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Vibronic Emission Spectra of Dithiophene and Terthiophene and Their Complexes with H₂S and (H₂S)₂

In this work, the vibronic emission spectra of dithiophene (T2) and terthiophene (T3) molecules and their complexes with hydrogen sulfide and its dimer were calculated at the TD-DFT / CAM-B3LYP / 6-31G(d) theory level. The solvent was taken into account within the PCM model. Vibronic spectra were calculated considering both the Herzberg-Teller and Duschinsky effects. Good agreement between the computed and experimental spectra was obtained. The vibration promoting modes forming vibronic progressions were found. Vibronic bands for dithiophene and terthiophene were formed by their low-frequency modes (≤ 370 cm⁻¹), combinations of low-frequency modes with high-frequency modes (1497 and 1672 cm⁻¹ for T2 and 1516 and 1573 cm⁻¹ for T3), and with their composite high-frequency modes. The intensities of vibronic lines for the emission spectra of T2⋯H₂S, T3⋯H₂S and T2⋯(H₂S)₂, T3⋯(H₂S)₂ complexes were shown to decrease 3.7, 2.6 and 5.5, 3.6 times compared to T2 and T3, respectively. The bathochromic shifts of the vibronic bands of dithiophene and terthiophene complexes with H₂S and (H₂S)₂ did not exceed 130 cm⁻¹ for all bands.

Keywords: oligothiophenes, hydrogen sulfide, vibronic spectra, emission, complexes, vibration modes, Herzberg-Teller effect, Duschinsky effect.

Introduction

At present, many conjugated organic molecules are being actively studied for their use as light-emitting diodes [1–2]. Molecules based on polythiophenes and their derivatives are promising for implementation in organic electronics devices. This is due to their efficient charge transfer, low cost, high chemical stability [3–4], and compatibility with a flexible substrate in a technological process at a low operating voltage [5]. Shorter structures of such compounds, in particular oligothiophene molecules, are also promising as materials for organic electronics [6–7]. The possibility of modifying oligothiophene structures with different functional groups makes it possible to improve their chemical and radiation properties [8–9]. For example, the photoluminescence quantum yield for a dioctylphenyl-substituted polythiophene derivative is 24 % [10]. The photoluminescence efficiency of materials based on oxygen-containing benzothiophene is 21 %, and the electroluminescence brightness is 10500 cd/m² [11]. Recently, the thiazole-centered oligothiophene donor has provided the efficiency of 15.4 % [12]. In addition, such compounds in the crystal packing are prone to formation of intermolecular bonds [5]. It should be noted that thiophenes can be extracted from medium sulfur oil refining products [13]. Other reactions are also possible during this treatment, such as thermal cleavage of hydrocarbons to lighter hydrocarbons, complete sulfurization of some products to carbon disulfide, secondary reaction of some products with sulfur or hydrogen sulfide, leading to the formation of high sulfur content resin.

It is well-known that oligothiophenes have a pronounced vibronic structure of the emission spectra and a weak vibronic structure of the absorption spectra [14]. To interpret the spectral bands, it is necessary to determine the promoting vibration modes that form these vibronic spectra. Note that the quantum-chemical calculations of vibronic spectra for oligothiophenes were carried out in [15–17] using the FCclasses [18] and MidasCpp [19] codes. However, an analysis of promoting vibration modes is missing in these works. In the present work, such an analysis was performed on the example of oligothiophene compounds with 2 (dithiophene) and 3 (terthiophene) thiophene fragments. The influence of H₂S and (H₂S)₂ on vibronic spectra of dithiophene and terthiophene complexes with these molecules, which can be formed during the technological processes, were also studied.

