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Russian Text © The Author(s), 2019, published in Zhurnal Strukturnoi Khimii, 2019, Vol. 60, No. 10, pp. 1736-1745.

SUBSTITUENT EFFECT ON THE STRUCTURE AND PHOTOPHYSICAL PROPERTIES OF PHENYLAMINO- AND PYRIDYLAMINO-2,1,3-BENZOTHIADIAZOLES

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4-Bromo-7-phenylamino-2,1,3-benzothiadiazole (**1**) and 4-bromo-7-(3-pyridylamino)-2,1,3-benzo thiadiazole (**2**) are synthesized. Their crystal structure and photophysical properties are studied in comparison with the known phenylamino- and pyridylamino-derivatives of 2,1,3-benzothiadiazole. It is found that the aryl substituent and noncovalent interactions affect the absorption band positions and emission in a solid and a solution. It is shown that under the mechanical action on polycrystalline samples of compounds **1** and **2** a hypsochromic shift of the emission band occurs, which indicates the weakening of noncovalent intermolecular interactions.

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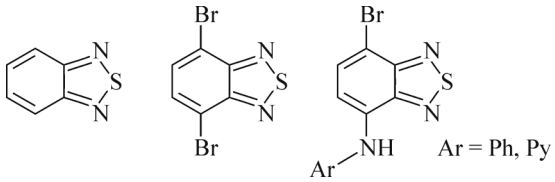
Keywords: 2,1,3-benzothiadiazole, crystal structure, noncovalent interactions, electronic absorption spectroscopy, photoluminescence.

INTRODUCTION

The chemistry of chalcogen-nitrogen heterocyclic compounds, in particular, 2,1,3-benzothiadiazole (btd, Scheme 1) derivatives, is one of the relevant trends in modern science because of tremendous opportunities of their application in materials science and biomedicine, which is explained by a combination of their unique physical properties and a high synthetic potential. Having a high electron acceptor [1, 2] and effective charge transfer [3] abilities, photoconductivty [4, 5], and intense fluorescence in the near UV and/or visible spectral ranges [6, 7], btd derivatives are promising materials for optoelectronic devices, e.g., organic light emitting diodes, solar cells, organic field transistors [8-11], as well as fluorescent



Scheme 1. Structure of btd, Br_2-btd, phenylamino-, and pyridylamino-benzothiadiazoles.

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biological labels and markers for PCR analyses [9]. This set of properties is favorably combined with a great number of variants of functionalizing btd by introducing various substituents into the carbon ring that enable the design of target compounds. For instance, the ease of btd bromination to 4,7-dibromo-2,1,3-benzothiadiazole (Br_2-btd, Scheme 1) makes it possible to perform Sonogashira or Suzuki cross-coupling reactions [10, 12-14], and also the Buchwald – Hartwig reaction. The latter was previously used for the synthesis of diverse mono- and disubstituted amines proposed as fluorescent dyes for living cells [10, 15-19], organic light emitting diodes [20], fluorescent sensors for different agents [21] and solar cells [8, 12, 22, 23].

In this work, 4-bromo-7-phenylamino-2,1,3-benzothiadiazole **1** and 4-bromo-7-(3-pyridylamino)-2,1,3-benzothiadiazole **2** were synthesized by the Buchwald–Hartwig reaction, their crystal structure was solved, and the substituent effect on the structure and photophysical properties was studied. The results were analyzed in comparison with the other known phenylamino- and pyridylamino-substituted btd.

EXPERIMENTAL

Reactions were conducted in the inert argon atmosphere using the standard Schlenk technique. The filtration of the reaction mixture and subsequent operations were performed in contact with air. Compound **1** was obtained by the described procedure [24]. Commercially available 4,7-dibromo-2,1,3-benzothiadiazole (Br_2-btd), (oxydi-2,1-phenylene)bis(diphenylphosphine) (DPEPhos), sodium *tert*-butylate (*t*-BuONa), and palladium acetate [$Pd(OAc)_2$] were used without additional purification. Toluene for the reaction was distilled above K/Na alloy in the argon atmosphere and stored in a Schlenk vessel in the argon atmosphere. Chemically pure solvents for column chromatography were used without additional purification and degassing. The C, H, N, S analysis of the samples was carried out on a vario MICRO cube analyzer. IR spectra were measured in KBr pellets on a FT-801 (Simex) IR–Fourier spectrometer. Electronic absorption and photoluminescence spectra of solutions (~10^{-5} M) were recorded on a Cary 60 spectrophotometer and a Cary Eclipse spectrofluorometer respectively. Diffuse reflectance spectra were measured on a Shimadzu UV-3101 PL spectrophotometer. To prepare the samples, a portion of the compound under study (0.005 g) and $BaSO_4$ (0.200 g) used as the standard were thoroughly mixed. The diffuse reflectance spectra were recalculated into absorption spectra by the Kubelka – Munk function [25].

