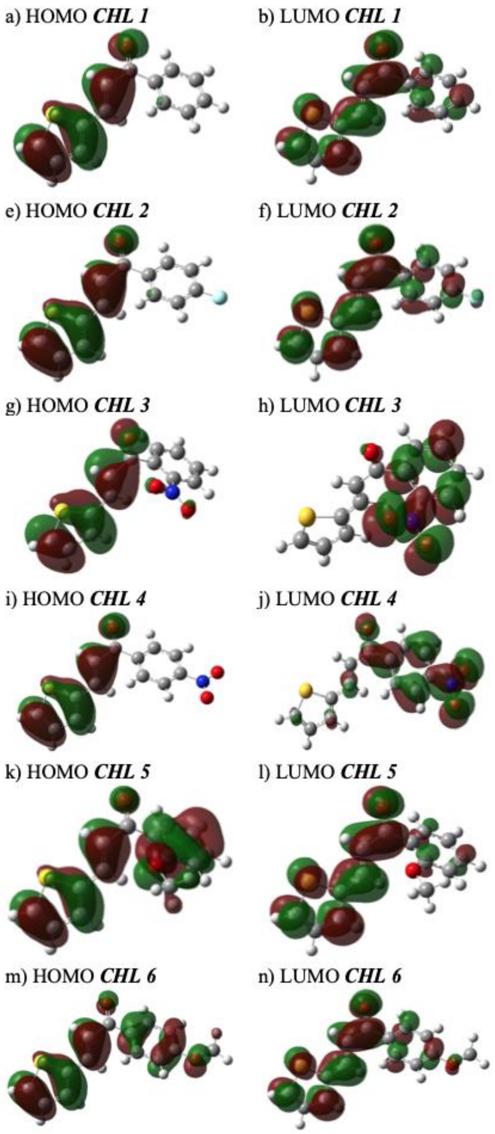

Figure 3. Computed frontier molecular orbitals of chalcones.

The HOMO–LUMO energy gap (***E_g***) represents the lowest energy for intermolecular charge transfer. The theoretical calculations demonstrate that the energy of the frontier molecular orbitals of these chalcones is modified by the substituent nature and their position on the aromatic ring. E_{HOMO}, E_{LUMO} and ***E_g*** of compounds ***CHL 1-6*** are resumed in Table 2.

Table 2. HOMO, LUMO and E_g values in eV obtained from theoretical calculations, UV-vis absorption spectrum and CV experiments.

Compound	Theoretical calculations			UV-vis			CV edge		
	HOMO	LUMO	E_g	λ_{max} (nm)	λ_{onset} (nm)	E_g	HOMO	LUMO	E_g
CHL 1 (-H)	-6.48	-2.67	-3.81	337	381	-3.26	-6.08	-3.27	-2.81
CHL 2 (4-F)	-6.51	-2.72	-3.79	336	380	-3.27	-6.08	-3.32	-2.76
CHL 3 (2-NO_2)	-6.56	-3.57	-2.98	331	378	-3.29	-6.20	-3.58	-2.61
CHL 4 (4-NO_2)	-6.58	-3.66	-2.92	351	407	-3.05	-5.68	-3.96	-1.72
CHL 5 (2-OCH_3)	-6.39	-2.63	-3.76	331	380	-3.27	-5.89	-3.19	-2.70
CHL 6 (4-OCH_3)	-6.53	-2.60	-3.93	336	381	-3.26	-6.01	-3.24	-2.77

The UV–Vis spectrum of the chalcones ***CHL 1-6*** are displayed in Figure 4 and the maximum absorption bands are resumed too in Table 2. The spectrums were characterized by two bands in the range of 230-290 nm (band II) and 300-400 nm (band I). This absorptions bands can be assigned to the Ph-C=O and Th-CH=CH- chromophores and they have been attributed to n–π* and π–π* transitions respectively [42,43].

