Full Articles

Nitrogen-containing analogues of boron difluoride benzoylacetonate: synthesis, structure, luminescence, and quantum chemical modeling

G. O. Tretyakova,[a,b]★ **B. V. Bukvetskii,**[a] **E. V. Fedorenko,**[a] **A. Yu. Beloliptsev,**[a] **and A. G. Mirochnik**[a]

[a] *Institute of Chemistry, Far Eastern Branch of the Russian Academy of Sciences,*
159 prosp. 100-letiya Vladivostoka, 690022 Vladivostok, Russian Federation.
Fax: +7 (423) 231 1889. E-mail: tretyakova_galin@list.ru
[b] *Far Eastern Federal University,*
8 ul. Sukhanova, 690950 Vladivostok, Russian Federation.
Fax: +7 (423) 243 2315

Nitrogen-containing analogues of boron difluoride benzoylacetonate (**1**), *i.e.*, boron difluoride ketoiminates (boron difluoride 3-amino-1-phenyl-2-buten-1-onate (**2**) and 3-methylamino-1-phenyl-2-buten-1-onate (**3**)), were taken as examples to study the influence of a substituent (H, Me) at the nitrogen atom on structure and spectral-luminescent properties. The replacement of the oxygen atom with the nitrogen atom in compound **1** led to a bathochromic shift of the monomeric luminescence maximum. Quantum chemical modeling of absorption spectra for compound **2** was carried out. In contrast to compounds **1** and **3**, crystals of compound **2** are characterized by the formation of J-aggregates and excimers on their basis, which leads to a bathochromic shift of the luminescence spectrum and an increase in the luminescence intensity.

Key words: boron difluoride ketoiminates, luminescence, quantum chemical modeling, crystal structure, stacking interaction.

In recent years, interest towards the study of photophysical and photochemical properties of boron difluoride β-diketonates has grown due to a possibility of the use of these compounds in laser technology[1—3] and in the development of mesomorphous systems based on them.[4,5] Boron difluoride β-diketonates exhibit strong luminescence in both solutions and crystals.[6] Nitrogen-containing analogues of boron difluoride β-diketonates, ketoiminates and diiminates, possess weak luminescence in solutions,[7,8] however, they strongly luminesce in the crystalline state.[8,9] Due to this, the studies of the relationship between the crystal structure and spectral-luminescent properties of boron difluoride ketoiminates is an interesting objective. The number of researched boron difluoride ketoiminates is limited: for the most part spectral-luminescent properties of compounds bearing bulky substituents at the nitrogen atom (phenyl, *tert*-butyl, *para*-bromophenyl, *para*-methoxyphenyl) are described.[7,10] At the same time,

Published in Russian in *Izvestiya Akademii Nauk. Seriya Khimicheskaya,* No. 10, pp. 2312—2318, October, 2015.

in the work[11] boron difluoride enaminedibenzoylmethanate was taken as an example to demonstrate that the presence of methyl substituent at the nitrogen atom considerably affects molecular structure.

In the present work, we take nitrogen-containing analogues of boron difluoride benzoylacetonate (**1**), *viz.*, boron difluoride 3-amino-1-phenyl-2-buten-1-onate (**2**) and 3-methylamino-1-phenyl-2-buten-1-onate (**3**), as model compounds to study the influence of a substituent at the nitrogen atom (H, Me) on the crystal structure and spectral-luminescent properties.

Experimental

Luminescence and excitation spectra were obtained on a Shimadzu-RF 5301 spectrofluorimeter. The kinetics of luminescence decay were measured on a FluoTime 200 (PicoQuant) laser picosecond spectrofluorimeter (λ_{exct} = 370 nm). Absorption spectra were recorded on a Shimadzu-UV 2550 spectrophotometer. Mass spectra were recorded in the positive and negative ion modes (electrospray ionization (ESI), a Shimadzu LCMS-2010EV mass spectrometric detector). The samples were injected in the system acetonitrile—water (9 : 1).

X-ray diffraction study. Crystals of compound **2** were obtained by recrystallization from isopropyl alcohol. X-ray diffraction studies were performed on a Bruker SMART-1000 CCD diffractometer. Experimental data were collected in three groups of 906 shots each at angles φ = 0, 90 and 180° using the ω-scan technique with a 0.2° step and 20 sec exposure for every shot. Data processing, refinement of unit cell parameters, and recalculation of integral intensities to the structural amplitude modules were performed using the standard Smart and Saint programs.[12] The structure was solved by direct method with subsequent refinement of positional and thermal parameters in the anisotropic approximation for all the nonhydrogen atoms using the SHELXTBL software package.[13] Hydrogen atoms were placed in geometrically calculated positions and refined using a riding model.