The X-ray crystallographic analysis of compounds **1** and **2** was performed by the standard procedure on an automated four-circle Bruker APEX DUO diffractometer equipped with an area CCD detector (molybdenum radiation $\lambda = 0.71073$ Å, graphite monochromator). Reflection intensities were measured by φ- and ω-scanning of narrow (0.5°) frames. Absorption correction was applied using the SADABS program [26]. The structures were solved by a direct method and refined by the full-matrix least-squares technique in the anisotropic approximation for non-hydrogen atoms using the SHELXTL program package [27] and the Olex2 interface [28]. Hydrogen atoms were located geometrically and refined in the rigid body approximation, except hydrogen atoms of amino groups found from the difference Fourier maps and refined with a DFIX restraint of the N–H bond length. Crystallographic data, details of the experiments and refinement are summarized in Table 1. The X-ray crystallographic data have been deposited with the Cambridge Crystallography Data Center (CCDC) under numbers 1899853 and 1899854 and can be obtained from the authors or at: http://www.ccdc.cam.ac.uk/conts/retrieving.html.

Synthesis of 7-bromo-4-phenylamino-2,1,3-benzothiadiazole 1 [24]. To a suspension of *t*-BuONa (0.135 g, 1.40 mmol), Br_2-btd (0.294 g, 1.00 mmol), DPEPhos (0.027 g, 0.050 mmol), and [$Pd(OAc)_2$] (0.012 g, 0.050 mmol) in 5 mL of toluene an aniline (109 μL, 1.19 mmol) solution in 5 mL of toluene was slowly added. The reaction mixture was stirred at 90 °C for 42 h, then cooled to T_{room}, and filtered through a kieselguhr layer. The filtrate was evaporated until dryness; target product **1** was purified by column chromatography on silica gel (hexane:methylene chloride = 1:1 eluent). Compound **1** is contained in the first fraction. The product is orange powder. Yield 0.204 g (67%). Crystals suitable for X-ray crystallography were grown by recrystallizing the compound from diethyl ether.

TABLE 1. Crystallographic Data, Data Collection Parameters, and Results of the Structure Refinement for 4-Bromo-7-Phenylamino-2,1,3-Benzothiadiazole (**1**) and 4-Bromo-7-(3-Pyridylamino)-2,1,3-Benzothiadiazole (**2**)

Parameter	**1**	**2**
Chemical formula	$C_{12}H_8BrN_3S$	$C_{11}H_7BrN_4S$
M	306.18	307.18
T, K	293(2)	150(2)
Space group	$P2_1/c$	$P2_1/c$
a, Å	9.1128(5)	8.0943(6)
b, Å	16.1399(9)	16.4445(12)
c, Å	8.5069(5)	8.3877(6)
β, deg	110.660(2)	92.590(2)
V, Å^3	1170.73(12)	1115.32(14)
Z	4	4
ρ_{calc}, g/cm^3	1.737	1.829
μ, mm^{-1}	3.667	3.852
F(000)	608.0	608.0
Crystal dimensions, mm	0.55×0.4×0.15	0.31×0.2×0.08
2θ data collection range, deg	5.048-52.728	4.954-55.81
h, k, l indices	$-11 \le h \le 9$, $-18 \le k \le 20$, $-10 \le l \le 10$	$-10 \le h \le 10$, $-21 \le k \le 20$, $-11 \le l \le 11$
Number of measured reflections	8768	13119
Number of independent reflections (R_{int}, R_σ)	2380 (0.0415, 0.0370)	2660 (0.0270, 0.0191)
Number of refined parameters	157	157
Number of restraints	1	1
GOOF on F^2	1.112	1.055
R-factor ($I > 2\sigma(I)$)	$R_1 = 0.0376$, $wR_2 = 0.0813$	$R_1 = 0.0250$, $wR_2 = 0.0722$
R-factor (all data)	$R_1 = 0.0452$, $wR_2 = 0.0849$	$R_1 = 0.0285$, $wR_2 = 0.0740$
$\Delta\rho_{max}$ / $\Delta\rho_{min}$, e/Å^3	0.59 / –0.56	0.47 / –0.46

