

Solid state structural and light emission color diversity from styrylbenzothiazole derivatives

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ABSTRACT

Here, 2-styryl-1,3-benzothiazole and seven para-substituted phenyl derivatives thereof were synthesized, structurally elucidated and assessed to photoluminescence, with theoretical approaches of their absorption spectra. One derivative substituted at ortho-position of phenyl adds to series of nine studied compounds, in which five of them had their crystal structures determined for the first time. These structures join to two others already known thus far, allowing us to get solid state structural knowledge from the compounds series such as molecular planarity and packing diversity given by different patterns of $\pi\cdots\pi$ stacking, $\text{CH}\cdots\pi$ and $\text{CH}\cdots\text{N}$ interactions even though their molecular simplicity and similarity. Isostructurality was observed only between the unsubstituted and the fluoro substituted compounds. Compounds with methoxy, *N,N*-dimethyl and thiomethoxy para-substituents presented high photoluminescence quantum yields above 10 %, with emission in the blue, yellow and green colour regions, respectively.

1. Introduction

The development of novel organic materials exhibiting distinctive optical and electronic properties has attracted significant attention in the field of optoelectronics, driven by their potential applications in organic light-emitting diodes, photovoltaic devices, flexible electronic systems, and biosensing [1–3]. Thiazole derivatives constitute a versatile family of heteroaromatic fluorophores whose luminescent properties can be finely tuned through structural and electronic modifications. Both simple and fused thiazole systems exhibit intense fluorescence, large Stokes shifts, and pronounced solvatochromic behavior, enabling emission across the visible spectrum in solution and in the solid state [4–7]. In this context, numerous thiazole-based derivatives have emerged as attractive platforms for the development of functional luminescent materials.

2-(2-Hydroxyaryl)benzothiazole derivatives (Fig. 1) are well-known luminophores owing to their efficient excited-state intramolecular proton transfer (ESIPT) process and, as a result, have been extensively

explored as luminescent probes for the selective detection of metal ions, anions, and biomolecules, as well as for applications in bioimaging and optoelectronic devices [8–10]. Thiazole derivatives containing extended unsaturated chains have also been investigated for their luminescent properties. In a study reported in 2013, Awad and co-workers examined the influence of aromatic system size on the photophysical and photochemical behavior of styrylbenzothiazoles by replacing the phenyl ring of 1-phenyl-2-(2-benzothiazolyl)ethene with naphthyl and phenanthryl moieties [11]. Their results demonstrated that the fluorescence quantum yield is strongly dependent on the size of the hydrocarbon group, with the naphthyl-substituted derivative (Fig. 1) displaying the highest quantum yields [11]. In a recent study, Stindt and co-workers reported the synthesis and systematic evaluation of the photochemical properties of a series of styrylbenzazoles, including benzoxazole, benzothiazole, benzimidazole, *N*-methylbenzimidazole, and *N*-methylbenzoxazolium salt derivatives [12]. The compound 2,6-dimethyl-4-(dimethylamino)-styrylbenzothiazole, a thiazole derivative (Fig. 1), demonstrated outstanding photochemical properties, combining high thermal

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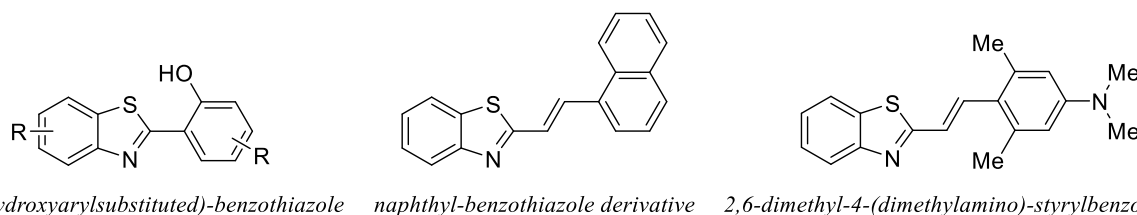
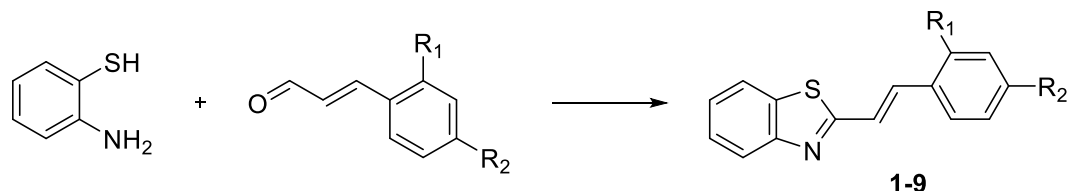


Fig. 1. Representative benzothiazole derivatives highlighting, from left to right, the effects of ESIPT, π -conjugation, and electron-donating substitution on luminescent properties.



1: $R_1 = R_2 = H$; **2:** $R_1 = H$, $R_2 = OCH_3$; **3:** $R_1 = H$, $R_2 = N(CH_3)_2$; **4:** $R_1 = OCH_3$, $R_2 = H$; **5:** $R_1 = H$, $R_2 = F$; **6:** $R_1 = H$, $R_2 = CN$; **7:** $R_1 = H$, $R_2 = SCH_3$; **8:** $R_1 = H$, $R_2 = Br$; **9:** $R_1 = H$, $R_2 = CF_3$.

Scheme 1. Synthesis of 2-styrylbenzothiazole derivatives. Aldehyde, o-aminothiophenol, $NaHSO_3$, *N,N*-dimethylacetamide, MWI, 80 °C.

Table 1

Summary of crystal data collected with CuK α and refinement statistics for the five compounds elucidated for the first time here.

	3	4	5	6	8
structural formula	$C_{17}H_{16}N_2S$	$C_{16}H_{13}NOS$	$C_{15}H_{10}FNS$	$C_{16}H_{10}N_2S$	$C_{15}H_{10}BrNS$
space group	$Pca2_1$	$Pna2_1$	$P2_1/c$	$P-1$	$Pccn$
Z/Z'	4/1	8/2	4/1	2/1	8/1
$T(K)$	290	301	300	301	301
a (Å)	11.1326(8)	27.8413(15)	6.13330(10)	6.46475(17)	28.8846(5)
b (Å)	16.828(2)	6.8920(3)	14.5585(3)	7.57684(19)	14.9105(2)
c (Å)	7.7639(5)	14.1365(6)	13.7600(3)	13.4650(4)	6.04476(10)
α (°)	90	90	90	94.358(2)	90
β (°)	90	90	95.729(2)	101.054(2)	90
γ (°)	90	90	90	96.761(2)	90
V (Å ³)	1454.5(2)	2712.5(2)	1222.52(4)	639.52(3)	2603.39(7)
calculated density (Mg/m ³)	1.280	1.309	1.387	1.362	1.614
θ range for data collection (°)	2.626–78.858	3.175–81.245	4.433–79.983	3.362–79.851	3.060–80.084
data collected	7823	25,254	23,845	13,602	35,633
unique reflections	2529	5349	2643	2727	2831
unique reflections with $I > 2s(I)$	1698	4340	2160	2335	2474
symmetry factor (R_{int})	0.0435	0.0666	0.0667	0.0380	0.0406
parameters refined	183	346	163	172	163
goodness-of-fit on F^2	1.062	1.049	1.069	1.026	1.066
final $R1$ factor for $I > 2s(I)$	0.0664	0.0674	0.0759	0.0458	0.0447
$wR2$ factor for all data	0.2017	0.2008	0.2110	0.1367	0.1230
largest Dr peaks ($e/\text{Å}^3$)	0.391/−0.249	0.362/−0.240	0.936/−0.520	0.310/−0.166	0.845/−0.364
CCDC deposit number	2485,380	2485,381	2505,702	2505,703	2505,704

stability, negative photochromism, and near-quantitative photoisomerization under visible-light irradiation up to 470 nm, with a quantum yield of 59 %, thus representing a highly efficient P-type photoswitch [12].

In summary, benzothiazole derivatives, particularly styrylbenzothiazoles, constitute a promising class of compounds; however, their photoluminescent properties remain relatively underexplored when compared with other widely investigated π -conjugated systems. A comprehensive understanding of the mechanisms driving their emission processes, including the influence of both electron-donating and electron-withdrawing substituents on the Stokes shift and fluorescence quantum yield, is essential for expanding their potential applications in optical devices and bioimaging. Herein, we report a detailed investigation of the crystal structures and luminescent properties of

styrylbenzothiazole derivatives, in which density functional theory (DFT) calculations helped us to understand.

2. Materials and methods

2.1. Synthesis

Styrylbenzothiazole derivatives 1–9 were synthesized following a previously reported methodology [13], with minor modifications (Scheme 1). Sodium bisulfite ($NaHSO_3$, 2 equiv.) was placed in a 50 mL round-bottom flask, followed by the addition of *N,N*-dimethylacetamide (DMA, 5 mL) and the corresponding aldehyde (1.5 mmol). Subsequently, o-aminothiophenol (1.0 mmol) was added, and the reaction mixture was subjected to microwave irradiation in an open system at 80

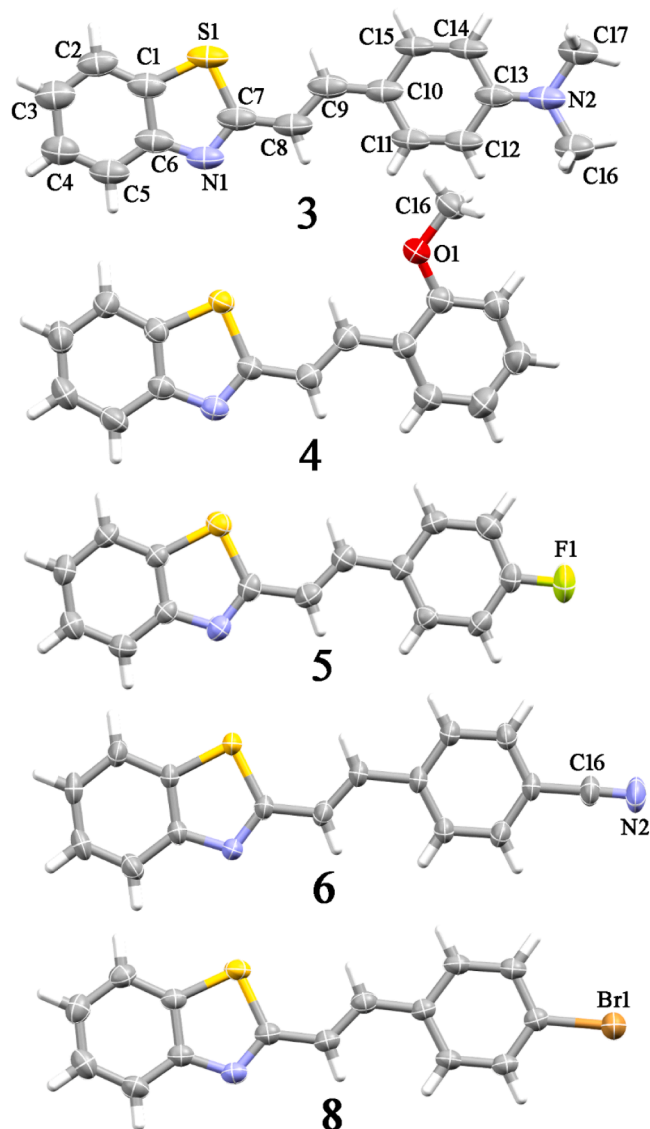


Fig. 2. Asymmetric unit of the compounds elucidated in this study. Non-hydrogen atoms are drawn with their 30 % probability ellipsoid, while hydrogen atoms are arbitrary radius spheres. The labelling scheme of non-hydrogen atoms and rings common to all compounds followed those shown once. Even though compound 4 has two crystallographically independent molecules in its asymmetric unit, just one molecule (labelled as A) is presented here because both molecules are well superimposed (RMSD = 0.164 Å).