Basic crystallographic parameters of the sample under study, characteristics of X-ray diffraction experiment, and details of refinement of structural model by the least squares method are given in Table 1, the principal distances are given in Table 2. The crystallographic data for compound **2** were deposited with the Cambridge Crystallographic Data Center (CCDC 910454) and can be obtained upon request at www.ccdc.cam.ac.uk/data_request/cif.

Quantum chemical modeling of electron absorption spectra of compounds in different conformations was carried out in the cluster approximation using the GAMESS-US software package.[14] Structural parameters, energy characteristics, and electron structure of compounds were determined with full optimization of geometry in the 6-311G(d, p) basis by *ab initio* method and density functional method with the B3LYP exchange-correlation potential. Electron absorption spectra with allowance for the excited singlet and triplet states were calculated by the TDDFT method in the 6-311G(d, p) basis with the B3LYP potential.

Boron difluoride benzoylacetonate (1) was obtained according to the procedure described earlier.[15]

Table 1. Crystallographic data for structure **2** and characteristics of the X-ray diffraction experiment

Parameter	Value
Molecular formula	$C_{10}H_{10}BF_2NO$
Temperature/K	243(2)
Molecular weight	209.00
Space group	$P\bar{1}$
a/Å	7.431(2)
b/Å	7.857(2)
c/Å	8.886(3)
α/deg	105.033(5)
β/deg	94.141(5)
γ/deg	91.257(5)
Z	2
d_{calc}/g cm^{-3}	1.390
μ/mm^{-1}	0.113
F(000)	216
Crystal size/mm^3	0.35×0.15×0.09
θ/deg range of data collection	2.38—25.04
Ranges of reflection indices	$-8 \le h \le 8$, $-9 \le k \le 9$, $-10 \le l \le 10$
Reflection collected	4592
Independent reflections	1774
R_{int}	0.0318
Completeness on θ = 25.04	99.8
Reflections with $I > 2\sigma(I)$	1199
Number of refinement parameters	142
S	1.042
R-factors on $I > 2\sigma(I)$	
R_1	0.0553
wR_2	0.1364
R-factors on all the reflections	
R_1	0.0850
wR_2	0.1513
Extinction ratio	0.027(9)
Residual electron density (min/max)/e Å^{-3}	−0.250/0.199

Table 2. Principal lengths distances for compound **2**

Bond	Length/Å	Bond	Length/Å
O—C(3)	1.317(3)	C(5)—C(3)	1.475(4)
O—B	1.463(3)	C(3)—C(2)	1.351(4)
F(1)—B	1.383(4)	C(2)—C(1)	1.400(4)
N—C(1)	1.300(3)	C(10)—C(9)	1.380(4)
N—B	1.536(4)	C(6)—C(7)	1.379(4)
F(2)—B	1.383(4)	C(9)—C(8)	1.373(4)
C(5)—C(10)	1.385(4)	C(8)—C(7)	1.371(4)
C(5)—C(6)	1.390(4)		

3-Amino-1-phenyl-2-buten-1-one was obtained according to the procedure described earlier.[16] Boron difluoride benzoylacetonate (3.75 g, 0.018 mol) was dissolved in acetonitrile (142 mL) with stirring. After 5 min of stirring, an aqueous solution of ammonia (3.5 mL, 0.054 mol) was added to the reaction mixture, and the stirring was continued for another 40 min (the reaction progress was monitored by TLC). Then, the reaction mixture was extracted with dichloromethane. The organic layer was washed with water and dried with sodium sulfate, the solvent was evaporated. The formed precipitate was filtered and washed with hexane. The yield was 2.3 g (61%). Found (%): C, 74.48; H, 6.92; N, 8.71. $C_{10}H_{11}NO$. Calculated: C, 74.51; H, 6.88; N, 8.69.

Boron difluoride 3-Amino-1-phenyl-2-buten-1-onate (2). A mixture of 3-amino-1-phenyl-2-buten-1-one (1 g, 0.0048 mol), boron trifluoride diethyl etherate (1.4 mL, 0.0096 mol), tributoxyborane (5.3 mL, 0.0096 mol), and freshly distilled toluene (9 mL) was refluxed for 30 min. Then, the reaction mixture was cooled, the formed precipitate was filtered, washed with toluene, and recrystallized from a mixture of isopropyl alcohol—acetonitrile. The yield was 0.83 g (82.69%), m.p. 164—165 °C. IR (KBr), ν/cm^{-1}: 3340, 1543, 1479, 1108, 1636, 1444, 1300, 770. Found (%): C, 56.98; H, 5.70; N, 6.61. $C_{10}H_{12}BF_2NO$. Calculated (%): C, 56.92; H, 5.73; N, 6.64.