^{1}H NMR (500 MHz, $CDCl_3$): δ, ppm = 7.07 (d, 1H, J = 8.0 Hz); 7.16 (t, 1H, J = 7.5 Hz); 7.36 (d, 2H, J = 8.0 Hz); 7.44 (t, 2H, J = 7.5 Hz); 7.67 (d, 1H, J = 8.5 Hz).

IR spectrum, ν, cm^{-1}: 3400 s., 3052 w., 3017 v.w., 2923 w., 2853 w., 1944 v.w., 1855 v.w., 1732 v.w., 1591 s., 1549 s., 1509 m., 1476 m., 1440 v.w., 1382 s., 1331 v.w., 1306 m., 1277 v.w., 1252 w., 1179 w., 1156 w., 1126 w., 1078 w., 1029 v.w., 995 v.w., 932 w., 883 m., 853 w., 813 w., 751 s., 690 m., 615 w., 563 w., 541 w., 504 w.

For $C_{12}H_8BrN_3S$ calculated, %: C 47.1, H 2.6, N 13.7, S 10.5. Found, %: C 48.9, H 2.8, N 13.8, S 10.7.

Synthesis of 7-bromo-4-(3-pyridylamino)-2,1,3-benzothiadiazole 2. To a suspension of *t*-BuONa (0.423 g, 4.40 mmol), Br_2-btd (1.176 g, 4.000 mmol), DPEPhos (0.054 g, 0.10 mmol), and [$Pd(OAc)_2$] (0.059 g, 0.10 mmol) in 10 mL of toluene solid 3-aminopyridine (0.395 g, 4.20 mmol) was added. The mixture was stirred at 100 °C for 72 h, then cooled to T_{room}, and filtered through a kieselguhr layer. The filtrate was evaporated until dryness; target product **2** was purified by column chromatography on silica gel (hexane:ethylacetate = 1:2 eluent). As a result, several fractions were obtained, main – first and second. During the slow evaporation of solutions from the first fraction initial Br_2-btd was extracted (0.459 g, conversion 60%). From the second fraction we obtained dark red crystals of compound **2**, suitable for X-ray crystallography. Yield 0.41 g (33%).

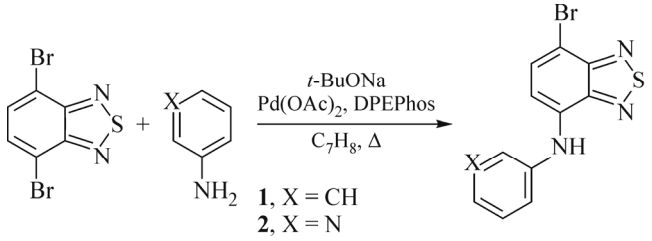
^{1}H NMR (500 MHz, $CDCl_3$, ppm): δ = 7.05 (d, 1H, J = 8.0 Hz); 7.13 (d, 1H); 7.36-7.39 (m, 1H); 7.70-7.73 (m, 2H); 8.40-8.41 (m, 1H); 8.70 (d, 1H, J = 3.0 Hz).

IR spectrum, ν, cm^{-1}: 3395 w., 3237 s., 3091 w., 3045 w., 2928 w., 1821 v.w., 1586 w., 1557 s., 1508 w., 1483 s., 1412 w., 1380 s., 1338 m., 1238 w., 1310 m., 1182 w., 1104 w., 1076 w., 1024 w., 936 w., 915 v.w., 879 m., 855 w., 837 v.w., 797 m., 715 m., 623 m., 571 w., 539 w.

For $C_{11}H_7BrN_3S$ calculated, %: C 43.0, H 2.3, N 18.2, S 10.4, Found, %: C 43.4, H 2.7, N 18.4, S 11.0.

