How to Cite: Sunchugashev, D.A., & Cherepanov, V.N. (2023). Vibronic Emission Spectra of Dithiophene and Terthiophene and Their Complexes with H_2S and $(H_2S)_2$. *Eurasian Journal of Chemistry, 111(3), 83-88.* https://doi.org/10.31489/2959-0663/3-23-8

Article

Received: 23 April 2023 | Revised: 25 May 2023 |
Accepted: 15 June 2023 | Published online: 26 July 2023

UDC 541.65/.654+535.372

https://doi.org/10.31489/2959-0663/3-23-8

Dmitry A. Sunchugashev*, Victor N. Cherepanov

National Research Tomsk State University, Tomsk, Russia
*(*Corresponding author's e-mail: dsunchugashev@gmail.com)*

Vibronic Emission Spectra of Dithiophene and Terthiophene and Their Complexes with H_2S and $(H_2S)_2$

In this work, the vibronic emission spectra of dithiophene (T2) and terthiophene (T3) molecules and their complexes with hydrogen sulfide and its dimmer 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 bithiophene 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 $T2\cdots H_2S$, $T3\cdots H_2S$ and $T2\cdots(H_2S)_2$, $T3\cdots(H_2S)_2$ 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 H_2S and $(H_2S)_2$ 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/m^2 [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 this 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 H_2S and $(H_2S)_2$ on vibronic spectra of dithiophene and terthiophene complexes with these molecules, which can be formed during the technological processes, were also studied.

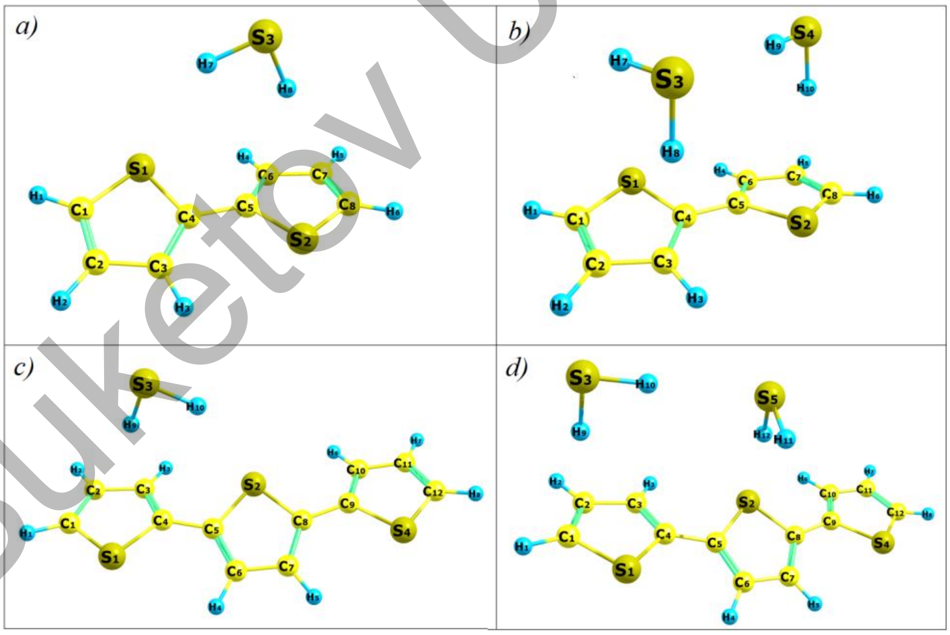
Computational Details

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 20º (the experimental value is 21º [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.