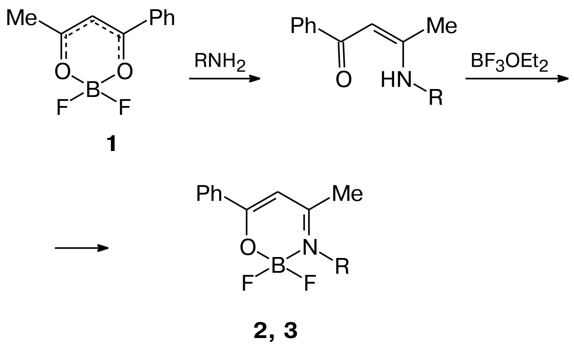
3-Methylamino-1-phenyl-2-buten-1-one. Boron difluoride benzoylacetonate (1.22 g, 0.0058 mol) was dissolved in acetonitrile (44 mL) with stirring. Then, a 40% aqueous solution of methylamine (0.57 mL, 0.0174 mol) was added to the reaction mixture, which was stirred for 2 h with the gradual addition of another 0.3 mL of an aqueous solution of methylamine (the reaction progress was monitored by TLC). Then, the reaction mixture was extracted with chloroform. The organic layer was washed with water and dried with sodium sulfate, the solvent was evaporated. The formed precipitate was recrystallized from aqueous ethanol. The yield was 0.5 g (50%). IR (Nujol), ν/cm^{-1}: 3331, 1600, 1568, 1556. HPLC-MS: Found: *m/z* 176 [M]$^+$; *m/z* 174 [M]$^-$. Calculated M = 175 g mol^{-1}. Found (%): C, 75.35; H, 7.51; N, 8.02. $C_{11}H_{13}NO$. Calculated (%): C, 75.40; H, 7.48; N, 7.99.

Boron difluoride 3-methylamino-1-phenyl-2-buten-1-onate (3). A mixture of 3-methylamino-1-phenyl-2-buten-1-one (0.5 g, 0.0029 mol), boron trifluoride diethyl etherate (0.53 mL, 0.0043 mol), calcium carbonate (0.29 g, 0.0029 mol), and freshly distilled toluene (9 mL) was refluxed for 8 h with stirring by a magnetic stirrer. Then, the reaction mixture was extracted with dichloromethane. The organic layer was washed with water and dried with a drying agent. The solvent was evaporated, the formed precipitate was filtered. The TLC data showed that the precipitate is an individual compound with a bluish violet luminescence. Compound **3** was obtained as fine white crystals, m.p. 139—140 °C; *cf.* Ref. 17: m.p. 136—137 °C. HPLC-MS: Found: *m/z* 224 [M]$^+$; *m/z* 222 [M]$^-$ Calculated: M = 223 g mol^{-1}. IR, ν/cm^{-1}: 3342, 2953, 2922, 2852, 1637, 1548 1494, 1462, 1105, 698. Found (%): C, 58.75; H, 6.36; N, 6.19. $C_{11}H_{14}BF_2NO$. Calculated (%): C, 58.71; H, 6.27; N, 6.22.

Results and Discussion

The synthesis of compounds **2** and **3** was carried out according to Scheme 1.

Scheme 1



R = H (**2**), Me (**3**)

The ligands were obtained by the reaction of boron difluoride benzoylacetonate with the corresponding amine. According to data in work,[16] the reaction of ammonia and primary amines with boron difluoride β-diketonates leads to the selective substitution of the oxygen atom next to the methyl group with the amino group. Compounds **2** and **3** were obtained based on the procedure for the preparation of compound **1** in the presence of tributoxyborane as a proton acceptor.[15] 3-Amino-1-phenyl-2-buten-1-one is less active than benzoylacetone, therefore, in the preparation of compound **2** we increased the reflux time of the reaction mixture from 10 to 40 min and the ratio ligand : boron trifluoride diethyl etherate to 1 : 2. For the preparation of compound **3**, the reaction of the ligand with boron trifluoride diethyl etherate was carried out under more drastic conditions than for the synthesis of compound **2**. Thus, a stronger base, namely calcium carbonate was used instead of tributoxyborane.