RESULTS AND DISCUSSION

Secondary amines **1** and **2** were synthesized by the Buchwald–Hartwig reaction from 4,7-dibromo-2,1,3-benzothiadiazole and respective primary arylamine (Scheme 2). Similar compounds with substituted 2- and 4-aminopyridines [19, 29], and also compound **1** [24] were obtained earlier while the 3-aminopyridine derivative was synthesized for the first time. [$Pd(OAc)_2$] was used as a catalyst precursor and (oxydi-2,1-phenylene)bis(diphenylphosphine) (DPEPhos) was used as a phosphine ligand. In the reaction with phenylamine, apart from monosubstituted compound **1**, known disubstituted 4,7-bis(phenylamino)-2,1,3-benzothiadiazole [30] is formed in the amount of 20% of the target product. The compounds obtained were separated by column chromatography. In the synthesis of compound **2**, a part of initial 4,7-dibromo-2,1,3-benzothiadiazole was extracted; the conversion was 60%. With regard to the conversion, the yield of compound **2** purified by column chromatography was 55%. Apart from the fractions containing 4,7-dibromo-2,1,3-benzothiadiazole and the target product, several fractions of other products were collected, which were not identified because of their low yield. Products **1** and **2** obtained were characterized by X-ray crystallography, ^1H NMR, elemental analysis, and IR spectroscopy. The NMR and IR spectroscopic results for product **1** are consistent with the literature data [24].



Scheme 2.

According to the X-ray crystallographic data, the C4–N10 bond lengths (atomic numbering is given in Fig. 1) in compounds **1** and **2** (Table 2) are shorter than the typical C–N bond (1.48 Å), which indicates the conjugation of the N lone pair of the amino group with the aromatic system of the benzothiadiazole moiety. Close bond lengths are observed in similar 4-pyridyl [17], 2-pyridyl [19], and phenyl derivatives [30] and also in 4-amino-2,1,3-benzothiadiazole [31]. Torsion angles C9–C4–N10–C11 are close to 180° for compounds **1** and **2**. These conformations are stabilized by the conjugation of the amino group with the aromatic system. On the other hand, the conjugation of the amino group can be partially violated, in some cases, stabilizing also other conformations due to intermolecular interactions and/or steric factors. In particular, in 4,7-bis(4-pyridylamino)-2,1,3-benzothiadiazole [17], 7-bromo-4-(4-pyridylammonium)-2,1,3-benzothiadiazole nitrate [17], and 4,7-bis(phenylamino)-2,1,3-benzothiadiazole [30] a substantial deviation of torsion angles C9–C4–N10–C11 from 180° is observed (Table 2). Another torsion angle (C4–N10–C11–C12) governing the molecular conformation is varied within 141-180°.

In compounds **1** and **2**, the H10 atom of the amino group makes a weak intramolecular hydrogen bond with the N3 atom of the thiadiazole ring. The presence of this hydrogen bond in the 4-amino-2,1,3-benzothiadiazole molecule was earlier confirmed by quantum chemical calculations [32]. In compound **2** there is also the intermolecular N10–H10···N13 hydrogen bond between the amino group and the nitrogen atom of the pyridine moiety with a N···N distance of 2.99 Å. Apart from the hydrogen bond, in the structure of **2** short pair S···N contacts (Table 2) and head-to-tail π–π interactions between the pairs of benzothiadiazole moieties are observed, which all together form layers along the (1 0 0) plane (Fig. 2). Similar short S···N

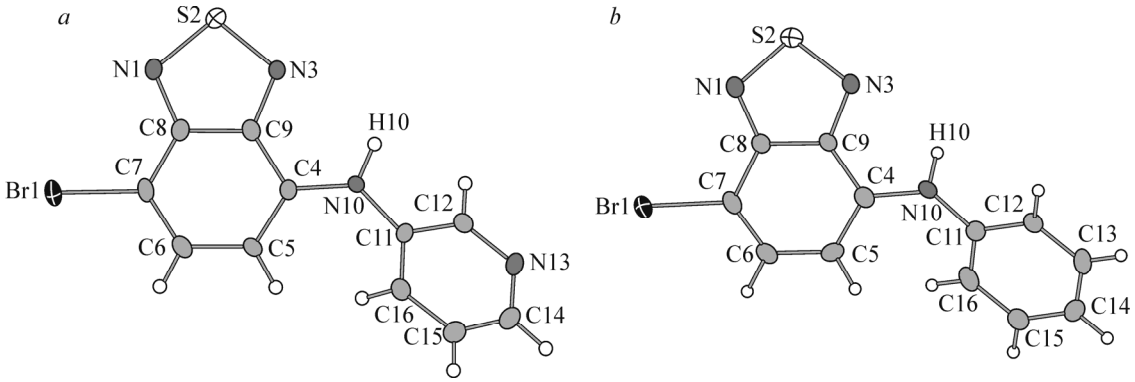
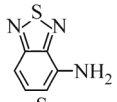
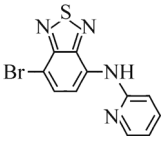
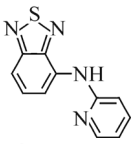
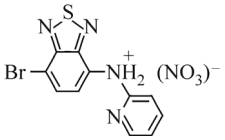
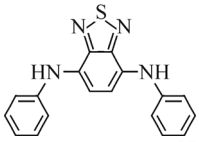
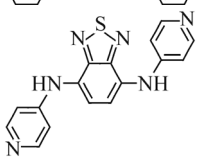