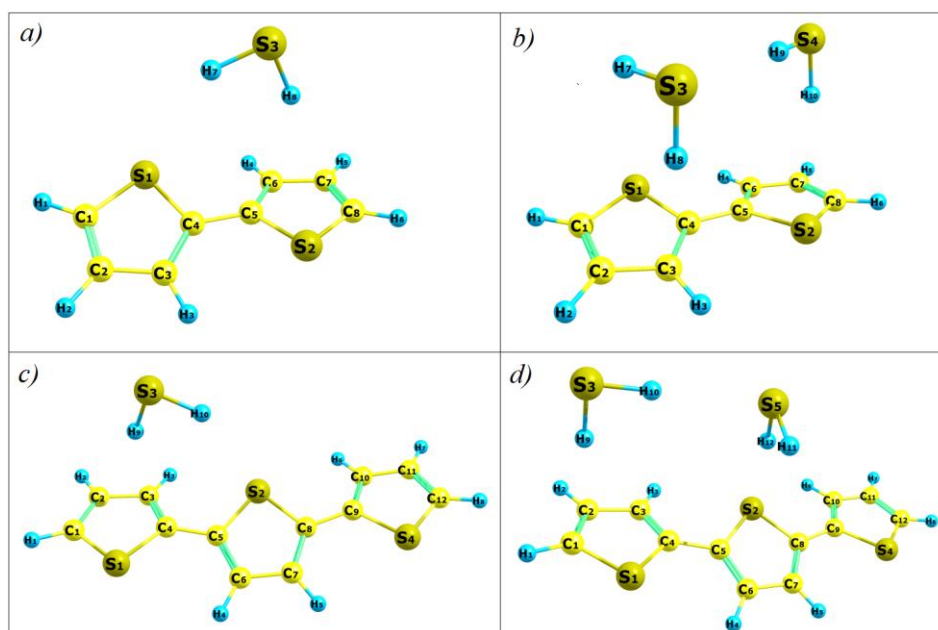
Computational Details

The equilibrium geometries of bithiophene and terthiophene molecules and their complexes with hydrogen sulfide molecules were optimized at the DFT level for the singlet state S_0 and at the TD-DFT level for the first excited state S_1 using the hybrid exchange-correlation functional CAM-B3LYP [23] with the basis set 6-31G(d) [24]. The choice of the method is due to its effectiveness for application to such compounds [15, 18]. The solvent (ethanol) used in the experiment [14] was taken into account within the PCM to compare the computational and experimental results. In this study, all vibronic spectra of the considered compounds were calculated using the Gaussian code [20] taking into account the Herzberg-Teller [21] and Duschinsky [22] effects.

Results and Discussion

Molecule structures. For all found equilibrium structures of molecules studied in the work, the calculated vibration frequencies turned out to be positive. It should be noted that the obtained equilibrium geometries of dithiophene (T2) and terthiophene (T3) molecules both in the ground and excited electronic states agree well with the results of [15-16]. Analysis shows that these compounds have a non-planar structure in the ground electronic state. The torsion angles calculated between the monomeric thiophene rings are 20° (the experimental value is 21° [25]). As a result, the conjugations between these fragments are disrupted. At the same time, oligothiophene molecules are practically planar in the excited electronic state.

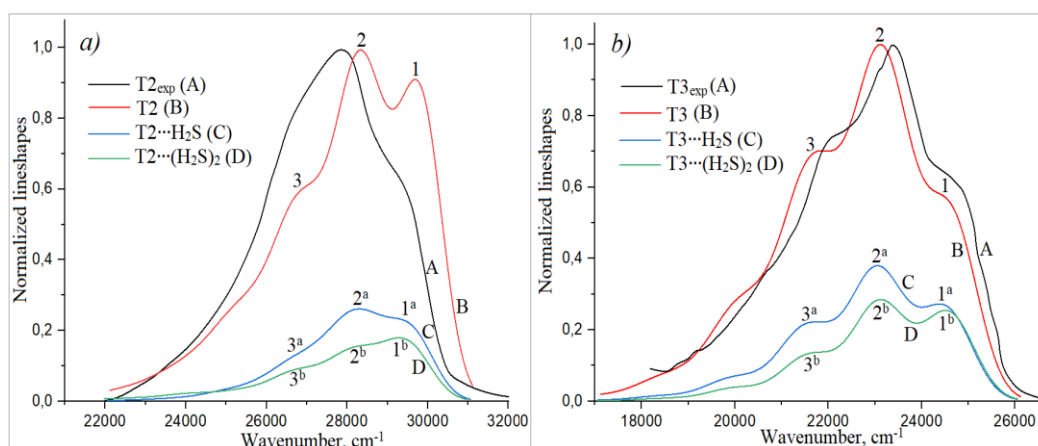
The structures of the complexes for their ground electronic states formed from T2 and T3 molecules and H_2S and $(H_2S)_2$ are shown in Figure 1. The coordinates of atoms, bond lengths and angles of $T2 \cdots H_2S$, $T2 \cdots (H_2S)_2$, $T3 \cdots H_2S$, $T3 \cdots (H_2S)_2$ are given in [Supplementary Materials](#). The calculations showed that for these complexes the bond lengths change by less than 0.016 \AA and the angles change by less than 0.41° compared to the free T2 and T3 molecules. For excited states, the structures of these complexes also change very slightly (for bond lengths $< 0.018 \text{ \AA}$, and for angles $< 0.65^\circ$). Thus, dithiophene and terthiophene molecules forming complexes with H_2S and $(H_2S)_2$ retain practically their non-planar structures in the ground electronic state and planar structures in the first excited states.