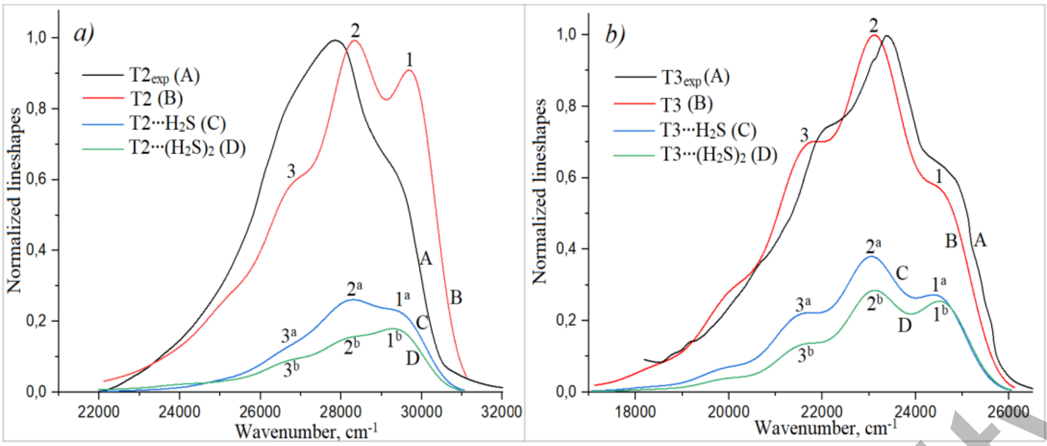
The structures of the complexes for their ground electronic states formed from T2 and T3 molecules and H_2S and $(H_2S)_2$ are shown in Figure 1. The coordinates of atoms, bond lengths and angles of $T2\cdots H_2S$, $T2\cdots (H_2S)_2$, $T3\cdots H_2S$, $T3\cdots (H_2S)_2$ are given in Supplementary Materials. The calculations showed that for these complexes the bond lengths change by less than 0.016 Å and the angles change by less than 0.41º 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 Å, and for angles < 0.65º). 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 ~ 600 cm^{-1} estimated from the experimental spectra [14] was used to simulate the vibronic spectra.



a — T2, T2···H_2S, T2···$(H_2S)_2$; *b* — T3, T3···H_2S, T3···$(H_2S)_2$

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 $\omega_i+\omega_j+\cdots$, square of the dipole moment of transitions μ^2) for vibronic spectra of bithiophene, terthiophene and their complexes with H_2S and $(H_2S)_2$

Peak number	$\omega_i + \cdots + \omega_j$cm^{-1}	μ^2, a.u.	$\omega_i + \cdots + \omega_j$cm^{-1}	μ^2, a.u	$\omega_i + \cdots + \omega_j$cm^{-1}	μ^2, a.u
	T2		T2···H_2S		T2···$(H_2S)_2$	
1	87+66 290+66 370+87+66	$0.54\cdot10^{-3}$ $0.65\cdot10^{-2}$ $0.24\cdot10^{-3}$	62+21 75+62+21 291+75+62+21	$0.24\cdot10^{-2}$ $0.49\cdot10^{-3}$ $0.18\cdot10^{-3}$	54+16 69+16 69+54+16	$0.11\cdot10^{-3}$ $0.13\cdot10^{-3}$ $0.18\cdot10^{-3}$
2	1497+66 1672+66 1497+290+66 1497+370+66 1672+370+66	$0.14\cdot10^{-1}$ $0.16\cdot10^{-1}$ $0.27\cdot10^{-2}$ $0.14\cdot10^{-2}$ $0.12\cdot10^{-2}$	1495+62+21 1670+62+21 1670+75+62+21 1495+75+62+21 1670+291+75+62+21 1495+291+75+62+21	$0.10\cdot10^{-3}$ $0.13\cdot10^{-3}$ $0.23\cdot10^{-3}$ $0.17\cdot10^{-3}$ $0.96\cdot10^{-4}$ $0.81\cdot10^{-4}$	1494+69+16 1670+69+16 1494+69+54+16 1670+69+54+16 1670+69+54+32+16 1494+69+54+32+16	$0.70\cdot10^{-4}$ $0.67\cdot10^{-4}$ $0.82\cdot10^{-4}$ $0.83\cdot10^{-4}$ $0.36\cdot10^{-4}$ $0.41\cdot10^{-4}$
3	1672+1497 +66 1672+1497+370+66	$0.22\cdot10^{-2}$ $0.14\cdot10^{-2}$	1670+1105+75+62+21 1670+1495+75+62+21	$0.59\cdot10^{-4}$ $0.91\cdot10^{-4}$	1670+1494+69+32+16 1670+1494+69+54+16	$0.14\cdot10^{-4}$ $0.11\cdot10^{-4}$
	T3		T3···H_2S		T3···$(H_2S)_2$	
1	71+53 174+53 174+70+53	$0.28\cdot10^{-3}$ $0.16\cdot10^{-3}$ $0.22\cdot10^{-3}$	204+70+51+20 204+70+51+35 204+70+51+35+20	$0.16\cdot10^{-4}$ $0.12\cdot10^{-4}$ $0.25\cdot10^{-4}$	57+52+19+10 57+52+29+10 57+52+29+19+10	$0.86\cdot10^{-5}$ $0.12\cdot10^{-4}$ $0.11\cdot10^{-4}$
2	1516+53 1573+53 1516+71+53 1573+71+53 1516+174+71+53 1573+174+71+53	$0.11\cdot10^{-4}$ $0.84\cdot10^{-4}$ $0.51\cdot10^{-3}$ $0.53\cdot10^{-3}$ $0.40\cdot10^{-3}$ $0.35\cdot10^{-3}$	1517+70+51+20 1572+70+51+20 1517+70+51+35+20 1572+70+51+35+20 1517+70+51+35+20 1572+70+51+35+20 1517+204+70+51+35+20 1572+204+70+51+35+20	$0.13\cdot10^{-4}$ $0.14\cdot10^{-4}$ $0.23\cdot10^{-4}$ $0.31\cdot10^{-4}$ $0.11\cdot10^{-4}$ $0.14\cdot10^{-4}$ $0.16\cdot10^{-4}$ $0.12\cdot10^{-4}$	1513+57+52+29+10 1571+57+52+19+10 1571+57+52+29+10 1513+57+52+29+19+10 1513+204+57+52+29+10 1571+204+57+52+29+10 1513+204+57+52+29+10 1571+204+57+52+29+19+10	$0.11\cdot10^{-5}$ $0.61\cdot10^{-5}$ $0.62\cdot10^{-5}$ $0.12\cdot10^{-4}$ $0.77\cdot10^{-5}$ $0.62\cdot10^{-5}$ $0.67\cdot10^{-5}$ $0.59\cdot10^{-5}$
3	1573+1516+53 1573+1516+71+53 1573+1516+174+71+53	$0.16\cdot10^{-3}$ $0.46\cdot10^{-3}$ $0.28\cdot10^{-3}$	1572+1517+61+59+70+51+20 1572+1517+61+59+70+51+35+20	$0{,}17\cdot10^{-4}$ $0{,}19\cdot10^{-4}$	1513+1571+57+52+29+10 1513+1571+57+52+29+19+10	$0.71\cdot10^{-5}$ $0.69\cdot10^{-5}$