Fig. 1. Structure of the molecules of **1** (*a*) and **2** (*b*). Atomic displacement ellipsoids are given with a 50% probability.

TABLE 2. Selected Bond Distances and Bond Angles in Phenylamino- and Pyridylamino-2,1,3-Benzothiadiazoles

Compound	C4–N10, Å	C9–C4–N10–C11, deg	C4–N10–C11–C12, deg	S···N, Å	Center C_6–center C_2N_2S, Å	References
1	1.38	167.3	156.2	–	3.51	This work
2	1.37	180.0	149.4	2.99	3.58	This work
	1.39	–	–	3.12	3.79	[31]
	1.38	177.6	173.8	2.99	3.65	[19]
	1.38, 1.38	175.3, 178.6	168.1, 179.8	3.10	3.71, 3.66	[19]
	1.40	146.2	163.2	–	3.65, 3.81	[17]
	1.39, 1.40	171.5, 154.4	141.0, 159.8	–	3.80	[30]
	1.41, 1.40	149.5, 56.0	167.5, 178.5	–	3.58	[17]

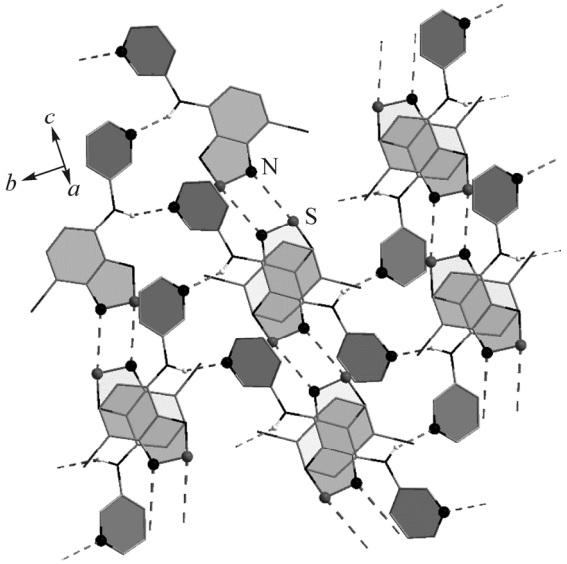


Fig. 2. Layer structure in compound **2** made by intermolecular hydrogen bonds and S···N contacts (dashed lines). Aromatic rings are shown by gray, H atoms, except the H atom of the amino group, are omitted.

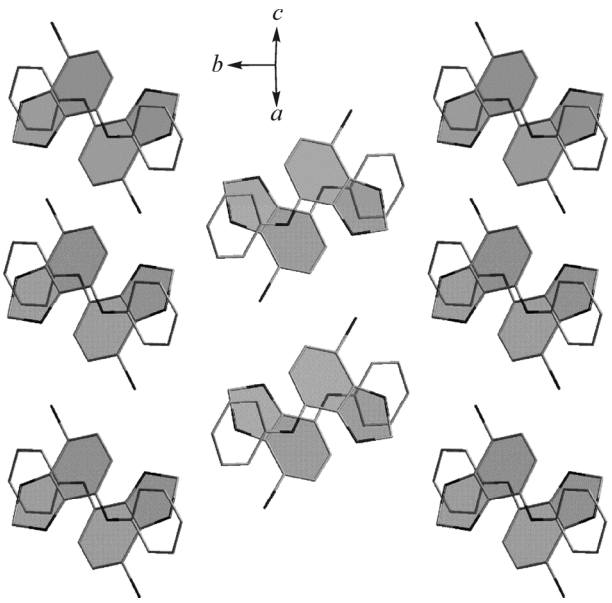


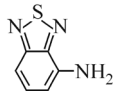
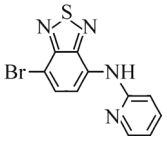
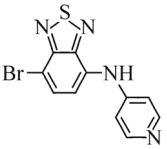
Fig. 3. Fragment of the crystal packing in compound **1**. Aromatic rings involved in the π–π interaction are shown by gray; H atoms are omitted.