a — $T2 \cdots H_2S$; *b* — $T2 \cdots (H_2S)_2$; *c* — $T3 \cdots H_2S$; *d* — $T3 \cdots (H_2S)_2$

Figure 1. The equilibrium geometries optimized for the ground electronic states of the complexes

Vibronic spectra. The calculation results of vibronic spectra for bithiophene and terthiophene molecules and their complexes with H_2S and $(H_2S)_2$ in comparison with experimental spectra are shown in Figure 2 and Table. A half-width of $\sim 600 \text{ cm}^{-1}$ estimated from the experimental spectra [14] was used to simulate the vibronic spectra.



a — T2, T2·H₂S, T2·(H₂S)₂; *b* — T3, T3·H₂S, T3·(H₂S)₂

Figure 2. Experimental (A) (Reprinted with permission from [14]. Copyright 1996 American Chemical Society) and calculated (B, C, D) vibronic emission spectra at room temperature

Table

Parameters (harmonic frequencies $\omega_i + \omega_j + \dots$, square of the dipole moment of transitions μ^2) for vibronic spectra of bithiophene, terthiophene and their complexes with H₂S and (H₂S)₂

Peak number	$\omega_1 + \dots + \omega_i \text{ cm}^{-1}$	μ^2 , a.u.	$\omega_1 + \dots + \omega_i \text{ cm}^{-1}$	μ^2 , a.u.	$\omega_1 + \dots + \omega_i \text{ cm}^{-1}$	μ^2 , a.u.
	T2		T2·H ₂ S		T2·(H ₂ S) ₂	
1	87+66	$0.54 \cdot 10^{-3}$	62+21	$0.24 \cdot 10^{-2}$	54+16	$0.11 \cdot 10^{-3}$
	290+66	$0.65 \cdot 10^{-2}$	75+62+21	$0.49 \cdot 10^{-3}$	69+16	$0.13 \cdot 10^{-3}$
	370+87+66	$0.24 \cdot 10^{-3}$	291+75+62+21	$0.18 \cdot 10^{-3}$	69+54+16	$0.18 \cdot 10^{-3}$
2	1497+66	$0.14 \cdot 10^{-1}$	1495+62+21	$0.10 \cdot 10^{-3}$	1494+69+16	$0.70 \cdot 10^{-4}$
	1672+66	$0.16 \cdot 10^{-1}$	1670+62+21	$0.13 \cdot 10^{-3}$	1670+69+16	$0.67 \cdot 10^{-4}$
	1497+290+66	$0.27 \cdot 10^{-2}$	1670+75+62+21	$0.23 \cdot 10^{-3}$	1494+69+54+16	$0.82 \cdot 10^{-4}$
	1497+370+66	$0.14 \cdot 10^{-2}$	1495+75+62+21	$0.17 \cdot 10^{-3}$	1670+69+54+16	$0.83 \cdot 10^{-4}$
	1672+370+66	$0.12 \cdot 10^{-2}$	1670+291+75+62+21	$0.96 \cdot 10^{-4}$	1670+69+54+32+16	$0.36 \cdot 10^{-4}$
3	1672+1497+66	$0.22 \cdot 10^{-2}$	1670+1105+75+62+21	$0.59 \cdot 10^{-4}$	1670+1494+69+32+16	$0.14 \cdot 10^{-4}$
	1672+1497+370+66	$0.14 \cdot 10^{-2}$	1670+1495+75+62+21	$0.91 \cdot 10^{-4}$	1670+1494+69+54+16	$0.11 \cdot 10^{-4}$
	T3		T3·H ₂ S		T3·(H ₂ S) ₂	
1	71+53	$0.28 \cdot 10^{-3}$	204+70+51+20	$0.16 \cdot 10^{-4}$	57+52+19+10	$0.86 \cdot 10^{-5}$
	174+53	$0.16 \cdot 10^{-3}$	204+70+51+35	$0.12 \cdot 10^{-4}$	57+52+29+10	$0.12 \cdot 10^{-4}$
	174+70+53	$0.22 \cdot 10^{-3}$	204+70+51+35+20	$0.25 \cdot 10^{-4}$	57+52+29+19+10	$0.11 \cdot 10^{-4}$
2	1516+53	$0.11 \cdot 10^{-4}$	1517+70+51+20	$0.13 \cdot 10^{-4}$	1513+57+52+29+10	$0.11 \cdot 10^{-5}$
	1573+53	$0.84 \cdot 10^{-4}$	1572+70+51+20	$0.14 \cdot 10^{-4}$	1571+57+52+19+10	$0.61 \cdot 10^{-5}$
	1516+71+53	$0.51 \cdot 10^{-3}$	1517+70+51+35+20	$0.23 \cdot 10^{-4}$	1571+57+52+29+10	$0.62 \cdot 10^{-5}$
	1573+71+53	$0.53 \cdot 10^{-3}$	1572+70+51+35+20	$0.31 \cdot 10^{-4}$	1513+57+52+29+19+10	$0.12 \cdot 10^{-4}$
	1516+174+71+53	$0.40 \cdot 10^{-3}$	1517+70+51+35+20	$0.11 \cdot 10^{-4}$	1513+204+57+52+29+10	$0.77 \cdot 10^{-5}$
	1573+174+71+53	$0.35 \cdot 10^{-3}$	1572+70+51+35+20	$0.14 \cdot 10^{-4}$	1571+204+57+52+29+10	$0.62 \cdot 10^{-5}$
3	1573+1516+53	$0.16 \cdot 10^{-3}$	1572+204+70+51+35+20	$0.16 \cdot 10^{-4}$	1513+204+57+52+29+10	$0.67 \cdot 10^{-5}$
	1573+1516+71+53	$0.46 \cdot 10^{-3}$	1572+1517+61+59+70+51+20	$0.17 \cdot 10^{-4}$	1571+204+57+52+29+19+10	$0.59 \cdot 10^{-5}$
	1573+1516+174+71+53	$0.28 \cdot 10^{-3}$	1572+1517+61+59+70+51+35+20	$0.19 \cdot 10^{-4}$	1513+1571+57+52+29+10	$0.71 \cdot 10^{-5}$