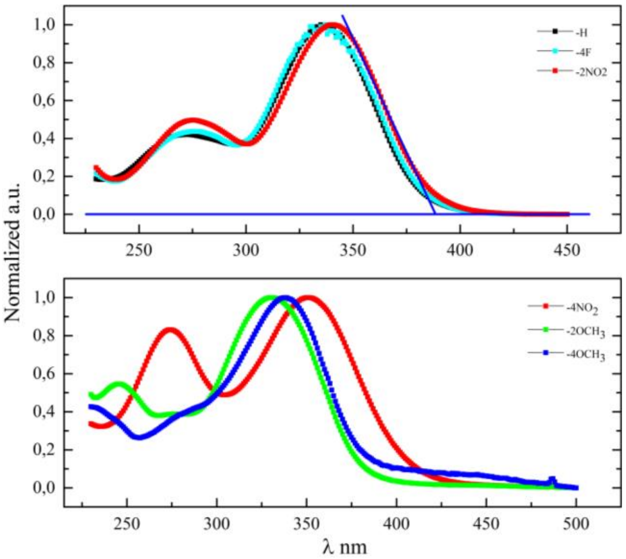

Figure 4. UV-vis spectrum of chalcone samples in acetonitrile.

The absorption bands could be correlated with the HOMO–LUMO band gap. The E_g can be estimated through a linear extrapolation of the low-energy side of the absorption maximum from the cross point of absorption onset line and corrected base line [44] (see Figure 4a blue line) and they are shown in Table 2. E_g corresponds to the energy of the long wavelength edge of the exciton absorption band [45]. The longest absorption wavelength λ_{onset} was used to calculate the optical gap energy, E_g [46], according to the following relation:

$$E_g = 1242/\lambda_{onset}$$

On the other hand, HOMO represents the energy required to extract an electron from a molecule, which is an *oxidation* process, and LUMO is the energy necessary to inject an electron to a molecule, thus implying a *reduction* process. For these reasons both processes can be measured using cyclic voltammetry [47,48]. The energy values could be estimated using the following empirical relations [49]:

$$E\ (\mathrm{HOMO}) = -e\ [E_{ox}{}^{onset} + 4.4]$$
$$E\ (\mathrm{LUMO}) = -e\ [E_{red}{}^{onset} + 4.4]$$

Where $E_{ox}{}^{onset}$ and $E_{red}{}^{onset}$ correspond to the potential which the current of oxidation or reduction began to increase. These values are independent of the scan rate and concentration of the electroactive molecule [50,51]. The HOMO and LUMO levels approximated from the CV experiments, as well as the band gap are shown in Table 2. The theoretical calculations show the same trend that the one obtained by CV.

Optical absorption and cyclic voltammetry measurements revealed that the compounds have a narrow-band gap, similar to semiconductors, with a high electron affinity (LUMO level ~ -3.0 to -3.29 eV) and a high positive oxidation potential. These properties indicates these compounds are potential candidates to be used as acceptor materials in organic heterojunction solar cells [52].

The energy gap determined from cyclic voltammetry experiments were smaller than the optical gap derived from UV-Vis absorption spectra. The differences between these values are related to the different approaches of each technique; were the optical spectra give information about the optical excitation of an electron from the ground to the first excited state, whereas electrochemical oxidation/reduction produces real charged species [53,54].

The theoretical and experimental band-gap values, suggest the potential suitability of this type of compound for optoelectronic applications [55]. It may also be noted that these band gaps are comparable with inorganic materials used in optoelectronic device applications [56-58].

CONCLUSIONS

We have synthetized heterocyclic chalcones with different substituents in 2- or 4-position on the benzene ring. The FMO analysis showed that the HOMO level are mainly concentrated on the thienyl vinylic moiety, nevertheless the LUMO level are delocalized over the whole molecule.

Optical absorption and cyclic voltammetry measurements have revealed that these compounds own a narrow-band gap semiconductors with high electron affinity (LUMO level ~ -3.0 to -3.29 eV) and high oxidation potential. The Eg values suggest the potential suitability of this type of compound for optoelectronic applications comparable with inorganic materials.

Finally, the theoretical and experimental results support that the insertion of substituents with an electron-donating or withdrawing group in 2- or 4-position on the aromatic ring, are key factors to modulate the electronic properties of these chalcones.

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