contacts and π–π interactions are quite often observed in btd derivatives [6]. On the other hand, no short intermolecular S···N contacts are observed in compound **1**, although there are head-to-tail π–π interactions between the pairs of benzothiadiazole moieties (Fig. 3). Specific contacts with bromine were not detected in compounds **1** and **2**.

The region of stretching NH vibrations in the IR spectrum of **1** contains a narrow band at 3400 cm^{-1}, while in the spectrum of **2**, the respective band is at a lower frequency (3235 cm^{-1}) and is broadened, which is consistent with the occurrence of the N–H···N hydrogen bond for **2**. The IR spectra of **1** and **2** are slightly different in the range 1400-1600 cm^{-1} because of distinctions in stretching C–C and C–N vibrations.

For compounds **1** and **2**, the photophysical properties were studied (Table 3). In the electronic absorption spectra of solutions in CH_2Cl_2 (Fig. 4*a*) bands are observed in the range 250-320 nm which are characteristic of benzothiadiazole derivatives and correspond to π–π* transitions. Long-wave bands at 443 nm (for **1**) and 458 nm (for **2**) correspond to

TABLE 3. Wavelengths of Peaks in the Electronic Absorption and Emission Spectra for Compounds **1** and **2** in the Solution in CH_2Cl_2 and the Solid State

Compound	Solution in CH_2Cl_2			Solid sample			References
	$\lambda_{max.abs.}$, nm ($\varepsilon\cdot10^{-3}$, $M^{-1}\cdot cm^{-1}$)	$\lambda_{max.em.}$ nm	Stokes shift, cm^{-1}	$\lambda_{max.abs.}$, nm	$\lambda_{max.em.}$, nm	Stokes shift, cm^{-1}	
1	263 (27.2), 304 (8.49), 318 (6.92), 458 (6.83)	601	5195	265, 470	575/567[b]	3885/3640[b]	This work
2	258 (22.6), 303 (10.4), 316 (8.74), 443 (5.85)	584	5450	265, 455	600/590[b]	5310/5030[b]	This work
	410 (2.4)[a]	575	7000	308, 410	550	6210	[7]
	441 (12.3)[a]	510	3070	–	–	–	[19]
	430 (–)[a]	550	5075	–	–	–	[17]

[a] Only data on the long-wave band are given.
[b] Data are given on the polycrystalline/ground sample.

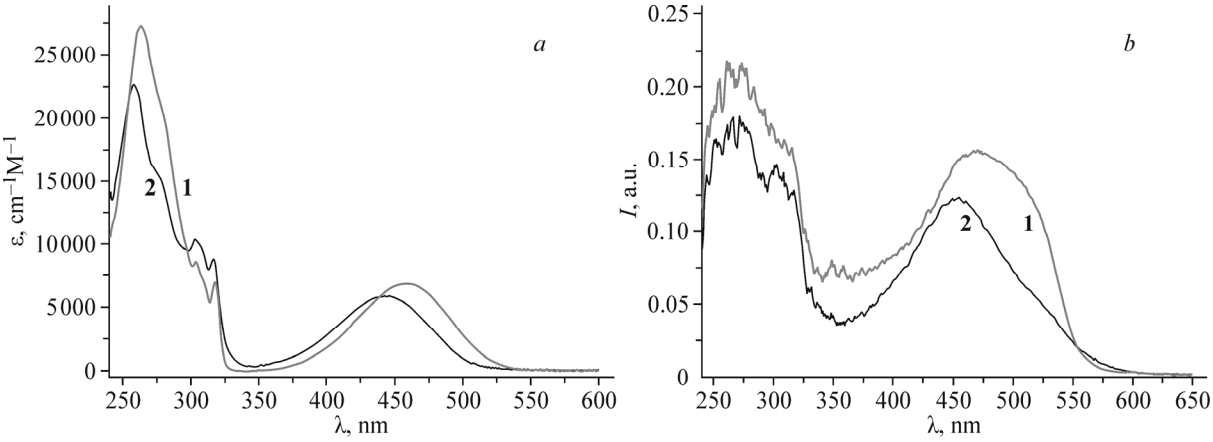


Fig. 4. Electronic absorption spectra of compounds **1** and **2** in the CH_2Cl_2 solution (*a*) and the solid state (*b*).