The X-ray diffraction analysis showed that molecule **2** has a planar structure (Fig. 1), like the molecule of its analogue compound **1**.[18] However, in contrast to molecule **1**, in which the C(1)—C(2), C(2)—C(3), C—O, and C—B bonds are equalized in pairs, in molecule **2** the quasiaromaticity of the chelate ring is disturbed. The C(1)—C(2) bond length (1.41 Å) is larger than that of the C(2)—C(3) bond (1.35 Å); the C(1)—N bond length (1.30 Å) corresponds to the double bond length;[19] the C(3)—O bond length (1.32 Å) is equal to that of the single C—O bond length in phenol,[19] which suggests the presence of a diene structure in the chelate ring of compound **2**. In molecule **2**, the C(1)—C(2), C(2)—C(3), and C(3)—C(5) bond lengths are longer as compared to the corresponding bonds in compound **1**.[18] Thus, it can be stated that in molecule **2** the π—π-conjugation is decreased in both the chelate ring and between the chelate and the phenyl rings of the molecule. A comparison of the X-ray diffraction data for compounds **3** (see Ref. 17) and **2** shows an even greater disturbance of quasiaromaticity in molecule **3**. Thus, the C—O bond length is increased to 1.33 Å, the C—C bond length at the methyl substituent is increased to 1.415 Å, whereas that of the phenyl group is decreased to 1.336 Å.

Since compounds **1**—**3** are isoelectron analogues, their electron absorption spectra are essentially similar (Fig. 2) (λ_{max} = 330 (**1**), 330 (**2**), 335 nm (**3**)). The luminescence

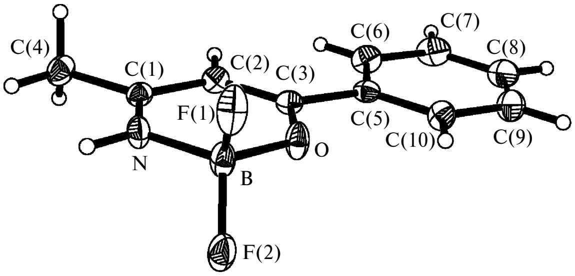


Fig. 1. Molecular structure of compound **2**.

and excitation spectra of solutions of compounds **2** and **3** are practically identical and are bathochromically shifted relative to the spectra of compound **1** (Fig. 3). The quantum yield of luminescence (φ) of compound **2** is considerably higher than that of compounds **1** and **3** (φ = 0.001 (**1**), 0.07 (**2**), 0.003 (**3**)).

In order to determine the reason for the difference of the excitation spectra from the absorption spectra of nitrogen-containing analogues of boron difluoride β-diketonates, for compound **2** we compared these spectra with the calculated spectra for the geometries of the ground and structurally relaxed excited states (Table 3).

Quantum chemical calculations showed that excitation of molecule **2** results in considerable changes in its geometric structure: the C(1)—C(2) bond length in the chelate ring and the C(3)—C(6) bond length between the phenyl and the chelate rings decreased, whereas the C(1)—N and C(2)—C(3) bond lengths increased (Fig. 4). In addition, bond lengths in the phenyl ring were changed, and it was transformed into the quinonoid ring (see Fig. 4). Consequently, the geometric structure of compound **2** in the structurally relaxed state undergoes a change corre-

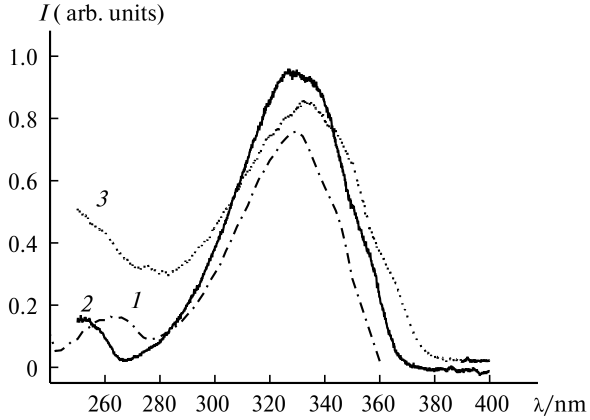


Fig. 2. Absorption spectra of solutions of compounds **1** (*1*), **2** (*2*), and **3** (*3*) ($C = 10^{-5}$ mol L^{-1}, chloroform).

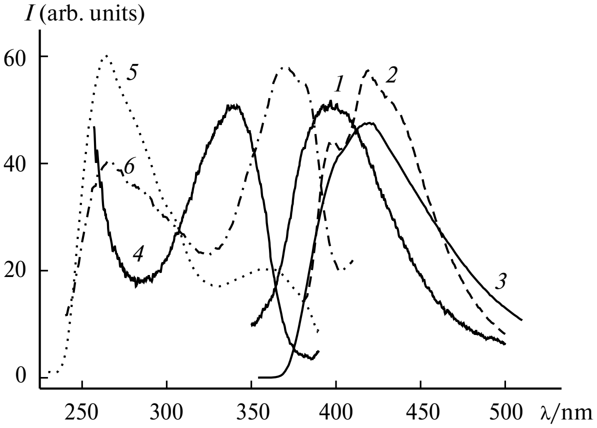


Fig. 3. Luminescence spectra of solutions of compounds **1** (*1*), **2** (*2*), and **3** (*3*) and excitation spectra of solutions of compounds **1** (*4*), **2** (*5*), and **3** (*6*) ($C = 10^{-5}$ mol L^{-1}, chloroform). The spectra are normalized on intensities.