°C, with a maximum power of 300 W, a ramp time of 5 min, and a reaction time of 60 min, under cooling. After completion of the reaction, the mixture was allowed to cool to room temperature and then poured into ice-cold water. The resulting solid was collected by vacuum filtration and purified by column chromatography using hexane/ethyl acetate as the eluent (in proportions optimized for each compound), followed by recrystallization when necessary. All synthesized compounds were fully characterized by melting point determination (MP), infrared (IR) spectroscopy, nuclear magnetic resonance (NMR) spectroscopy, and high-resolution mass spectrometry (HRMS) (Figs. S1–S36).

(E)-2-styrylbenzo[d]thiazole (1)

Yield, 67 %, m.p. 106–108 °C. FTIR cm^{-1} : 3058, 1630, 1446, 1316, 1192, 956, 754, 748, 723, 684. ^1H NMR (CDCl_3 , 400 MHz): δ (ppm): 8.00 (d, J = 8.0 Hz, 1H), 7.86 (d, J = 8.0 Hz, 1H), 7.62–7.50 (m, 3H), 7.50–7.33 (m, 6H). ^{13}C NMR (CDCl_3 , 100 MHz): δ : 167.2, 138.2, 135.3, 129.6, 129.0, 127.5, 126.5, 125.5, 122.8, 121.8, 126.6. HRMS (ESI) m/z , calcd. for $\text{C}_{15}\text{H}_{12}\text{NS}$ [$M + H$] $^+$, 238.0685; found 238.0686.

(E)-2-(4-methoxystyryl)benzo[d]thiazole (2)

Yield, 74 %, m.p. 145–147 °C. FTIR cm^{-1} : 2995, 1601, 1514, 1257, 1174, 1028, 956, 808, 805, 757, 729. ^1H NMR (CDCl_3 , 400 MHz): δ (ppm): 8.00 (d, J = 8.2 Hz, 1H), 7.87 (d, J = 8.2 Hz, 1H), 7.59–7.44 (m, 4H), 7.38 (t, J = 7.4 Hz, 1H), 7.34–7.26 (m, 1H), 6.96 (d, J = 8.6 Hz, 2H), 3.88 (s, 3H). ^{13}C NMR (CDCl_3 , 100 MHz): δ : 167.5, 160.8, 153.9, 137.4, 134.2, 128.9, 128.2, 126.3, 125.1, 122.8, 121.5, 119.9, 114.5, 55.4. HRMS (ESI) m/z , calcd. for $\text{C}_{16}\text{H}_{14}\text{NOS}$ [$M + H$] $^+$, 268.0791; found 268.0788.

(E)-2-(4-dimethylaminostyryl)benzo[d]thiazole (3)

Yield, 61 %, m.p. 205–208 °C. FTIR cm^{-1} : 2891, 1595, 1524, 1474, 1361, 1226, 1181, 1168, 960, 804, 756. ^1H NMR (CDCl_3 , 400 MHz): δ (ppm): 7.94 (d, J = 8.1 Hz, 1H), 7.82 (d, J = 8.1 Hz, 1H), 7.52–7.39 (m, 4H), 7.32 (t, J = 7.6 Hz, 1H), 7.20 (d, J = 16.2 Hz, 1H), 6.76–6.66 (m, 2H), 3.03 (s, 6H). ^{13}C NMR (CDCl_3 , 100 MHz): δ : 168.2, 154.0, 151.2, 138.3, 134.1, 130.7, 128.9, 126.1, 124.7, 123.4, 122.4, 121.4, 117.3, 112.1, 111.8, 40.3. HRMS (ESI) m/z , calcd. for $\text{C}_{17}\text{H}_{17}\text{N}_2\text{S}$ [$M + H$] $^+$, 281.1107; found 281.1104.

(E)-2-(2-methoxystyryl)benzo[d]thiazole (4)

Yield, 69 %, m.p. 265–267 °C. FTIR cm^{-1} : 2995, 1601, 1514, 1257, 1174, 1028, 757. ^1H NMR (CDCl_3 , 400 MHz): δ (ppm): 7.98 (d, J = 8.2 Hz, 1H), 7.87–7.79 (m, 2H), 7.62–7.57 (m, 1H), 7.52 (d, J = 16.4 Hz, 1H), 7.48–7.42 (m, 1H), 7.38–7.30 (m, 2H), 7.03–6.96 (m, 1H), 6.93 (d, J = 8.2 Hz, 1H), 3.93 (s, 3H). ^{13}C NMR (CDCl_3 , 100 MHz): δ : 168.2, 157.8, 153.9, 134.4, 133.4, 130.6, 128.1, 126.2, 125.2, 124.3, 122.9, 121.5, 120.9, 111.1, 55.5. HRMS (ESI) m/z , calcd. for $\text{C}_{16}\text{H}_{14}\text{NOS}$ [$M + H$] $^+$, 268.0791; found 268.0790.

(E)-2-(4-fluorostyryl)benzo[d]thiazole (5)

Yield, 82 %, m.p. 161–163 °C. FTIR cm^{-1} : 3061, 3039, 3001, 1598, 1509, 1222, 952, 816, 758. ^1H NMR (CDCl_3 , 400 MHz): δ (ppm): 8.00 (d, J = 8.2 Hz, 1H), 7.85 (d, J = 8.2, 1H), 7.59–7.44 (m, 4H), 7.41–7.35 (m, 1H), 7.28 (d, J = 16.2 Hz, 1H), 7.10 (t, J = 8.5, 2H). ^{13}C NMR (CDCl_3 , 100 MHz): δ : 166.8, 163.3 (d, $J_{\text{C-F}}$ = 250.0 Hz), 153.9, 136.3, 134.3, 131.7 (d, $J_{\text{C-F}}$ = 3.4 Hz), 129.2 (d, $J_{\text{C-F}}$ = 8.3 Hz), 126.4, 125.4, 123.0, 121.9 (d, $J_{\text{C-F}}$ = 2.5 Hz), 121.5, 116.1 (d, $J_{\text{C-F}}$ = 22.0 Hz). HRMS (ESI) m/z , calcd. for $\text{C}_{15}\text{H}_{11}\text{FNS}$ [$M + H$] $^+$, 256.0591; found 256.0589.

(E)-4-(2-(benzo[d]thiazol-2-yl)vinyl)benzonitrile (6)

Yield, 57 %, m.p. 192–193 °C. FTIR cm^{-1} : 3063, 2998, 2223, 1606, 1478, 1410, 1314, 1188, 1123, 942, 811, 762, 728, 667, 607. ^1H NMR (CDCl_3 , 400 MHz): δ (ppm): 8.03 (d, J = 8.0 Hz, 1H), 7.89 (d, J = 8.0, 1H), 7.73–7.61 (m, 4H), 7.57–7.38 (m, 4H). ^{13}C NMR (CDCl_3 , 100 MHz): δ : 165.6, 153.8, 139.8, 135.0, 134.6, 132.7, 127.7, 126.7, 125.9, 125.4, 123.4, 121.7, 118.6, 112.4. HRMS (ESI) m/z , calcd. for $\text{C}_{16}\text{H}_{11}\text{N}_2\text{S}$ [$M + \text{Na}$] $^+$, 285.0457; found 285.0455.

(E)-2-(4-(methylthio)styryl)benzo[d]thiazole (7)

Yield, 75 %, m.p. 206–207 °C. FTIR cm^{-1} : 1628, 1591, 1500, 1435, 1091, 951, 802, 758, 729. ^1H NMR (CDCl_3 , 400 MHz): δ (ppm): 7.99 (d, J = 8.0 Hz, 1H), 7.85 (d, J = 8.0 Hz, 1H), 7.53–7.43 (m, 4H), 7.40–7.32 (m, 2H), 7.29–7.22 (m, 2H), 2.52 (s, 3H). ^{13}C NMR (CDCl_3 , 100 MHz): δ : 167.1, 153.9, 140.7, 137.1, 134.3, 132.1, 127.8, 126.3 (2C), 125.3, 122.9, 121.5, 121.2, 15.3. HRMS (ESI) m/z , calcd. for $\text{C}_{16}\text{H}_{14}\text{NS}_2$ [$M + H$] $^+$, 284.0562; found 284.0562.

(E)-2-(4-bromostyryl)benzo[d]thiazole (8)

Yield, 83 %, m.p. 231–234 °C. FTIR cm^{-1} : 1478, 1399, 1235, 1190, 1070, 957, 943, 808, 753, 722. ^1H NMR (CDCl_3 , 400 MHz): δ (ppm): 8.00 (d, J = 8.0 Hz, 1H), 7.87 (d, J = 8.0 Hz, 1H), 7.56–7.52 (m, 2H), 7.51–7.42 (m, 4H), 7.42–7.35 (m, 2H). ^{13}C NMR (CDCl_3 , 100 MHz): δ : 166.5, 153.8, 136.2, 134.4 (2C), 132.2, 128.8, 126.5, 125.5, 123.5, 123.1, 122.7, 121.6. HRMS (ESI) m/z , calcd. for $\text{C}_{15}\text{H}_{11}\text{BrNS}$ [$M + H$] $^+$, 315.9790; found 315.9793.