a transition from the HOMO mainly localized on amino and phenyl/pyridyl groups to the LUMO localized on the thiadiazole moiety, which was previously revealed for similar compounds [7, 19], i.e. this transition is characterized by a charge transfer band. Note that in the series of substituents phenyl > 3-pyridyl ~2-pyridyl > 4-pyridyl for the respective bromoaryl derivatives, a decrease in the wavelength of the absorption maximum is observed (Table 3). This phenomenon may be assumed to be caused by a decrease in the electron donor effect of aryl substituents in the amino group in the above compounds.

The absorption spectra of solid polycrystalline samples of compounds **1** and **2** are close to those in the solution (Fig. 4*b*), except the long-wave band with a long-wave shoulder, shifted to the red range, which can be explained by the occurrence of intermolecular interactions in the crystal. The maximum of this band for derivative **1** is in the longer-wave range as compared to that in **2** in both solution and solid state.

The obtained compounds exhibit luminescence in the solution (Fig. 5*a*). In the series of phenyl, 3-pyridyl, 4-pyridyl derivatives, a bathochromic shift of the maxima of emission bands is also observed (Table 3), which correlates with the absorption spectra. In this series, 7-bromo-4-(2-pyridylamino)-2,1,3-benzothiadiazole stands out: its Stokes shift is much smaller than that of the other derivatives. The possible reason for this distinction in the properties from those of the other compounds is that the molecule of this compound is planar. This conformation is stabilized by the intramolecular noncovalent interaction of the N atom of the pyridyl group with the H atom of the benzene moiety [19]. It is worth noting that according

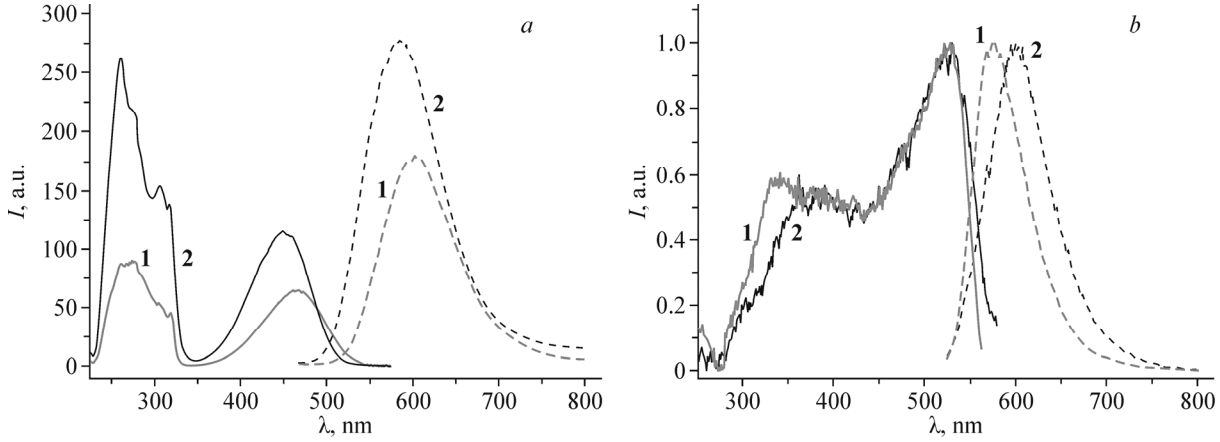


Fig. 5. Excitation (solid line) and luminescence (dashed line) spectra of compounds **1** and **2** in the CH_2Cl_2 solution (λ_{exc}= 260 nm (*a*) and normalized in the solid state, λ_{exc} = 350 nm for **1** and 380 nm for **2**) (*b*).