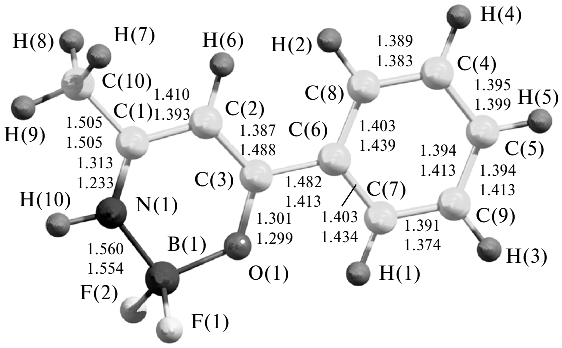
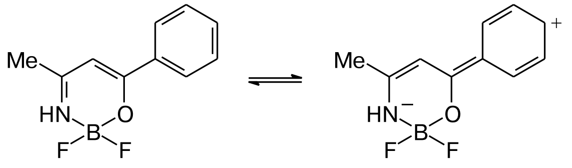


Fig. 4. Molecular geometry of compound **2**. The upper bond lengths (in Å) are given for the ground state, the lower bond lengths for the structurally relaxed state.

Table 3. Positions of absorption maxima in calculated and experimental spectra and the excitation spectrum of compound **2**

Band	Calculated absorption spectrum		Experimental absorption spectrum λ/nm (log ε)	Excitation spectrum λ/nm
	Ground state	Structurally relaxed state		
	λ/nm (*f*)			
1	250 (0.093)	260 (0.248)	252 (3.73)	270
2	306 (0.472)	358 (0.385)	327 (4.39)	380

Scheme 2



2a **2b**

sponding to the resonance structure given in Scheme 2. As it is seen from Table 3, the calculated absorption spectrum for the ground state is in good agreement with the experimental absorption spectrum, while the excitation spectrum agrees better with the theoretical absorption spectrum of compound **2** in the structurally relaxed excited state.

Quantum chemical calculations indicate that compound **2** exists in two tautomeric forms: **2a** and **2b** (see Scheme 2). An increase in the bond order between the phenyl and the chelate rings hinders the rotation of the phenyl ring, thus decreasing the nonradiative deactivation of the excited state, which leads to an increase in the quantum yield of luminescence of compound **2**. In summary, quantum chemical studies indicate the presence of the tautomeric form **2b**, which leads to a bathochromic shift of the excitation spectrum of compound **2** with respect to the absorption spectrum.

The absorption and the excitation spectra are practically identical for compound **1** (see Figs 2 and 3), in contrast to compounds **2** and **3**. It is probable that the asymmetry of the chelate ring in compounds **2** and **3**, unlike for compound **1**, favors the formation of the tautomeric form **2b**, which leads to a bathochromic shift of the excitation and the luminescence spectra of compounds **2** and **3** as compared to the spectrum of compound **1** (see Fig. 3).

Another pattern is observed when comparing the luminescence and excitation spectra of crystals of compounds **1**—**3** (Fig. 5). The luminescence and the excitation spectra of crystals **1**, similar to the case of dilute solutions, are hypsochromically shifted relative to the corresponding spectra of crystals **2**. However, for luminescence and excitation spectra of crystals **3** a hypsochromic shift relative to the spectra of crystals **2** and **1** is also observed.

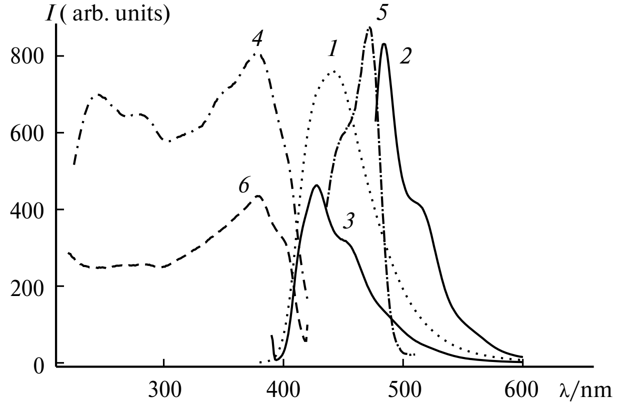


Fig. 5. Luminescence spectra of crystals **1** (*1*), **2** (*2*), and **3** (*3*) and excitation spectra of crystals **1** (*4*), **2** (*5*), and **3** (*6*).