(E)-2-(4-(trifluoromethyl)styryl)benzo[d]thiazole (9)

Yield, 55 %, m.p. 162–163 °C. FTIR cm^{-1} : 3071, 3000, 2934, 1614, 1557, 1483, 1413, 1316, 1158, 1104, 1066, 1013, 948, 865, 821, 760, 730, 666, 617. ^1H NMR (CDCl_3 , 400 MHz): δ (ppm): 8.03 (d, J = 8.1 Hz, 1H), 7.88 (d, J = 8.1 Hz, 1H), 7.70–7.64 (m, 4H), 7.58–7.37 (m, 4H). ^{13}C NMR (CDCl_3 , 100 MHz): δ : 166.1, 153.8, 138.8, 135.7, 134.5, 130.9 (q,

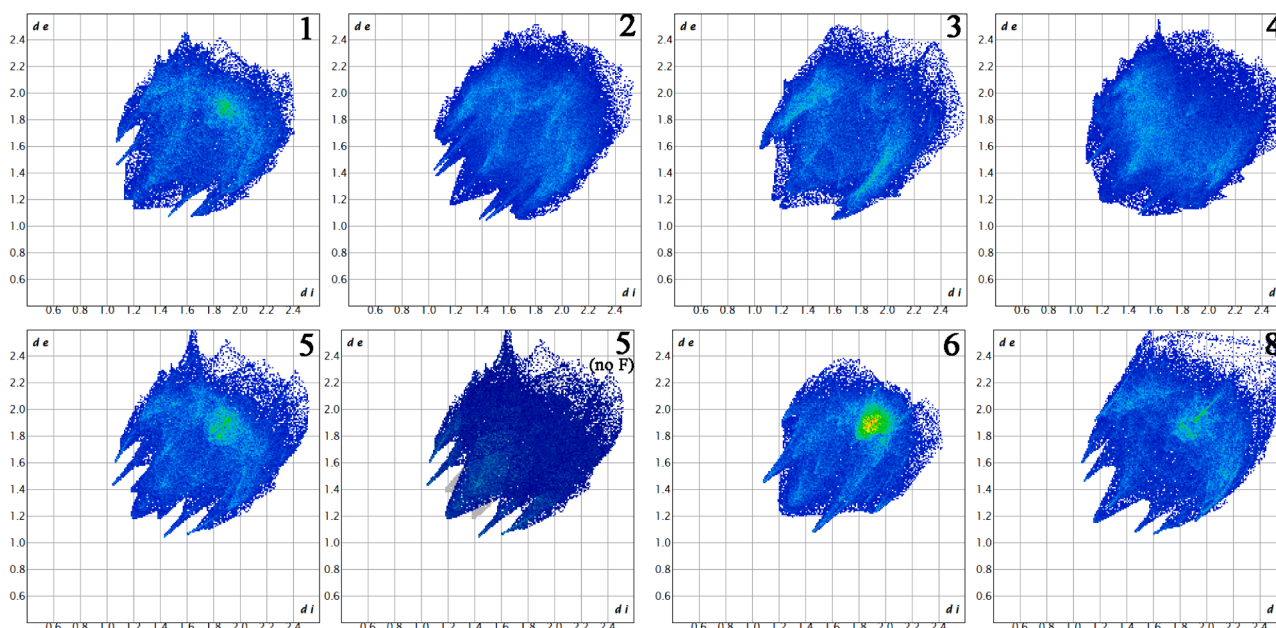


Fig. 3. Full fingerprint graphics of the Hirshfeld surface calculated for the styrylbenzothiole series studied here. One of the fingerprints of compound **5** has not the contribution of fluorine atom, and the gray shadow draws the distances involving this element. The blue colour indicates lower proportions of a (d_i, d_e) pair; green outlines an intermediary frequency; and red draws an upper limit fraction greater than 0.1 % of the surface points with the same (d_i, d_e) combination.

$J_{C-F} = 32.0$ Hz), 127.5, 126.6, 126.0 (q, $J_{C-F} = 270.0$ Hz), 125.9 (q, $J_{C-F} = 4.0$ Hz), 125.8, 124.4, 123.2, 121.6. HRMS (ESI) m/z , calcd. for $C_{16}H_{11}F_3NS$ [$M + H$] $^+$, 306.0559; found 306.0553.

2.2. Single-crystal X-ray structure determination

Single crystal X-ray diffraction data for compounds **3**, **4**, **5**, **6** and **8** were collected in a Rigaku Synergy diffractometer using $CuK\alpha$ ($\lambda = 1.54184$ Å) radiation at room temperature (298 K). The data collection, cell refinements and data reduction were performed using the CRYSA-LISPRO software [14]. The structures were resolved and refined by SHELX [15] using OLEX2 system [16], and all non-hydrogen atoms were refined with anisotropic thermal parameters. H atoms connected to carbon were placed in idealized positions and treated by rigid model, with $U_{iso}(H) = 1.2U_{eq}$ for aromatic rings and $U_{iso}(H) = 1.5U_{eq}$ for CH_3 groups. CCDC 2485380, 2485381, 2505702, 2505703, and 2505704 have supplementary crystallographic data for **3**, **4**, **5**, **6** and **8**, respectively. Summary of these data is in Table 1 and their complete set can be obtained free of charge from The Cambridge Crystallographic Data Centre at <http://www.ccdc.cam.ac.uk/conts/retrieving.html>. The figures were drawn using ORTEP-3 for Windows [17] and Mercury [18] programs.

To further compare the intermolecular interactions patterns found in the studied structures, Hirshfeld surfaces were calculated using Crystal Explorer software (version 21.5) [19]. The surfaces were also analysed by the fingerprint plots of external distance (d_e , the distance between the calculated Hirshfeld surface and the nearest atom of a packed molecule out of the calculated surface) versus internal distance (d_i , the shortest separation from the calculated Hirshfeld surface to an atom of the molecule within the calculated surface) [20].

2.3. Diffuse reflectance and photoluminescence measurements

The diffuse reflectance spectra were collected in a PerkinElmer spectrophotometer, model Lambda WB1050, using a Praying Mantis accessory and barium sulphate powder (Sigma-Aldrich) as a reference. The band gap was calculated from the Kubelka-Munk function [21]:

$$F(R_\infty) = (1 - R_\infty)^2 / (2R_\infty) = K/S \quad (1)$$

being R_∞ the ratio between the reflectance of the sample divided by the reference one ($R_{\text{sample}}/R_{\text{reference}}$), and absorption coefficient (K), and scattering coefficient (S), by using the Tauc relation [21]:

$$\alpha h\nu = A(h\nu - E_g)^{1/2} \quad (2)$$

where A is a proportionality constant, h is the Planck constant, α is the absorption coefficient, the band gap E_g , and considering that the absorption coefficient K becomes equal to 2α , and the scattering coefficient S is constant with respect to wavelength, the following expression can be written:

$$(F(R_\infty)h\nu)^2 = A(h\nu - E_g)^{1/2} \quad (3)$$

From the plot of $(F(R_\infty)h\nu)^2$ versus $h\nu$, the value of E_g could be obtained by extrapolating the linear fitted region to $(F(R_\infty)h\nu)^2 = 0$ [22].

Photoluminescence excitation and emission spectra were recorded at room temperature using a Horiba Jobin-Yvon Fluorolog FL3-221 spectrofluorometer equipped with a Hamamatsu photomultiplier and dual monochromators, in which a 450 W Xe lamp was used as an excitation source. A bandpass of 1.0 nm, increment of 0.5 nm, and integration times of 0.2 s were used for both emission and excitation measurements. Photoluminescence decay curves were recorded using pulsed NanoLEDs with excitations at 290, 340, and 390 nm, and ~ 1 ns width pulses and 1 MHz frequency. The CIE 1931 (Commission International d'Eclairage) chromaticity diagram was determined from emission spectra obtained for the samples by using the methods defined by Wyman et al. [23]. The correlated colour temperature (CCT) was calculated using the McCamy formula [24]: $CCT = -437n^3 + 360n^2 - 6861n + 5514.31$, where $n = (x - x_c)/(y - y_c)$, x and y the chromaticity coordinates, and $x_c = 0.3320$ and $y_c = 0.1858$ the coordinates of chromaticity epicentre. The internal and external QY's (iQY and eQY) were calculated following the method developed by Wrighton et al. [25].

2.4. Computational details

The electronic structure calculations and molecular geometry optimizations were performed at the DFT level using as starting geometry the coordinates from crystal structures. Vibrational harmonic fre-

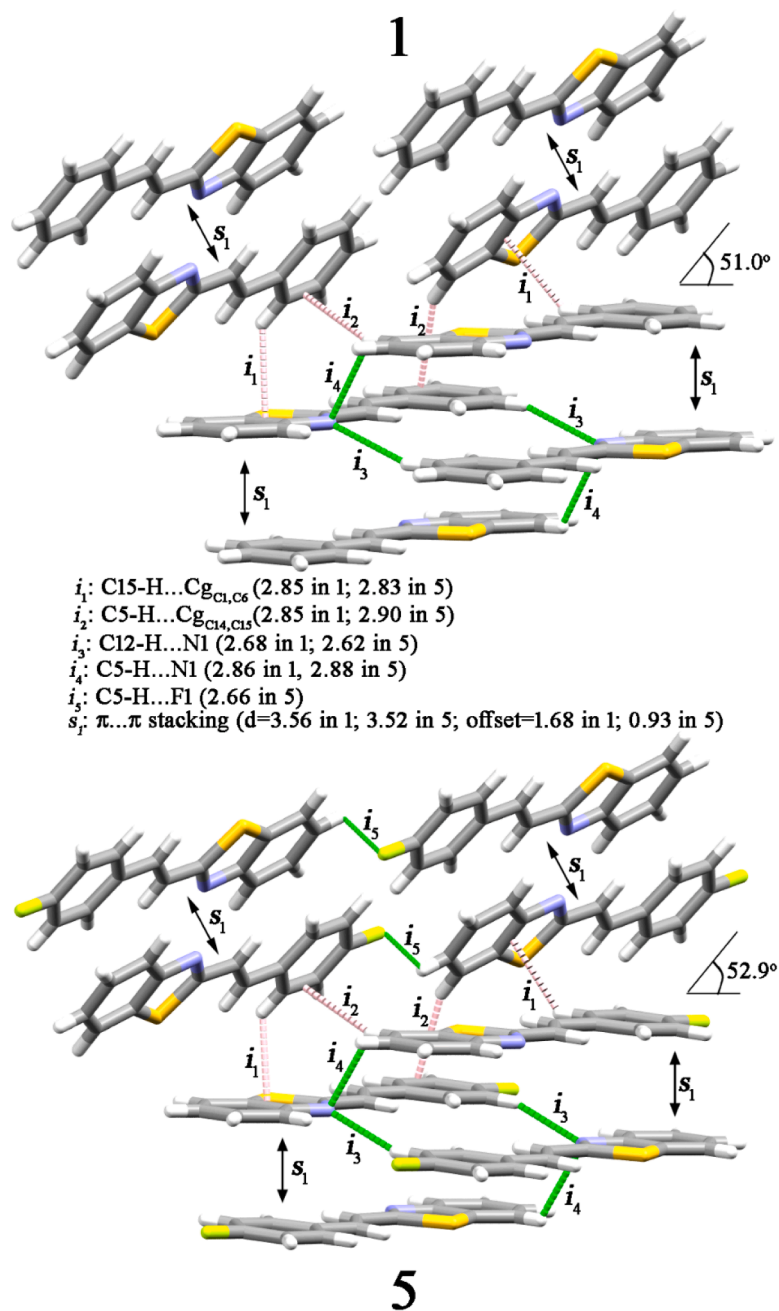


Fig. 4. A crystal packing view of isostructural compounds **1** and **5**. In this picture and hereinafter, up to Fig. 8, green and pink dashed lines depict CH...N and CH... π interactions, respectively. Likewise, the displayed angle was calculated between the least-square (LS) planes calculated for all non-hydrogen atoms of L-shaped (or T-shaped in Fig. 8) interacting molecules, as well as the interplanar distance (d) between π ... π -stacked ones were calculated for their LS planes (in order to calculate the offset between the stacked molecules, the molecular centroid was taken together with d). Except for the angle in°, all other values refer to distances in Å, and these were measured between hydrogen atom and either nitrogen or centroid (Cg) in the case of CH... π interactions.

quencies were computed for the optimized structures presenting only real values for all normal modes. The wavelengths of the electronic transitions and oscillator strengths were computed by the TD-DFT. All calculations were performed with Gaussian 16 [26]. The CAM-B3LYP [27] exchange correlation functional and the def2-TZVP [28] base set were employed in the computations. Electronic descriptors, chemical potential, $\mu = \frac{(E_{\text{HOMO}} + E_{\text{LUMO}})}{2}$, chemical hardness, $\eta = \frac{(E_{\text{LUMO}} - E_{\text{HOMO}})}{2}$ and electrophilicity index, $\omega = \frac{\mu^2}{2\eta}$ [29,30], are computed from the energies of the frontier molecular orbital corresponding to the highest occupied (HOMO) and lowest unoccupied (LUMO) molecular orbitals, respectively.