Figure 2 shows the calculated and experimental emission spectra of the molecules and complexes in question. It is well visible that the spectra contain a vibronic structure. Here, the intensity was normalized to the maximum peak 2 for T2 and T3 molecules, respectively, for comparison with experimental work [14]. The calculated absolute values of these peaks are $0.23 \times 10^3 \mu\text{J/mol}$ for T2 and $0.26 \times 10^2 \mu\text{J/mol}$ for T3. It should be noted that a good agreement between the experimental and calculated positions of the spectral peaks was obtained when the solvent (ethanol) was taken into account in the PCM model. In particular, for the maximum peaks 2 of T2 and T3 molecules, the difference between these positions is about 533 cm^{-1} and 246 cm^{-1} , respectively. Analysis of Figure 2 also shows that the shifts (bathochromic) of the vibronic bands of dithiophene and terthiophene complexes with H₂S and (H₂S)₂ do not exceed 130 cm^{-1} for all bands. In addition, the purely electronic transition (0-0) in the complexes is also slightly shifted. Indeed, the calculated frequencies of the electronic transition (0-0) are 30112 cm^{-1} , 30059 cm^{-1} , 29977 cm^{-1} for T2, T2·H₂S,

$T2 \cdots (H_2S)_2$ and 25119 cm^{-1} , 25056 cm^{-1} , 25053 cm^{-1} for $T3$, $T3 \cdots H_2S$, $T3 \cdots (H_2S)_2$, respectively. At the same time, a significant decrease of emission line intensity for these complexes as compared to that for individual free molecules of dithiophene and terthiophene is clearly seen in Figure 2: 3.7 and 2.6 times for $T2 \cdots H_2S$ and $T3 \cdots H_2S$ and by 5.5 and 3.6 times for $T2 \cdots (H_2S)_2$ and $T3 \cdots (H_2S)_2$, respectively. It is also seen that the complexity of the complexes' structures also leads to a decrease in the emission intensity.

Table shows the composite frequencies ($\omega_i + \omega_j + \dots$) of the harmonic oscillations of the promoting modes, which make the main contributions to the emission spectrum under study, and the squares of the dipole moment (μ^2) of transitions for these modes calculated taking into account the Herzberg-Teller and Duschinsky effects. The calculation results presented in Table and Figure 2 also show that the vibronic bands 1 for bithiophene and terthiophene are formed by their low-frequency modes ($\leq 370 \text{ cm}^{-1}$). The band 2 corresponds to combinations of low-frequency modes with high-frequency modes 1497 cm^{-1} , 1672 cm^{-1} for $T2$ and 1516 cm^{-1} , 1573 cm^{-1} for $T3$. The band 3 is formed by combinations of low-frequency modes and composite high-frequency modes.