A comparative study of the crystal structure of compounds **1**—**3** shows a significant role of crystal packing in the formation of the luminescent properties of the complexes. The X-ray diffraction data show that molecules **2** in the crystal are arranged as alternated stacks with two types of overlap (Fig. 6) and the formation of an N—H...F hydrogen bond between molecules of neighboring stacks. The bond distance value (2.930 Å) for the bond formed between the hydrogen at the nitrogen atom of one of the molecules and atom F(2) of the second molecule, as well as the value of the NHF angle (166°) (see Fig. 6), are a sufficient basis to regard the forming bond as that of hydrogen nature.[20,21] For the first type of overlap, the overlap exists between the chelate rings of neighboring molecules (the symmetry center of the type (0, 0.5, 0)). The distance between the planes of these molecules in the region of their overlap is 3.50 Å, the distance between the centroids is 3.90 Å. For the second type of overlap, the chelate ring of one of the molecules is located over the phenyl ring of the neighboring molecule, with the distance between the planes of these molecules being 3.58 Å (the symmetry center of the type (0, 0, 0)) and the distance between the centroids being 3.96 Å. The distance between the molecules is equal to the sum of the van der Waals radii for the carbon in the sp^2-hybridized state,[19] which is a favorable condition for the formation of excimers.[22] In fact, the luminescence spectrum of crystals **2** is shifted to the red region by 90 nm relative to spectrum of the dilute solution.

The presence of the excimeric luminescence in crystals **2** was confirmed by time-resolved spectroscopy (Fig. 7). The study of the kinetics of luminescence of crystals **2** showed the presence of two luminescent centers (τ_1 = 2.75 ns, τ_2 = 1.25 ns). At time zero in the time-resolved luminescence spectrum only a short wavelength component (λ_{max} = 400 nm) was observed, which belonged to monomeric luminescence and corresponded to the maximum of the luminescence spectrum of the solution. Within 0.5 ns, a new long wavelength band appeared in the luminescence spectrum (λ_{max} = 470 nm) attributed to the excimeric luminescence of crystal **2**.

According to the data in the work,[18] the molecules of compound **1**, the oxygen analogue of compound **2**, are packed as stacks with the intermolecular distance of 3.44 Å and a partial overlap of the chelate and the phenyl rings of neighboring molecules. The distance between molecules **1** in the crystal is limiting for excimer formation, since electrostatic repulsion forces come into play at small distances between molecules.[23—25] In work[26] it was shown that similar to crystal **2**, the formation of excimers was observed in crystal **1**. However, the shift of the luminescence spectrum of crystals relative to that of solutions for crystals **1** is

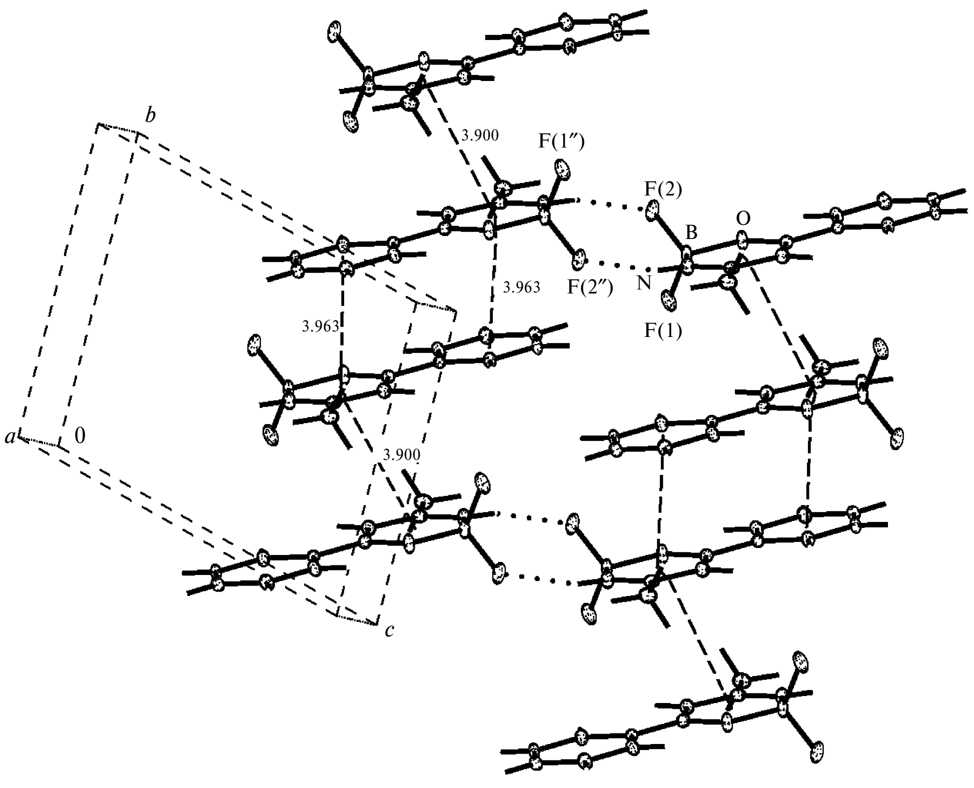


Fig. 6. Crystal structure of compound **2**.