3. Results and discussion

3.1. X-ray diffraction analysis

Here we have obtained single crystals suitably sized and shaped to X-ray structure experiment determination for six compounds of the studied series, namely, **2** to **6** and **8**. However, five of them were unknown thus far, because compound **2** has been already elucidated in the same crystal structure which we obtained here [Cambridge Structural Database (CSD) reference code OJEGAM, found in the CSD version 6.01, November 2025]. Furthermore, another compound of the series was previously elucidated by X-ray crystallography, that is compound **1**

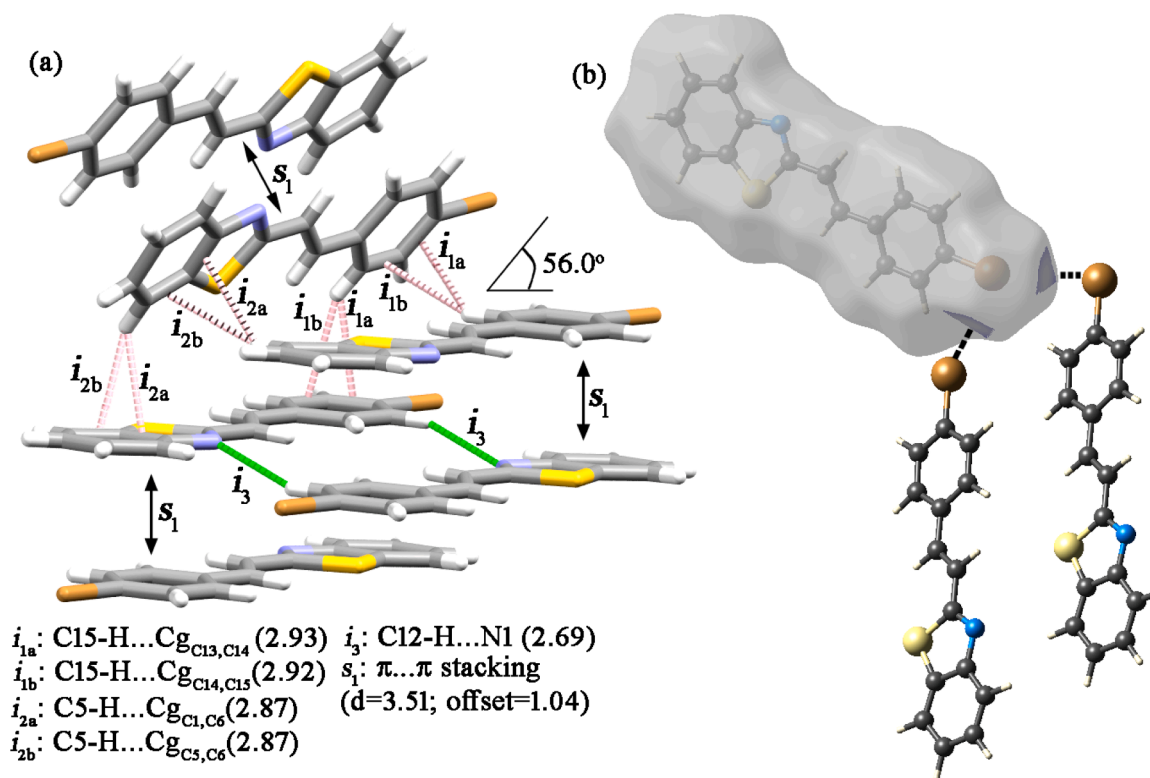


Fig. 5. (a) The main supramolecular motif in the crystal structure 8. For guidance, see Fig. 4 caption. (b) The weak Br...Br contacts points selected in the Hirshfeld surface (d_{norm} mapped) of compound 8. Observe that these regions in the surface are weakly blue coloured, indicating long contacts. All other contacts were not coloured in the surface.

(CSD reference code NINDIY). Therefore, our structural description will be based on five new crystal structures provided in this study and two others from CSD repository, whose data will be used to prepare artworks and to measure geometrical parameters of 1 and 2.

Two compounds have crystallized in non-centrosymmetric space groups even though they don't own molecular chiral centres (compounds 3 and 4, *Pca*2₁ and *Pna*2₁ space groups, respectively). The other three novel crystal structures were solved in centrosymmetric space groups (compounds 5, 6 and 7, *P*2₁/*c*, *P*-1 and *Pccn* space groups, respectively), as well as those already deposited in the CSD (compounds 1 and 2, *P*2₁/*c* and *P*-1 space groups, respectively). Except for methoxylated compounds 2 and 4, which are present with two crystallographically independent molecules in their asymmetric unit, all others have just one molecule in its asymmetric unit, which are nearly perfect molecular planes [root mean square deviation (RMSD) for all non-hydrogen atoms fitted on of the least-square plane is 0.044 (1), 0.183/123 (molecules A/B of 2), 0.118 (3), 0.160/0.255 (molecules A/B of 4), 0.038 (5), 0.034 (6) and 0.074 (8) Å], which denotes resonance encompassing the entire molecular backbone. An ORTEP-3 plot [17] is shown in Fig. 2 for each compound elucidated here.

Despite the molecular simplicity of the compounds, in both features of atoms assembly and conformation, and consequently their molecular similarity, just two compounds are isostructural in the solid state. Compounds 1 and 5 crystallize in the same space group with similar cell constants (Table 1) and disposition of the molecules in their crystal structures, showing that fluorine substitution in para position of the phenyl ring keeps the same intermolecular array of the unsubstituted compound. This can be viewed in Fig. 2, where the main supramolecular motif of these crystal structures is depicted, and in Fig. S37, where their overall packing is illustrated. The same CH... π and CH...N contacts are conserved in both structures, which is also reflected in the fingerprints of their Hirshfeld surfaces present with outermost wings and neighbouring spikes referring respectively to H...C (29.1 % and 27.4 % in 1 and 5) and

H...N (6.7 % and 6.9 % in 1 and 5) contacts (Fig. 3). Indeed, it is possible see in Fig. 3 that these fingerprints of 1 and 5 are similar if contacts involving F atom are not considered.

Therefore, structural variability is predominant in the series, which is a consequence of the intermolecular contacts pattern. This phenomenon can be observed in the Hirshfeld surface fingerprints of the structures, which, except for 1 and 5, present different shapes resulted from distinct sets of molecular distances to their surfaces (Fig. 3). Furthermore, just the two isostructural compounds 1 and 5 and compound 8 have tilted L-shaped intermolecular geometry occurring together with offset face-to-tail $\pi \dots \pi$ stacking interactions between centrosymmetry related molecules (Figs. 4 and 5). However, the halogen change impacts on their overall crystal packing, with CH...F contacts positioning benzothiazole and phenyl rings side-to-side in 5 (Fig. 4), while weak Br...Br interactions put in contact the phenyl rings of near molecules of 8 (Fig. 5). In fact, the bromine separation in 8 (3.8165(7) Å) is longer than its vdW diameter (3.70 Å). Therefore, different than other compounds exhibiting aggregation induced emission enhancement from Br...Br contacts in the solid state, as, for instance in tetraphenylethylenes present with Br...Br separations measuring 3.47/3.63 Å [31], the intermolecular role of halogen in the photophysical properties assessed here could not be established for compound 8. On the other hand, compounds 2 and 3 are present only with the first type of contacts (Fig. 6), while compound 6 has only the second pattern (Fig. 7). Already compound 4 has an offset face-to-tail $\pi \dots \pi$ stacking interactions pattern between its crystallographically independent molecules besides a slightly tilted T-shaped intermolecular geometry (Fig. 8). In addition, compounds 4 and 6 have also similar orientation of their sulfur atoms in nearly packed molecules. While in 4, however, the S...S distance (3.682(2) Å; vdW radius of sulfur is 1.80) and the C-S...S (138.8(2)°) angle do not allow us to state such interaction occurs, which is reinforced by the absence of these contacts in its Hirshfeld surface (Fig. 9), this interaction can be considered as strong in 6 (S...S = 3.4791(7) Å; C-S...S = 147.53(6)°),

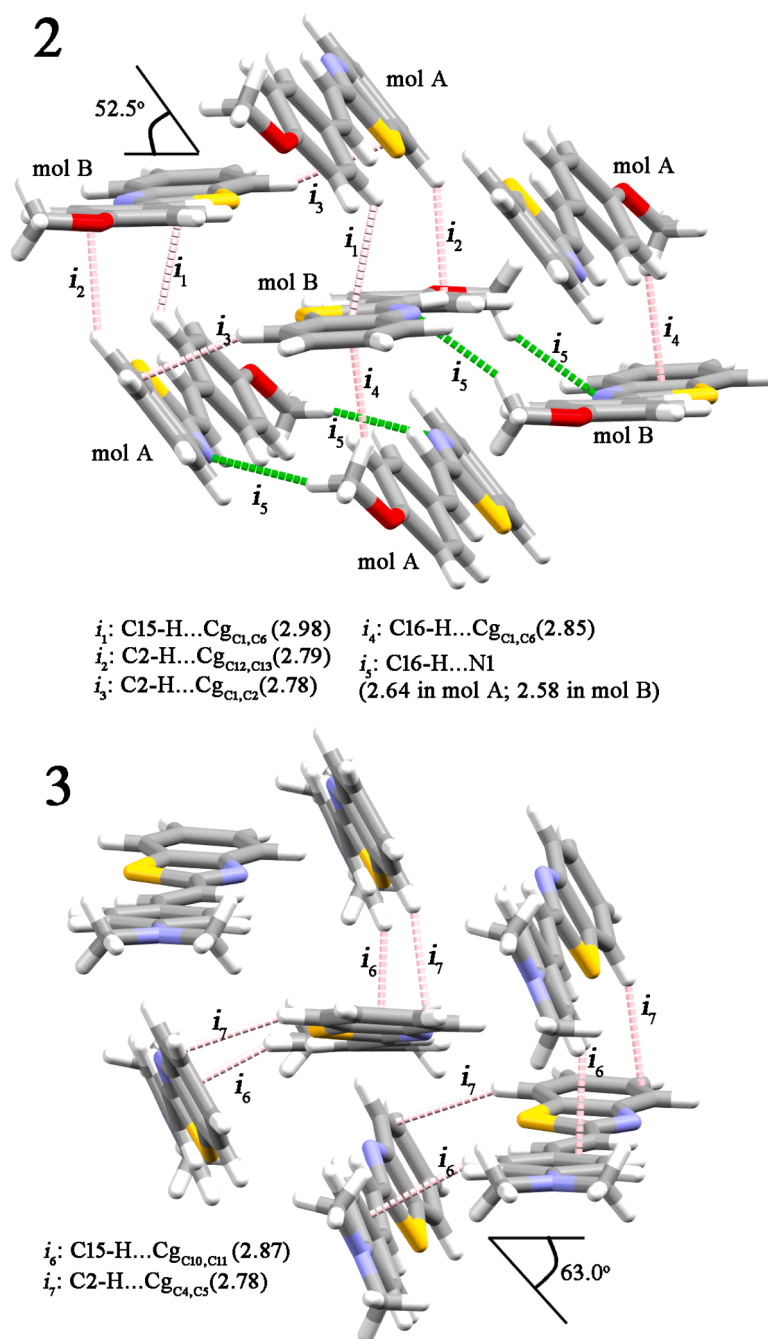


Fig. 6. Compounds 2 and 3 have not $\pi\cdots\pi$ interactions in their crystal structure. For guidance, see Fig. 4 caption.

appearing as a red region of short contact in its Hirshfeld d_{norm} map (Fig. 9). One can see an angle deviation from linearity for this contact, which is due to the fact that both sulfur atoms are electron donors and acceptors in the reciprocal contact, with their σ -hole in the line of the C-S bonds dislocated from each other to interact with the electron lone pairs almost perpendicularly oriented. Except in compound 3, in which thiazole nitrogen is not interacted with its neighbourhood, heterocyclic nitrogen is a non-classical hydrogen bonding acceptor from different donors in the crystal structures of the series (Figs. 4–8, where one can directly find some geometrical parameters of the main interactions responsible for the supramolecular architectures).