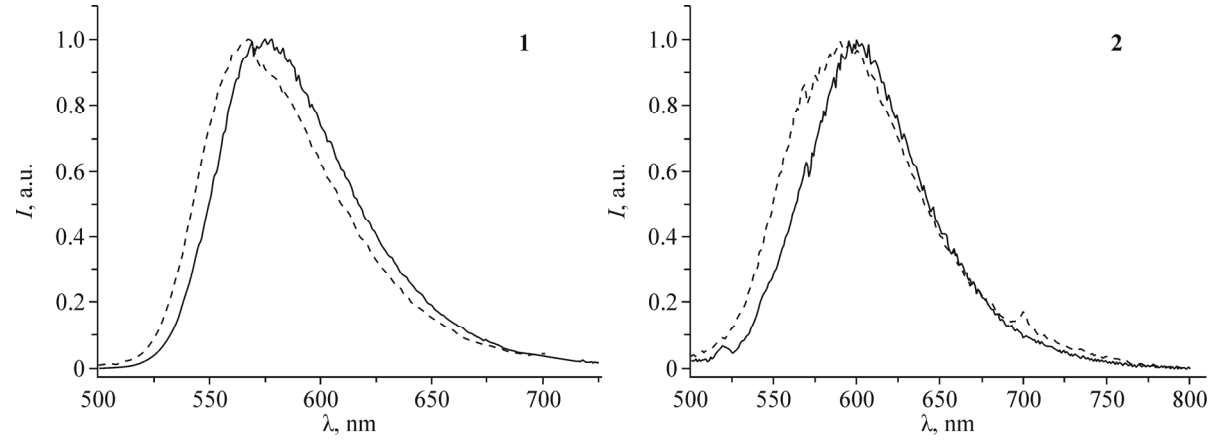


Fig. 6. Normalized emission spectra of compounds **1** (*a*) and **2** (*b*) in the solid state, (λ_{exc}= 350 nm for **1** and 380 nm for **2**) (solid line) and after grinding (λ_{exc} = 350 nm) (dashed line).

to quantum chemical calculations, the excited-state intramolecular proton transfer (ESIPT) from the N atom of the amino group to the N atom of the heterocycle does not occur in similar compounds [33]. In this case, a large Stokes shift (5100-5400 cm^{-1}) is only due to a considerable electron density redistribution during the transition to the excited state.

Solid compounds **1** and **2** also exhibit luminescence (Fig. 6). For compound **2**, the expected bathochromic shift of the emission band by 455 cm^{-1} as compared to the solution is observed, which may be due to the occurrence of intermolecular interactions in the solid state. For compound **1** an inverse effect is observed – a hypsochromic shift by 750 cm^{-1} as compared with the solution. The hypsochromic shift is also observed for 4-amino-2,1,3-benzothiadiazole [7]. This behavior is explained by different causes: molecular conformation, presence/absence of intermolecular interactions. However, it is possible to state that in the solid state the position of the emission band is very sensitive to the environment of the btd moiety. In particular, because of the metal ion coordination a significant shift of the band of intraligand transitions of btd derivatives to both long- and short-wave ranges can be observed [6, 7, 29, 32, 34, 35].

For compounds **1** and **2**, mechanofluorochromism is found: when polycrystalline samples are ground, a hypsochromic shift of the emission band by 245 cm^{-1} and 280 cm^{-1}, respectively, occurs. This behavior may mean that the luminescence of polycrystalline samples has the excimer nature [36, 37], and the grinding of the samples causes the weakening of intermolecular interactions. For instance, these may be π–π interactions present in both compounds **1** and **2**.

CONCLUSIONS

Thus, in this work, 4-bromo-7-phenylamino-2,1,3-benzothiadiazole **1** and 4-bromo-7-(3-pyridylamino)-2,1,3-benzothiadiazole **2** were synthesized and their crystal structures and photophysical properties are compared with other phenylamino- and pyridylamino-2,1,3-benzothiadiazoles. The greatest effect on the positions of absorption and emission bands in solutions is likely to be made by the electron donor properties of the aryl substituent, however, the effect of the molecular geometry and noncovalent interactions is not excluded. In the solid state, the molecular conformation and packing produce a much more significant effect, which may result in both hypsochromic (for **1**) and bathochromic (for **2**) shifts of the maxima of emission bands in comparison with the solutions. The effect of intermolecular interactions can be weakened during the grinding of polycrystalline samples **1** and **2**: the hypsochromic shift of the emission band occurs.

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CONFLICT OF INTERESTS

The authors declare that they have no conflict of interests.

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