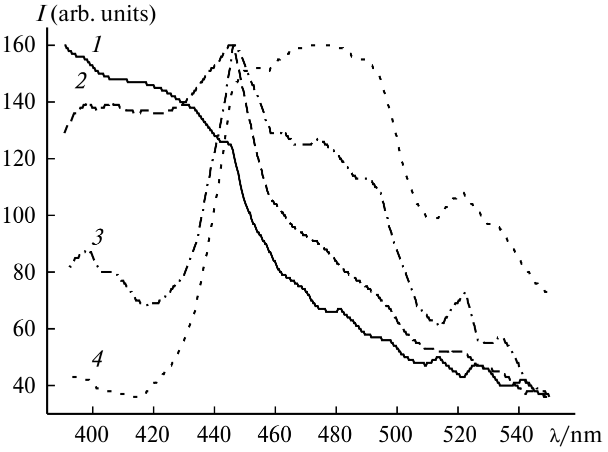


Fig. 7. Time-resolved luminescence spectra of crystal **2**: 75.6 ns (*1*); 75.8 ns (*2*); 75.9 ns (*3*); 76.1 ns (*4*) measured from the time of the laser pulse.

smaller than for **2**, and is 65 and 90 nm, respectively (see Figs 3 and 5). It should be noted that the structure corresponding to the structure of J-aggregates of the "deck-of-cards" type exists in crystals **2**, in contrast to compound **1**.[27] The formation of J-aggregates in crystals **2** leads to a bathochromic shift and a decrease in the half-width of the long wavelength band in the excitation spectra (see Figs 3 and 5). The formation of excimers based on J-aggregates in crystals **2** leads to an increase in the luminescence intensity by a factor of two relative to crystals **1**.

Two types of overlap[16] exist between molecules in crystal **3**, similar to the case of crystal **2**, with the molecules being arranged as alternated stacks, however, the degree of overlap between molecules is insignificant. Apparently, the presence of the methyl group at the nitrogen atom in compound **3** is responsible for a decrease in the efficiency of the overlap of molecules in crystals **3** compared to **2**, which decreases the probability of the formation of aggregates in solution of compound **3**. Thus, despite the distance between the molecules in crystal of compound **3** is optimal for the formation of excimers, the inefficient π—π-stacking interaction leads to a hypsochromic shift of the luminescence spectra of crystals **3** relative to crystals **2** by 70 nm. The study of the kinetics of luminescence of compound **3** showed the presence of a biexponential process (τ_1 = 0.48 ns (82%), τ_2 = 2.5 ns (18%)). A predominance of the short-lived process for crystals **3** and the similarity of the luminescence spectra of solutions and crystals indicate the monomeric character of the luminescence of crystals **3**. The absence of excimeric luminescence of J-aggregates in crystals **3** leads to a four-fold decrease in luminescence intensity in comparison with crystals **2**.

In conclusion, a comparative study of boron difluoride ketoiminates **2** and **3** and their oxygen analogue boron difluoride benzoylacetonate showed that the replacement of the oxygen atom with the nitrogen leads to a considerable change in the spectral-luminescent properties. The existence of the tautomeric form with a geometry that corresponds to the structure of the molecule of ketoiminates in the structurally relaxed excited state leads to a bathochromic shift of the luminescence excitation and the luminescence spectra relative to the spectra of boron difluoride benzoylacetonate. The crystal packing and an efficient π—π-stacking interaction in crystals **2** result in the formation of J-aggregates and excimers on their basis and in the increase in the luminescence intensity relative to **1** and **3**.

Physicochemical studies of compounds and quantum chemical modeling were supported by the "Far East" Program for Fundamental Studies of the Far Eastern Branch of the Russian Academy of Sciences (Grant 0265-2015-0038). Synthesis of complexes was supported by the Far Eastern Federal University Science Foundation (Grant 14-08-3/6-31_i).