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 0.23×10^3 μJ/mol for T2 and 0.26×10^2 μJ/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 H_2S and $(H_2S)_2$ 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···H_2S, T2···$(H_2S)_2$ and 25119 cm^{-1}, 25056 cm^{-1}, 25053 cm^{-1} for T3, T3···H_2S, T3···$(H_2S)_2$, 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···H_2S and T3···H_2S and by 5.5 and 3.6 times for T2···$(H_2S)_2$ and T3···$(H_2S)_2$, 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 ($\omega_i+\omega_j+\cdots$) 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 (≤ 370 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 tertiophene 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···H_2S and T3···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···$(H_2S)_2$ and 1513 cm^{-1}, 1571 cm^{-1} for T3···$(H_2S)_2$.

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 $(H_2S)_2$.

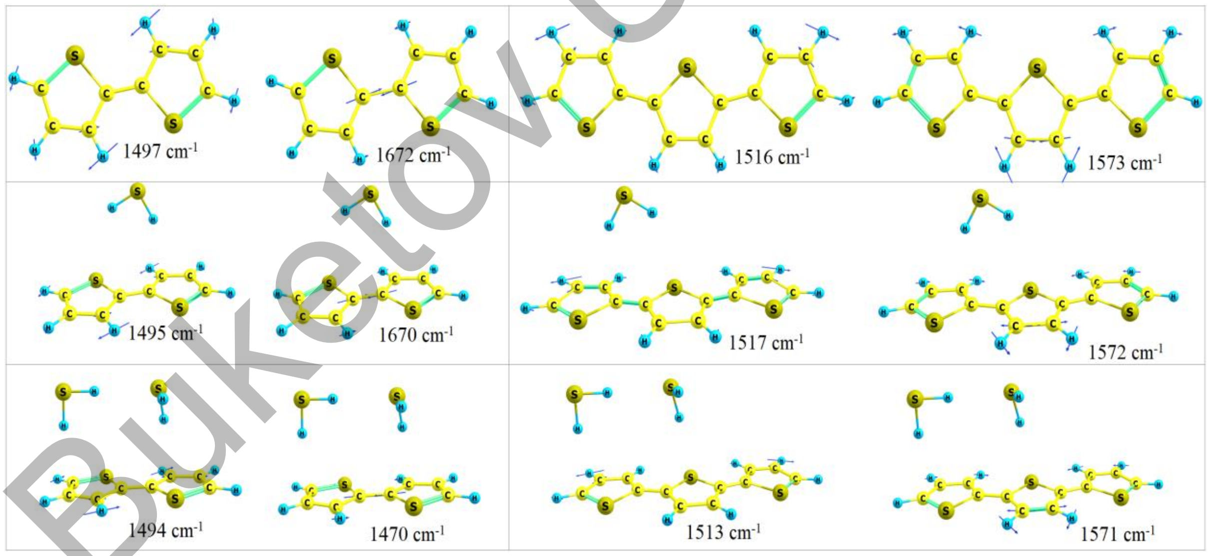


Figure 3. High-frequency promotion modes for T2 and T3 and for their complexes with H_2S and $(H_2S)_2$

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 H_2S and $(H_2S)_2$ 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.