A similar situation is observed for bithiophene and terthiophene complexes with H_2S and $(H_2S)_2$, where the vibronic structure of bands 1^a and 1^b (the subscripts a and b denote complexes with H_2S and $(H_2S)_2$, respectively) is a combination of low-frequency modes formed by intramolecular vibrations of bithiophene and terthiophene as well as intermolecular vibrations. The bands 2^a and 2^b correspond to combinations of low-frequency modes with high-frequency modes 1495 cm^{-1} , 1670 cm^{-1} and 1517 cm^{-1} , 1572 cm^{-1} for $T2 \cdots H_2S$ and $T3 \cdots H_2S$, respectively. It can also be seen that the vibronic spectra of the complexes containing $(H_2S)_2$ are close to ones of the corresponding complexes with H_2S (Fig. 2). At the same time, high-frequency modes are practically unchanged, namely 1494 cm^{-1} , 1670 cm^{-1} for $T2 \cdots (H_2S)_2$ and 1513 cm^{-1} , 1571 cm^{-1} for $T3 \cdots (H_2S)_2$.

Figure 3 illustrates the high-frequency promotion modes for bithiophene and terthiophene and their complexes with H_2S and $(H_2S)_2$. As can be seen, the contribution to the vibronic bands comes from high-frequency vibrations of C–C bonds in the central part of the molecules. The low-frequency modes (Table) correspond to out-of-plane vibrations of bithiophene and terthiophene molecules as well as to intermolecular vibrations of their complexes with H_2S and $(H_2S)_2$.

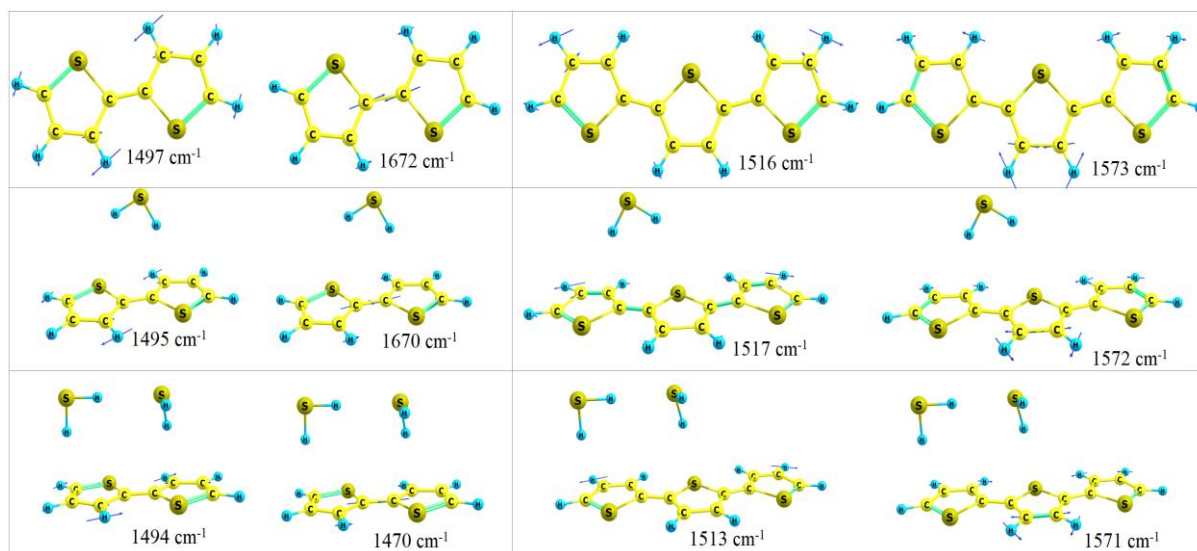


Figure 3. High-frequency promotion modes for $T2$ and $T3$ and for their complexes with H_2S and $(H_2S)_2$

Conclusions

The emission spectra of bithiophene and terthiophene molecules had a clear vibronic structure. As a result of calculations, it was found that the positions of bands (peaks) in the vibronic emission spectra of these compounds agreed well with the experimental data. It was established that vibronic progressions for bithiophene and terthiophene, as well as for oligofluorenes [26], are caused by low-frequency modes and some combinations of low-frequency modes with high-frequency modes and their combinations. A similar situation occurred for complexes of dithiophene and terthiophene molecules with H_2S and $(H_2S)_2$. The presence

of H₂S and (H₂S)₂ molecules in these complexes led to a 2.6–5.5-fold decrease in the vibronic band intensity in the emission spectra and to small bathochromic band shifts (< 130 cm⁻¹).

Acknowledgments

This study was carried out under RFBR grant No. 20-32-90110.

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