References

1. N. N. Vasil´ev, A. Ya. Gorelenko, I. I. Kalosha, V. A. Mezhentsev, I. G. Tishchenko, V. A. Tolkachev, V. Ya. Tulach, A. P. Shkadarevich, *Zh. Prikl. Spektr.*, 1985, **42**, 51 [*J. Appl. Spectr.* (*Engl. Transl.*), 1985, **42**].
2. K. Gustav, U. Bartsch, W. Gunther, *Monatsh. Chem.*, 1994, **125**, 1321.
3. E. Cogne-Laage, J.-F. Allemand, O. Ruel, J.-B. Baudin, V. Croquette, M. Blanchard-Desce, L. Jullien, *Chem. Eur. J.*, 2004, **10**, 1445.
4. O. A. Turanova, A. N. Turanov, D. V. Lapaev, O. I. Gnezdilov, S. V. Lokov, Yu. G. Galyametdinov, *Russ. J. Gen. Chem.* (*Engl. Transl.*), 2006, **76**, 730 [*Zh. Obshch. Khim.*, 2006, **76**, 767].
5. O. A. Turanova, G. G. Garifzyanova, A. N. Turanov, *Russ. J. Gen. Chem.* (*Engl. Transl.*), 2010, **80**, 2317 [*Zh. Obshch. Khim.*, 2010, **80**, 1854].
6. A. G. Mirochnik, E. V. Gukhman, V. E. Karasev, P. A. Zhikhareva, *Russ. Chem. Bull.* (*Int. Ed.*), 2000, **49**, 1024 [*Izv. Akad. Nauk, Ser. Khim.*, 2000, 1030].
7. Y. Kubota, H. Hara, S. Tanaka, K. Funabiki, M. Matsui, *Org. Lett.*, 2011, **13**, 6544.
8. R. Yoshii, A. Hirose, K. Tanaka, Y. Chujo, *Chem. Eur. J.*, 2014, **20**, 8320.
9. R. Yoshii, A. Nagai, K. Tanaka, Y. Chujo, *Chem. Eur. J.*, 2013, **19**, 4506.
10. F. P. Macedo, C. Gwengo, S. V. Lindeman, M. D. Smith, J. R. Gardiner, *Eur. J. Inorg. Chem.*, 2008, **20**, 3200.
11. M. Xia, B. Wu, G. Xiang, *J. Fluor. Chem.*, 2008, **129**, 402.
12. *SMART and SAINT-Plus. Versions 5.0. Data Collection and Processing Software for the SMART Sistem,* Bruker AXS Inc., Madison, Wisconsin, USA, 1998.
13. G. M. Sheldrick, *SHELXTBL/PC. Versions 5.10. An Integrated System for Solving, Refining and Displaying Crystal Structures From Diffraction Data*, Bruker AXS Inc., Madison, Wisconsin, USA, 1998.
14. M. W. Schmidt, K. K. Baldridge, J. A. Boatz, S. T. Elbert, M. S. Gordon, J. H. Jensen, *J. Comput. Chem.*, 1993, **14**, 1347.
15. V. E. Karasev, O. A. Korotkich, *Russ. J. Inorg. Chem.* (*Engl. Transl.*), 1986, **31**, 869 [*Zh. Neorg. Khim.*, 1986, **31**, 869].
16. B. Stefane, S. Polanc, *New J. Chem.*, 2002, **26**, 28.
17. K. Itoh, M. Fujimoto, M. Hashimoto, *Acta Crystallogr.*, 1998, **54**, 1324.
18. A. W. Hanson, E. W. Macaulay, *Acta Crystallogr.*, 1972, **28**, 1961.
19. A. Gordon, R. Ford, *The chemist's companion*, Wiley Interscience, New York, 1972, 541 pp.
20. R. Flonish, T. Rosen, O. Meyer, K. Rissanen, G. Haufe, *J. Mol. Struct.*, 2006, **787**, 50.
21. P. Murray-Rust, W. Stalling, C. Monti, R. Preston, J. Glusker, *J. Am. Chem. Soc.*, 1983, **105**, 3206.
22. N. N. Barashkov, T. V. Sachno, R. N. Nurmukhametov, O. A. Khakhel´, *Russ. Chem. Rev.*, 1993, **62**, 539.
23. M. L. Glowka, D. Martynowski, K. Koztowska, *J. Mol. Struct.*, 1999, **474**, 81.
24. E. M. Gordon, W. R. Ware, *The Exciplex*, Akadem Press, New York, 1975, 156 pp.
25. B. V. Bukvetskii, E. V. Fedorenko, A. G. Mirochnik, A. Yu. Beloliptsev, *J. Struct. Chem.* (*Engl. Transl.*), 2010, **51**, 545 [*Zh. Struktur. Khim.*, 2010, **51**, 563].
26. E. V. Fedorenko, B. V. Bukvetskii, A. G. Mirochnik, T. B. Emelina, V. E. Karasev, *Russ. Chem. Bull.* (*Int. Ed.*), 2009, **58**, 2240 [*Izv. Akad. Nauk, Ser. Khim.*, 2009, 2174].
27. B. I. Shapiro, *Russ. Chem. Rev.*, 2006, 75, 433.

Received March 27, 2015;
in revised form September 7, 2015