References

1 Xu, R.-P., Li, Y.-Q. & Tang J.-X. (2016). Recent advances in flexible organic light-emitting diodes. *Journal of Materials Chemistry C*, *4*(39), 9116–9142. https://doi.org/10.1039/C6TC03230C

2 Choi, S., Kwon, S., Kim, H., Kim, W., Kwon, J.H., Lim, M.S., Lee, H.S. & Choi, K.C. (2017). Highly flexible and efficient fabric-based organic light-emitting devices for clothing-shaped wearable displays. *Scientific Reports*, *7*(1). https://doi.org/10.1038/s41598-017-06733-8

3 Barbarella, G., Favaretto, L., Zambianchi, M., Pudova, O., Arbizzani, C., Bongini, A. & Mastragostino, M. (1998). From easily oxidized to easily reduced thiophene-based materials. *Advanced Materials*, *10*(7), 551–554. https://doi.org/10.1002/(SICI)1521-4095(199805)10:7<551::AID-ADMA551>3.0.CO;2-Y

4 Perepichka, I. F., Perepichka, D. F. & Meng, H. (2009). Thiophene-based materials for electroluminescent applications. Handbook of Thiophene-Based Materials, 695–756. https://doi.org/10.1002/9780470745533.ch19

5 Zhang, L., Colella, N.S., Cherniawski, B.P., Mannsfeld, S.C.B. & Briseno, A.L. (2014). Oligothiophene semiconductors: synthesis, characterization, and applications for organic devices. *ACS Applied Materials & Interfaces*, *6*(8), 5327–5343. https://doi.org/10.1021/am4060468

6 Murphy, A.R. & Fréchet, J.M.J. (2007). Organic semiconducting oligomers for use in thin film transistors. *Chemical Reviews*, *107*(4), 1066–1096. https://doi.org/10.1021/cr0501386

7 Zade, S.S., Zamoshchik, N. & Bendikov, M. (2011). From short conjugated oligomers to conjugated polymers. Lessons from studies on long conjugated oligomers. *Accounts of Chemical Research*, *44*(1), 14–24. https://doi.org/10.1021/ar1000555

8 Mishra, A., Ma, C.-Q. & Bäuerle, P. (2009). Functional oligothiophenes: molecular design for multidimensional nanoarchitectures and their applications. *Chemical Reviews*, *109*(3), 1141–1276. https://doi.org/10.1021/cr8004229

9 Lim, S.T., Kwon, M.S. & Shin, D.-M. (2001). Organic light emitting diodes(OLEDs) with oligothiophene and silicon monoxide. *Molecular Crystals and Liquid Crystals Science and Technology. Section A. Molecular Crystals and Liquid Crystals*, *371*(1), 171–176. https://doi.org/10.1080/10587250108024715

10 Granlund, T., Theander, M., Berggren, M., Andersson, M., Ruzeckas, A., Sundström, V., Bjork, G., Granstrom, M. & Inganäs, O. (1998). A polythiophene microcavity laser. *Chemical Physics Letters*, *288*(5-6), 879–884. https://doi.org/10.1016/s0009-2614(98)00320-0

11 Mazzeo, M., Pisignano, D., Favaretto, L., Barbarella, G., Cingolani, R. & Gigli, G. (2003). Bright oligothiophene-based light emitting diodes. *Synthetic Metals*, *139*(3), 671–673. https://doi.org/10.1016/s0379-6779(03)00304-7

12 Duan, T., Chen, Q., Yang, Q. Hu, D., Cai, G., Lu, X., Lv, J., Song, H., Liu, F., Yu, D. & Lu, S. (2021) Simple thiazole-centered oligothiophene donor enables 15.4% efficiency all small molecule organic solar cells. *Journal of Materials Chemistry A*, *10*(6), 3009-3017. https://doi.org/10.1039/D1TA09058E