3.2. Optical spectroscopy

Fig. 10a shows the diffuse reflectance spectra (DRS) of all studied

benzothiazole derivatives, which were recorded in the range of 200 to 1800 nm, using finely ground powder samples. The spectra present the band edge absorption near 370 to 900 nm, depending of the substituent and its position in the aromatic terminal ring, and also the spectra show a high reflectance greater than 80 % in the spectral range from 600 to 1700 nm, except for compounds 4, 6 and 9. The spectra present some bands due to the absorptions of the molecular moieties, at 1090–1160 nm and 1600–1850 nm that are assigned to the third and second overtones of the aromatic C-H vibrations, respectively, and the third band at 1360–1410 nm region, due to overtones of the CH₃ stretching vibrations. The optical bandgap was calculated from the graphs $[F(R_{\infty})/h\nu]^2$ vs. $h\nu$ based on the Kubelka-Munk theory (see Fig. 10b for compound 1 and Fig. S38 for all other compounds). The values are given in Table 2, varying from 2.55 eV for 2 to 3.19 eV for 6. These values indicate that styrylbenzothiazole compounds could be considered as non-conducting

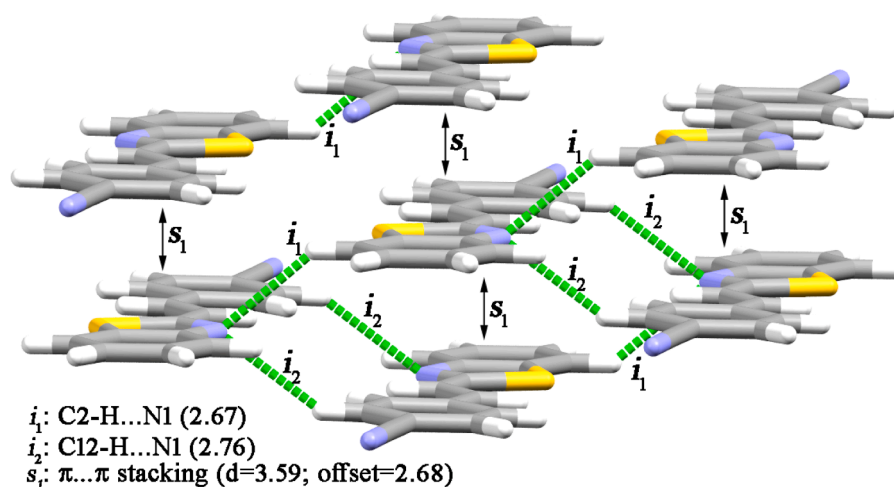


Fig. 7. Offset face-to-tail $\pi\cdots\pi$ stacking and CH...N interactions keeping in contact the molecules of compound 6 in its crystal structure. For guidance, see Fig. 4 caption.

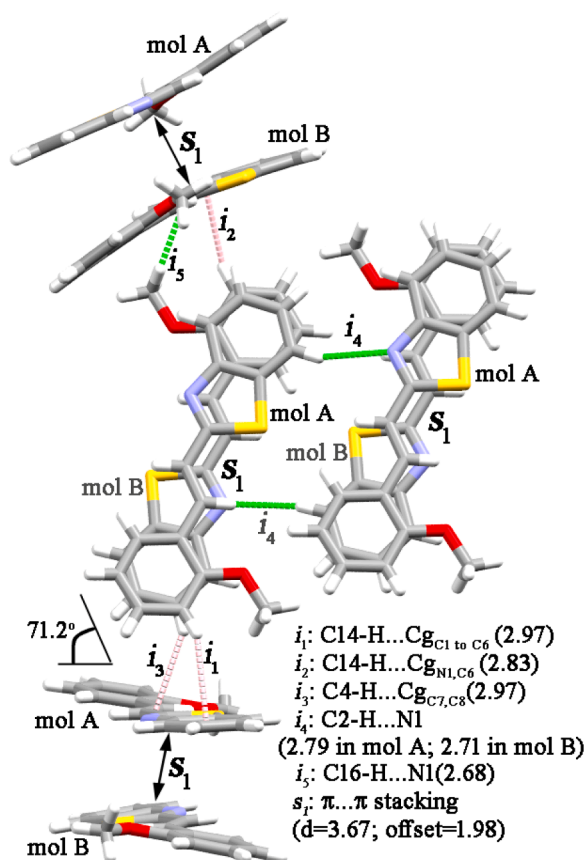


Fig. 8. The T-shaped pattern of CH... π interactions occurring in the crystal structure of 4, aided by $\pi\cdots\pi$ and CH...N contacts. For guidance, see Fig. 4 caption.

materials and are all lower than those found by Wang et al. [32] for a related benzothiazole derivative series obtained via cyclic voltammetry measurements, (ΔE_g , 3.45 – 3.69 eV).

3.3. Photoluminescence

The normalized excitation spectra are shown in Fig. 11a, by monitoring the maximum of emission band, λ_{emi} , of each sample at room

temperature (see Table 3). All spectra consist of sum of wide bands spread from ultraviolet to blue region of the optical spectrum. Some similarities can be observed among them. All present a well-defined band centred in $\sim 315 - 350$ nm. On the other hand, the absorption spectrum of 1, 4, 5 and 9 also present another absorption centred at $\sim 405 - 415$ nm, being that it is the greater band in 4 and 5 spectra, while on the 1 and 9 the greater is that one with maximum at ~ 325 nm.

Fig. 11b show the normalized emission spectra of the compounds investigated here, acquired by exciting the maxima of excitation spectra, λ_{exc} , of each sample (see Table 3 and Fig. 11a). All of them are consisted of a broad emission spread from 400 to 750 nm, were the maxima of each one given in column λ_{emi} in Table 3. Compounds 2 and 9 also exhibit a well-defined secondary peak at 440 nm and 435 nm, respectively. Moreover, it can be noted that the emission spectra of 2 and 9, as well as those of 4 and 8, are overlapped showing similar patterns. The emission peak at 461 nm of 9 exhibits a 14 nm blueshift comparing to emission of the other fluorinated compound 5, and a redshift of 40 nm in comparison with the similar benzothiazole derivative present without the $-C = C-$ bridge between the phenyl and bezothiazole rings [32]. On the other hand, in comparing 2 with its analogue absent of the $-C = C-$ motif, the redshift is ~ 71 nm, while for 1 the emission peak is blue shifted by ~ 67 nm if withdrawn the *E*-ethene moiety [32]. Also, it is important to note that *N,N*-dimethyl amine derivative 3 displays the largest redshift compared to the emission of the unsubstituted compound 1 (~ 105 nm).

The PL decay curves were taken at room temperature and are shown in Fig. 12, and these were measured by monitoring the peak position of the emission spectra of each sample, and using the energy excitation corresponding to the maxima of each excitation spectra (see Fig. 11 and Table 3). The curves of 1 to 4 were best fitted with a double-exponential functions ($\chi^2 = 0.995$), while for compounds 5 to 9 the best results were acquired with three-exponential functions ($\chi^2 = 0.991$). The obtained τ values are presented in Table 3, where it can be viewed again that the molecular similarity into the series was not reflected in the τ values. Similar results were obtained by Wang et al. [32] for a series of six benzothiazole derivatives in both dichloromethane solution and in the solid state, with lifetimes up to 4.77 ns.

The internal and external quantum yield values are presented in Table 3, and an inspection of this table reveals an interesting similarity between the iQY and eQY values, indicating that the studied compounds are good UV absorbers, being that the difference in their QYs resides in the emission efficiency. Also, it can be noted that, compound 1 had the lower eQY among all the assessed styrylbenzothiazoles. For the para substituted compounds, the eQY follows the trend 7 (SCH₃) > 3 (N

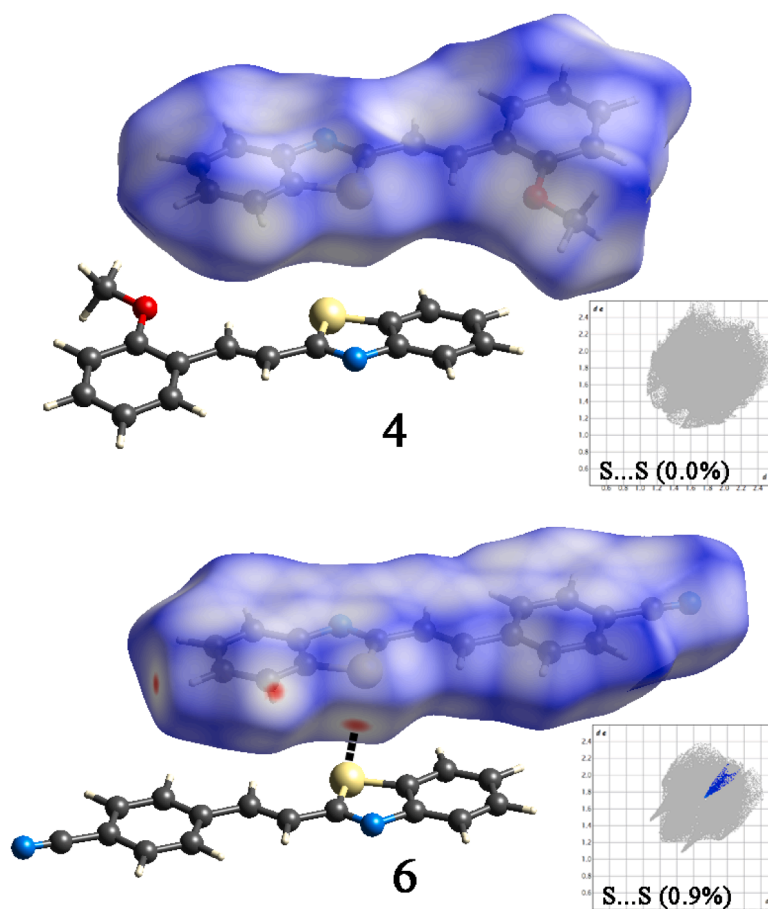


Fig. 9. The Hirshfeld surface (d_{norm} mapped) of compounds **4** and **6** and another packed molecule showing the C-S...S alignment. The corresponding fingerprints are shown at right, in which the gray shadow outlines the full fingerprint (the distances of the S...S contact are in blue in the fingerprint of **6**, together with their contribution to the surface). On the surface, red regions have closer contacts.