13 Sharipov, A.K. (2002). Chemistry and technology of fuels and oils, 38(5), 340–344. https://doi.org/10.1023/a:1021294917644

14 Becker, R.S., Seixas de Melo, J., Maçanita, A.L. & Elisei, F. (1996). Comprehensive evaluation of the absorption, photophysical, energy transfer, structural, and theoretical properties of α-oligothiophenes with one to seven rings. *The Journal of Physical Chemistry*, *100*(48), 18683–18695. https://doi.org/10.1021/jp960852e

15 Improta, R., Ferrer, F.J. A., Stendardo, E. & Santoro, F. (2014). Quantum-classical calculation of the absorption and emission spectral shapes of oligothiophenes at low and room temperature by first-principle calculations. *ChemPhysChem*, *15*(15), 3320–3333. https://doi.org/10.1002/cphc.201402323

16 Stendardo, E., Avila Ferrer, F., Santoro, F. & Improta, R. (2012). Vibrationally resolved absorption and emission spectra of dithiophene in the gas phase and in solution by first-principle quantum mechanical calculations. *Journal of Chemical Theory and Computation*, *8*(11), 4483–4493. https://doi.org/10.1021/ct300664d

17 Madsen, D., Christiansen, O., Norman, P. & König, C. (2019). Vibrationally resolved emission spectra of luminescent conjugated oligothiophenes from anharmonic calculations. *Physical Chemistry Chemical Physics*, *21*(31), 17410–17422. https://doi.org/10.1039/C9CP03039E

18 Santoro, F. & Cerezo, J. FCclasses. CNRICCOM, http://www.iccom.cnr.it/en/fcclasses/

19 Christiansen, O., Artiukhin, D. & Godtliebsen, I.H. Midascpp GITLAB, https://gitlab.com/midascpp/midascpp

20 Frisch, M.J., Trucks, G.W., Schlegel, H.B., Scuseria, G.E., Robb, M.A., Cheeseman et. al. (2009). Gaussian, Inc., Wallingford CT. https://gaussian.com/glossary/g09

21 Herzberg, G. & Teller, E. (1933). Schwingungsstruktur der elektronenübergänge bei mehratomigen molekülen. *Zeitschrift Für Physikalische Chemie*, *21B*(1). https://doi.org/10.1515/zpch-1933-2136

22 Duschinsky, F. (1937). The importance of the electron spectrum in multi atomic molecules. Concerning the Franck-Condon principle *Acta Physicochim. URSS* 7. 551–566.

23 Yanai, T., Tew, D.P., & Handy, N.C. (2004). A new hybrid exchange–correlation functional using the Coulomb-attenuating method (CAM-B3LYP). *Chemical Physics Letters*, *393*(1–3), 51–57. https://doi.org/10.1016/j.cplett.2004.06.011

24 Francl, M.M., Pietro, W.J., Hehre, W.J., Binkley, J.S., Gordon, M.S., DeFrees, D.J. & Pople, J.A. (1982). Self-consistent molecular orbital methods. XXIII. A polarization-type basis set for second-row elements. *The Journal of Chemical Physics*, *77*(7), 3654–3665. https://doi.org/10.1063/1.444267

25 Takayanagi, M., Gejo, T. & Hanazaki, I. (1994). Geometry and torsional potential of 2,2'-bithiophene in a supersonic jet. *The Journal of Physical Chemistry*, *98*(49), 12893–12898. https://doi.org/10.1021/j100100a014

26 Valiev, R.R., Sunchugashev, D.A., Gadirov, R.M., Nasibullin, R.T. & Cherepanov, V.N. (2022). Vibronic spectra of bifluorene and terfluorene. *Russian Physics Journal*, *64*(11), 2082–2088. https://doi.org/10.1007/s11182-022-02559-8

Information about authors*

Cherepanov, Victor Nikolaevich — Doctor of Physical and Mathematical Sciences, Head of Optics and Spectroscopy Department, National Research Tomsk State University, Lenin ave., 36, 634050, Tomsk, Russia; e-mail: vnch@phys.tsu.ru; https://orcid.org/0000-0002-5952-5202

Sunchugashev, Dmitry Andreevich (*corresponding author*) - 4th year PhD student, Department of Physics, National Research Tomsk State University, Lenin ave., 36, 634050, Tomsk, Russia; e-mail: dsunchugashev@gmail.com; https://orcid.org/0009-0006-6069-3410

---

*The author's name is presented in the order: *Last Name, First and Middle Names*