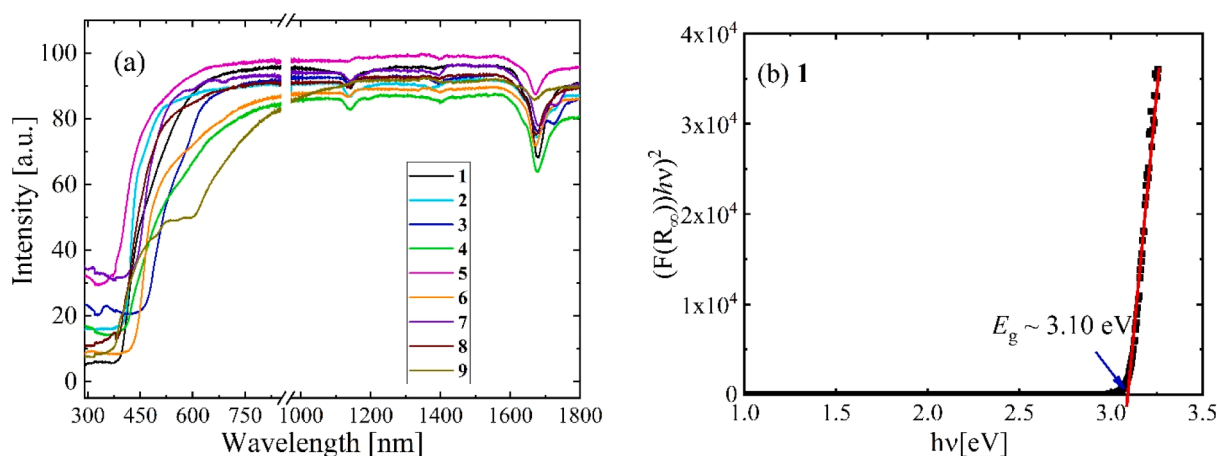


Fig. 10. (a) Diffuse reflectance spectra of **1–9** (left) and (b) the plot of $(F(R_{\infty}) \times hv)^2$ versus photon energy for compound **1**.

$(\text{CH}_3)_2 > \mathbf{2} (\text{OCH}_3) > \mathbf{8} (\text{Br}) > \mathbf{5} (\text{F})$, which, except for the best emitter **7**, follow the trend of the moiety to encompass in a resonance path with phenyl ring. On the other hand, introducing an electron withdrawing group in **6** (CN) and **9** (CF_3), respectively, or changing the position of methoxy group to ortho in **4**, resulting in a shorter resonance path, reduces the eQY of these compounds by up to four times, as shown in Table 3. An interesting crystal packing feature found in **2** and **3** correlates with its higher efficiency, that is the absence of $\pi \dots \pi$ interactions (Fig. 6). These interactions are present in all other structures evaluated

here and are known to quench photoluminescence, as, for instance, in diphenyldiacetylene [33] and phenylamine dyes [34]. This also helps to explain the lower emission efficiency of **4**, which, despite of owing an electron donor group at ortho position, is present with $\pi \dots \pi$ interactions in the solid state (Fig. 8).

On the other hand, no evident correlation between lifetimes and eQY values was found for studied compounds, but some interesting points can be noted. For example, compound **1** presents both lower lifetime and quantum yield values (0.90 ns and 0.49 %) among all studied

Table 2
Band gap E_g values for 1–9. (± 0.05 eV) .

Compound	E_g
1	3.10
2	2.97
3	2.55
4	2.89
5	3.05
6	2.81
7	2.70
8	3.07
9	3.19

derivatives, while compound **7** has both the greatest values in all series, 5.41 ns and 22.22 %, indicating that the presence of SCH₃ has a huge influence in the molecule electronic properties responsible to convert ultraviolet radiation into this visible spectral. Another interesting point can be noted, that is the fact that compounds **2** and **3** have the lower lifetimes among all nine ones (~ 1.48 ns), with good eQY values (8.60 and 12.65 %, respectively), which, together with the greatest values of **7**, may indicate that polarizability plays a key role in the eQY performance as verified by our theoretical approaches below.

From the emission spectra, the photometric parameters CIE 1931 (x , y) chromaticity coordinates and the correlated colour temperature (CCT) were calculated using the McCamy's formula [24]. Fig. 13 presents the CIE coordinates of all studied compounds whose values, taken

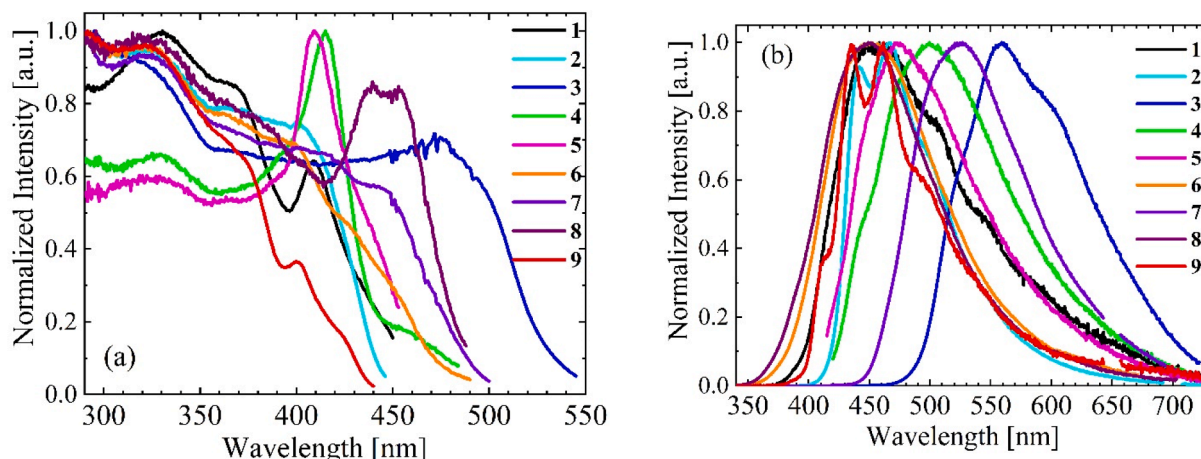


Fig. 11. Normalized (a) excitation and (b) emission spectra of 1–9.

Table 3

Photometric parameters for 1–9 (λ_{exc} and λ_{emis} in nm), experimental lifetimes τ (in ns) of the fitted decay curves, photoluminescent quantum yields (%), CIE (x , y) chromaticity coordinates, and CCT values (in K) .

Compound	λ_{exc}	λ_{emi}	τ_1	τ_2	τ_3	τ_{av}	A_1 (%)	A_2 (%)	A_3 (%)	iQY	eQY	(x , y)	CCT
1	368	453	0.65	3.23	–	0.90	90.2	9.8	–	0.58	0.49	0.226, 0.258	24,636
2	350	467	1.06	2.92	–	1.48	77.3	22.7	–	10.20	8.60	0.179, 0.211	–
3	365	558	1.07	2.95	–	1.48	77.7	22.3	–	14.82	12.65	0.463, 0.526	3379
4	415	500	1.07	2.99	–	1.49	78.0	22.0	–	2.75	2.35	0.266, 0.392	8084
5	409	475	5.65	23.33	1.18	2.84	22.1	2.0	75.8	2.78	2.12	0.227, 0.307	14,474
6	325	502	5.72	104.6	2.82	4.81	46.6	0.7	52.7	3.55	3.05	0.263, 0.436	7676
7	325	523	8.26	16.82	0.92	5.41	30.2	3.2	66.6	26.16	22.22	0.332, 0.535	5510
8	330	505	–	–	–	–	–	–	–	4.03	3.29	0.269, 0.454	7326
9	325	461	3.19	97.4	0.92	3.41	9.3	2.4	88.3	0.93	0.78	0.192, 0.196	–

$$y(x) = A1 \cdot \exp(-x/\tau_1) + A2 \cdot \exp(-x/\tau_2) + A3 \cdot \exp(-x/\tau_3) + y_0.$$

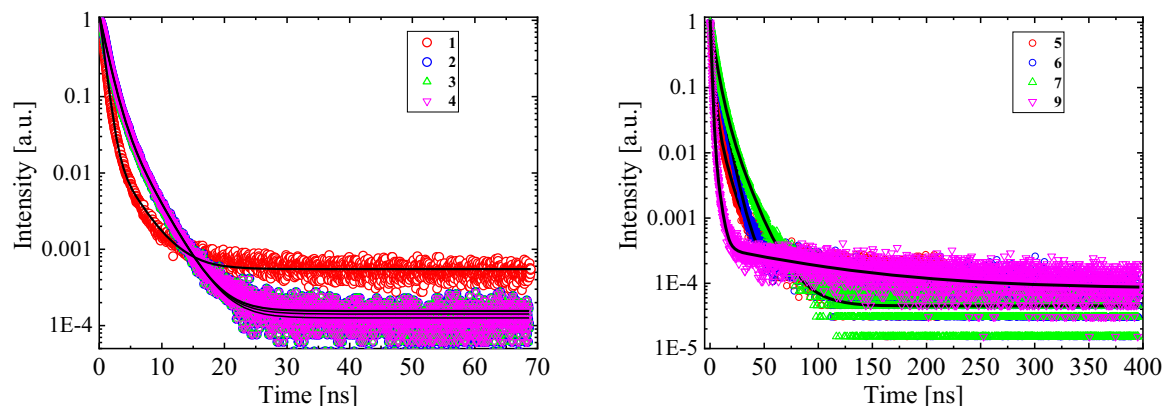


Fig. 12. Normalized emission decay curves of 1–9.

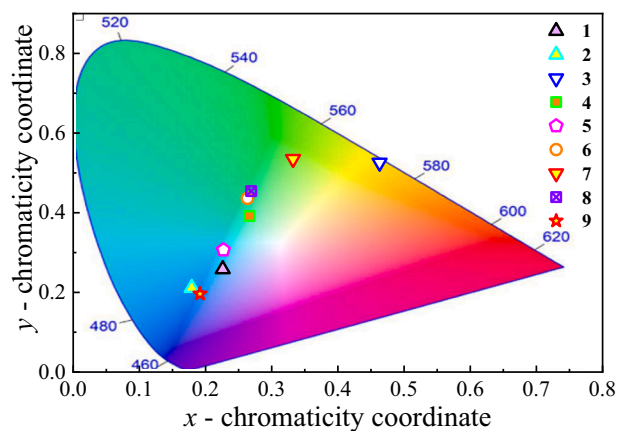


Fig. 13. CIE (x,y) coordinates for 1 to 9.

Table 4

Root-mean-square deviation (RMSD) between the optimized and crystallographic molecular geometries (excluding hydrogen atoms), and electronic descriptors chemical potential (μ), chemical hardness (η), and electrophilicity index (ω), for the 1 to 6 and 8.

Compound	RMSD/Å	Electronic Descriptors		
		μ /eV	η /eV	ω /eV
1	0.0655	-4.1996	3.1591	2.7914
2	0.1701	-3.9472	3.0762	2.5324
3	0.0957	-3.5954	2.9061	2.2241
4	0.1271	-4.0207	3.1151	2.5948
5	0.0775	-4.2392	3.1546	2.8484
6	0.0353	-4.6908	3.0374	3.6220
8	0.0560	-4.3280	3.1063	3.0152

at room temperature, are given in Table 3. It can be noted that the CIE coordinates lie from a blueish region to a yellowish region in the colour diagram, including greenish one. The best emitters with largest QY are

into the blue (2), yellow (3) and green (7) colour regions, opening the possibility of modulating the colour of the emission by changing the substituent in the phenyl ring of the simple 2-styryl-1,3-benzothiazole framework, aiming its application as light emitter under UV excitation. The CCT values for all compounds (Table 3) varied from 3379 K (3) to 24,636 K (2). As pointed by Singh et al. [35], when CCT value is greater than 5000 K, the compound could be used as a component for cold white light applications. In this sense, 4, 6 to 9 can be considered as good candidates for this application. In addition, the photophysical parameters resumed in Table 3 are compatible with those reported by Godogu et al. [36] for a series of 21 2-aminothiazole derivatives, and by Song et al. [37] for benzothiazole derivatives with varied π -conjugation, measured also in the solid state, were the substituent dependent emissions can be also modulated from blue to green colour, such as in our compounds 1–9.

3.4. Theoretical approach

From a theoretical point of view, only minor variations are observed between the experimental geometries and single isolated molecular structures for 1 to 6 and 8. This behaviour is viewed in Table 4, which presents the RMSD values with respect to the crystallographic experimental and optimized theoretical structures excluding hydrogen atoms. Table 4 also presents the electronic descriptors chemical potential (μ), chemical hardness (η), and electrophilicity index (ω). All parameters were calculated from the energies of the frontier molecular orbitals (HOMO and LUMO), according to Koopmans theorem [29,30]. The chemical potential reflects the tendency of a system to lose electron density, whereas the global hardness quantifies the intrinsic resistance of the system to electronic redistribution. The electrophilicity index expresses the ability of a species to accept electrons. These parameters are in agreement with the substitution profile of the compounds, with the lower μ values and the higher ω ones for those with electron withdrawing groups (5, 6 and 8 in Table 4). With respect to η , compound 1 was present with the highest value, due to absence of substituents introducing further resonance path, which correlates well with its lowest lifetime and QY values. On the other hand, compound 3 had the lowest η value, showing to be the derivative with the lowest hardness in the

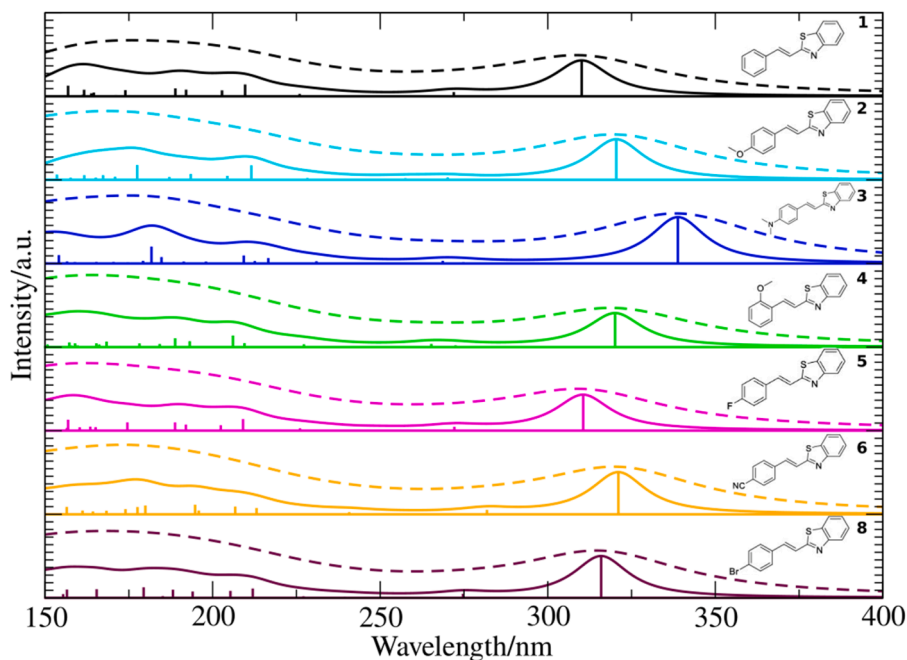


Fig. 14. Electronic transition spectra of compounds 1–6 and 8 computed at the TDDFT/CAM-B3LYP/def2-TZVP level using optimized isolated single-molecule geometries. Solid and dashed curves represent Lorentzian convolutions of the calculated discrete transitions with FWHM of 20 and 60, respectively.

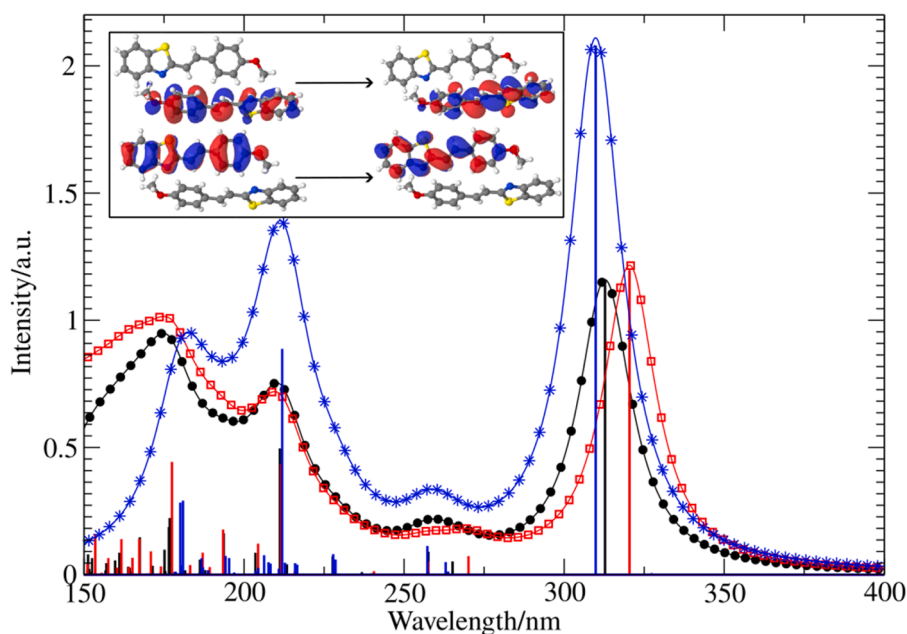


Fig. 15. Electronic transition spectra of compound **2** computed at the TDDFT/CAM-B3LYP/def2-TZVP level. Single-molecule spectra from the experimental (non-optimized, black) and optimized crystallographic (red) geometries, as well as for the non-optimized L-shaped dimer derived from the asymmetric unit (blue). Bars denote discrete transitions, and solid lines show Lorentzian convolutions with FWHM of 20. The molecular orbitals involved in the first dimer transition are shown in the upper left corner.

series. This thus can be correlated with its high QYs, indicating theoretically the role of the polarizability in this efficiency.

Fig. 14 shows the theoretical spectra for isolated units of **1** to **6** and **8**. The computed bar spectra with the frequency and oscillator strength intensities were convoluted with Lorentzian function with different full widths at half maximum (FWHM) values of 20 and 60 (solid and dashed lines, respectively). It is observed that, for a FWHM of 60 (dashed lines), a better agreement with the experimental spectrum is achieved by the comparison of the theoretical absorption spectra of isolated single molecule (Fig. 14) with the experimental excitation results in the solid state (Fig. 11a). The spectral behaviour is similar for all molecules, differing only in the shift of the first electronic transition. In all cases, the orbitals that contribute to the first electronic transitions correspond to the HOMO $\rightarrow$ LUMO transition. Interestingly, HOMO is well distributed over the substituent, the phenyl carbons and their bonds involving the 1,4-carbons, the styryl central double bond, the benzothiazole atoms, the N-C-S bonds, besides the rings fusion bond and another phenyl one parallel to that, while LUMO can be viewed out of the substituent and on the bonds alternate to those where HOMO laid, in which the orbital distribution would encompass the double bonds of a resonance structure (Fig. 15).

At last, we have further investigated if the tilted L-shaped intermolecular array, typical in the crystal structures of the series, could have some influence in the spectral profile found. Fig. 15 shows the theoretical spectra of the experimental crystallographic and theoretical optimized single molecule geometries of **2**. The spectrum of a dimer, consisting of the two crystallographic independent molecules of **2**, which are tilted L-shaped oriented in the unit cell (CSD reference code OJEGAM; see Fig. 6), with the molecular coordinates corresponding to its crystallographic geometry, is also included for comparison. The spectra of the single molecules between the crystallographic and optimized structures shows a blue shift for the theoretical optimised structure in relation to the latter one. The first band in the spectrum of the unit molecules present the biggest oscillator strength and it consists of the HOMO $\rightarrow$ LUMO transition. The comparison between the single molecule and the dimer crystallographic geometries shows that spectral profile is preserved with the dimer presenting doubled absorption

intensities, due to its two-units input. The electronic transition shown in the inset left upper corner of Fig. 15 corresponds to the first electronic transition observed in the dimer spectrum. The transition is a combination of two transitions localized in each individual molecule. The orbitals involved in the electronic transition have the same spatial distribution of the HOMO $\rightarrow$ LUMO transition observed for the spectra of the single molecules in both optimized theoretical and experimental crystallographic molecular geometries, showing no significant effect of the tilted L-shaped packing in this compound.

4. Conclusions

In this study, we prepare nine styrylbenzothiazole compounds, and five of them were elucidated by single-crystal X-ray diffraction for the first time. The inspection of these five structures and of two ones already deposited in the CDS belonging to the series allowed us to find packing variability despite of molecular similarity and simplicity reflected on the planar conformation found in all them. For example, isostructurality was observed only in two compounds related by one fluoro substitution in phenyl ring. Indeed, this supramolecular diversity was consequence of one substitution in either para or ortho position of phenyl ring, which also drive the photoluminescence profile towards variable light emission maxima. This is a desirable optical property, due to possibility of tuning light emission colour in devices through unique substitution in a simple and versatile molecular scaffold such as styrylbenzothiazole. Such result is further emphasized taken into account three compounds presented QY above 10 %, with emissions in blue, yellow and green tuned by choosing OCH_3 , $\text{N}(\text{CH}_3)_2$ or SCH_3 to append at para position of phenyl ring. Given these desirable features of molecular simplicity with high-efficiency colour tuneable emission, substituted styrylbenzothiazoles can be explored as promising emitter layers in OLEDs and biomedical sensing applications.

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CRediT authorship contribution statement

Nara Rúbia Pereira: Methodology, Investigation. **Meiry Edvirges Alvarenga:** Methodology, Investigation. **Renata Diniz:** Writing – review & editing, Methodology, Investigation. **Ricardo Costa de Santana:** Writing – review & editing, Methodology, Investigation. **Lauro June Queiroz Maia:** Methodology, Investigation. **Bárbara Júlia Gonçalves Dutra:** Methodology, Investigation. **Freddy Fernandes Guimarães:** Writing – review & editing, Methodology, Investigation. **Cleiton Moreira da Silva:** Writing – review & editing, Writing – original draft, Visualization, Validation, Project administration, Methodology, Investigation, Funding acquisition, Formal analysis, Conceptualization. **Felipe Terra Martins:** Writing – review & editing, Writing – original draft, Visualization, Validation, Methodology, Investigation, Formal analysis, Conceptualization.

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.

Supplementary materials

Supplementary material associated with this article can be found, in the online version, at [doi:10.1016/j.molstruc.2026.146043](https://doi.org/10.1016/j.molstruc.2026.146043).

Data availability

Data will be made available on request.

References

- [1] O. Ostroverkhova, Organic optoelectronic materials: mechanisms and applications, *Chem. Rev.* 116 (2016) 13279–13412, <https://doi.org/10.1021/acs.chemrev.6b00127>.
- [2] E.H. Cho, Y.W. K, J. Sim, H. Yeon, S. Baek, S.M. Jeong, J. Lee, Y. Jeon, K.C. Choi, Recent advances in flexible and wearable oleds for biomedical applications: a review, *Mater. Horiz.* 12 (2025) 8862–8894, <https://doi.org/10.1039/d5mh00742a>.
- [3] K. Gutmańska, A. Podborska, A. Sławek, R. Sivasamy, L. Alluhaibi, A. Maximenko, A. Ordyszewska, K. Szacilowski, A. Dolega, T. Mazur, Structural insights and advanced spectroscopic characterization of thiazolothiazoles: unveiling potential for optoelectronic and sensing applications, *Chemistry* 31 (2025), <https://doi.org/10.1002/chem.202501664> article e202501664.
- [4] A. Woodward, J. Kolesar, S. Hall, N. Saleh, D. Jones, M. Walter, Thiazolothiazole fluorophores exhibiting strong fluorescence and viologen-like reversible electrochromism, *J. Am. Chem. Soc.* 139 (2017) 8467–8473, <https://doi.org/10.1021/jacs.7b01005>.
- [5] R. Kammel, D. Tarabová, J. Vána, O. Machalický, M. Nepraš, J. Hanusek, StructureFluorescence relationships in 2Aryl5(2Aminophenyl) 4Hydroxyl,3Thiazoles, *J. Mol. Struct.* 1175 (2018) 804–810, <https://doi.org/10.1016/j.molstruc.2018.08.017>.
- [6] N. Sayresmith, A. Saminathan, J. Sailer, S. Patberg, K. Sandor, Y. Krishnan, M. Walter, Photostable voltage sensitive dyes based on simple, solvatofluorochromic, asymmetric thiazolothiazoles, *J. Am. Chem. Soc.* 141 (2019) 18780–18790, <https://doi.org/10.1021/jacs.9b08959>.
- [7] D. Bayramin, G. Öztürk, Synthesis and solvatochromism of new thiazole derivatives bearing N,N-bis(2-methoxyethyl) benzenesulfonamide moiety, *J. Fluoresc.* 35 (2025) 12173–12196, <https://doi.org/10.1007/s10895-025-04430-8>.
- [8] Y. Chen, T. Wei, Z. Zhang, T. Chen, J. Li, J. Qiang, J. Lv, F. Wang, X. Chen, A benzothiazole-based fluorescent probe for ratiometric detection of Al³⁺ in aqueous medium and living cells, *Ind. Eng. Chem. Res.* 56 (2017) 12267–12275, <https://doi.org/10.1021/acs.iecr.7b02979>.
- [9] F. Yan, J. Sun, Y. Zang, Z. Sun, H. Zhang, X. Wang, Benzothiazole applications as fluorescent probes for analyte detection, *J. Iran. Chem. Soc.* 17 (2020) 3179–3203, <https://doi.org/10.1007/s13738-020-01998-9>.
- [10] D. Shi, Y. Yang, L. Tong, L. Zhang, F. Yang, J. Tao, M. Zhao, A novel benzothiazole-based fluorescent AIE probe for the detection of hydrogen peroxide in living cells, *Molecules* 29 (2024), <https://doi.org/10.3390/molecules29215181> article 5181.
- [11] M.K. Awad, M.M. El-Hendawy, T.A. Fayed, S.E.H. Etaiw, N.J. English, Aromatic ring size effects on the photophysics and photochemistry of styrylbenzothiazole, *Photochem. Photobiol. Sci.* 12 (2013) 1220–1231, <https://doi.org/10.1039/c3pp25367h>.
- [12] C.N. Stindt, S. Crespi, B.L. Feringa, Synthesis of styrylbenzazole photoswitches and evaluation of their photochemical properties, *Chem. Eur. J.* 30 (2024) e202401409, <https://doi.org/10.1002/chem.202401409> article.
- [13] D.P. Araújo, V.S. Morais, Á.D. Fátima, L.V. Modolo, Efficient sodium bisulfite-catalyzed synthesis of benzothiazoles and their potential as ureases inhibitors, *RSC Adv.* 5 (2015) 28814–28821, <https://doi.org/10.1039/C5RA01081K>.
- [14] CrysAlisPro. Rigaku Oxford Diffraction. CrysAlisPro. Rigaku Corporation, Tokyo, Japan. 2015.
- [15] G.M. Sheldrick, Crystal structure refinement with SHELXL, *Acta Crystallogr. Sect. C Struct. Chem.* 71 (2015) 3–8, <https://doi.org/10.1107/S2053229614024218>.
- [16] O.V. Dolomanov, L.J. Bourhis, R.J. Gildea, J.A.K. Howard, H. Puschmann, OLEX2: a complete structure solution, refinement and analysis program, *J. Appl. Crystallogr.* 42 (2009) 339–341, <https://doi.org/10.1107/S0021889808042726>.
- [17] L.J. Farrugia, WinGX and ORTEP for Windows: an update, *J. Appl. Crystallogr.* 45 (2012) 849–854, <https://doi.org/10.1107/S0021889812029111>.
- [18] C.F. MacRae, I. Sovago, S.J. Cottrell, P.T.A. Galek, P. McCabe, E. Pidcock, M. Platings, G.P. Shields, J.S. Stevens, M. Towler, P.A. Wood, Mercury 4.0: from visualization to analysis, design and prediction, *J. Appl. Crystallogr.* 53 (2020) 226–235, <https://doi.org/10.1107/S1600576719014092>.
- [19] M.A. Spackman, D. Jayatilaka, Hirshfeld surface analysis, *CrystEngComm* 11 (2009) 19–32, <https://doi.org/10.1039/B818330A>.
- [20] P.R. Spackman, M.J. Turner, J.J. McKinnon, S.K. Wolff, D.J. Grimwood, D. Jayatilaka, M.A. Spackman, CrystalExplorer: a program for Hirshfeld surface analysis, visualization and quantitative analysis of molecular crystals, *J. Appl. Crystallogr.* 54 (2021) 1006–1011, <https://doi.org/10.1107/S1600576721002910>.
- [21] S. Som, S.K. Sharma, T. Shripathi, Influences of doping and annealing on the structural and photoluminescence properties of Y₂O₃ nanophosphors 23, *J. Fluoresc.* 23 (2013) 439–450, <https://doi.org/10.1007/s10895-013-1160-7>.
- [22] A.E. Morales, E.S. Mora, U. Pal, Use of diffuse reflectance spectroscopy for optical characterization of Un-supported nanostructures, *Rev. Mex. Fis.* 53 (2007) 18–22, <https://www.redalyc.org/articulo.oa?id=57028299004>.
- [23] C. Wyman, P.-P. Sloan, P. Shirley, Simple analytic approximations to the CIE XYZ color matching functions, *J. Comput. Graph. Tech.* 2 (2013) 1–11, <http://jcgct.org/published/0002/02/01/>.
- [24] C.S. McCamy, Correlated color temperature as an explicit function of chromaticity coordinates, *Color Res. Appl.* 17 (1992) 142–144, <https://doi.org/10.1002/col.5080170211>.
- [25] M.S. Wrighton, D.S. Ginley, D.L. Morse, Technique for the determination of absolute emission quantum yields of powdered samples, *J. Phys. Chem.* 78 (1974) 2229–2233, <https://doi.org/10.1021/j100615a009>.
- [26] T. Yanai, D.P. Tew, N.C. Handy, A new hybrid exchange–Correlation functional using the coulomb-attenuating method (CAM-B3LYP), *Chem. Phys. Lett.* 393 (2004) 51–57, <https://doi.org/10.1016/j.cplett.2004.06.011>.
- [27] F. Weigend, R. Ahlrichs, Balanced basis sets of split valence, triple zeta valence and quadruple zeta valence quality for H to Rn: design and assessment of accuracy, *Phys. Chem. Chem. Phys.* 7 (2005) 3297–3305, <https://doi.org/10.1039/B508541A>.
- [28] M.J. Frisch et al., Gaussian 16 Revision B.01, Gaussian Inc., Wallingford CT, 2016.
- [29] R.G. Parr, R.G. Pearson, Absolute hardness: companion parameter to Absolute electronegativity, *J. Am. Chem. Soc.* 105 (1983) 7512–7516, <https://doi.org/10.1021/ja00364a005>.
- [30] R.G. Parr, L.V. Szentpály, S. Liu, Electrophilicity Index, *J. Am. Chem. Soc.* 121 (1999) 1922–1924, <https://doi.org/10.1021/ja983494x>.
- [31] W. Huang, X. Zhao, S. Zhang, L. Ying, X. Miao, W. Deng, Bromine substituent position of tetraphenylethylene-based luminogens effect on enhanced AIE and reversible mechanofluorochromic properties by halogen bonding, *dyes pigments*, 225 (2024), article 112063, <https://doi.org/10.1016/j.dyepig.2024.112063>.
- [32] C. Wang, G. Ren, Y. Song, C. Wu, R. Liu, S. Zhu, H. Zhu, Benzothiazole derivatives with varied substituents: synthesis, aggregated luminescence properties, and application in single-component WLEDs, *J. Mol. Struct.* 1328 (2025), <https://doi.org/10.1016/j.molstruc.2025.141352> article 141352.
- [33] H. Wu, Z. Chen, W. Chi, A.K. Bindra, L. Gu, C. Qian, B. Wu, B. Yue, G. Liu, G. Yang, L. Zhu, Y. Zhao, Structural engineering of luminogens with high emission efficiency both in solution and in the solid State, *Angew. Chem. Int. Ed.* 58 (2019) 11419–11423, <https://doi.org/10.1002/anie.201906507>.
- [34] M.P. Szymanski, A. Czapik, M. Banasiewicz, K. Chuchracka, M. Kwit, A. Szumna, P. Skowronek, Multi-state emission of TICT luminophores, *J. Mater. Chem. C* 14 (2026) 3337–3344, <https://doi.org/10.1039/d5tc03748d>.

- [35] D.K. Singh, J. Manam, Investigation of structural, spectral and photometric properties of CaTiO₃:dy³⁺ nanophosphors for the lighting applications, *Electron. Mater. Lett.* 13 (2017) 292–301, <https://doi.org/10.1007/s13391-017-6285-4>.
- [36] K. Godugu, S. Shaik, M.K.M. Pinjari, T.R. Gundala, D.V.C. Subramanyam, S. S. Loka, H. Divi, V. Venkatramu, C.G.R. Nallagondur, Solid State thiazole-based fluorophores: promising materials for white organic light emitting devices, *Dyes Pigments*. 187 (2021), <https://doi.org/10.1016/j.dyepig.2020.109077> article 109077.
- [37] Y. Song, L. Hu, Q. Cheng, Z. Chen, H. Su, H. Liu, R. Liu, S. Zhu, H. Zhu, Benzothiazole derivatives with varied p-conjugation: synthesis, tunable solid-State emission, and application in single-component LEDs, *J. Mater. Chem. C*. 10 (2022) 6392–6401, <https://doi.org/10.1039/D2TC00440B>.