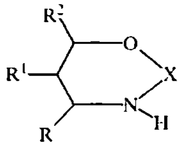
Chemistry of Heterocyclic Compounds, Vol. 35, No. 9, 1999

ANALYSIS OF THE CONFORMATIONAL COMPOSITION OF THE 4,5- AND 5,6-DIMETHYL-1,3,2-OXAZABORINANE STEREOISOMERS

V. V. Kuznetsov

An energy for the molecules of cis and trans 4,5- and 5,6-dimethyl-1,3,2-oxazaborinanes, and of model 1,3,2-oxazaborinanes and tetrahydro-1,3-oxazines with full geometric optimization has been calculated using empirical (MM2) and semiempirical (AM1) methods. From a comparison of experimental and calculated coupling constants and the relative energies of individual conformers it follows that molecules of the cyclic boron esters form a multicomponent equilibrium system, comprizing sofa and half-chair forms with an equatorial orientation of the N–H bond.

Systematic stereochemical investigations of substituted 1,3,2-oxazaborinanes have shown that a sofa or an equilibrium state between sofa invertomers is the preferred conformation for the majority of these compounds [1,2]. The possibility of one of the flexible forms participating in a conformational equilibrium has been assumed for the interpretation of the NMR data in several studies [2-5]. The complexity of assessing the relative stability of such forms within the framework of CNDO [6], due to incomplete estimates of the energy of electron exchange in the heteroatomic fragment [7,8], makes it probable that conformational assignments based on NMR data are mistaken. The aim of the present work was therefore to investigate the conformational composition for molecules of individual stereoisomers of 4,5- and 5,6-dimethyl-1,3,2-oxazaborinanes (I,II) and of model oxazaborinanes (III-V) and tetrahydro-1,3-oxazines (VI-X) by the methods of MM2 molecular mechanics [9] and SSP MO LCAO in AM1 parametrization [10,11] in combination with NMR data [3].

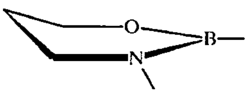


I X = B–H, R = R^1 = Me, R^2 = H; II X = B–H, R = H, R^1 = R^2 = Me; III X = B–H, R = R^2 = H, R^1 = Me;
IV X = B–H, R = Me, R^1 = R^2 = H; V X = B–H, R = R^1 = H, R^2 = Me; VI X = CH_2, R = R^2 = H, R^1 = Me;
VII X = CH_2, R = Me, R^1 = R^2 = H; VIII X = CH_2, R = R^1 = H, R^2 = Me; IX X = CH_2, R = R^1 = Me, R^2 = H;
X X = CH_2, R = H, R^1 = R^2 = Me

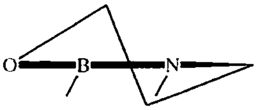
As a result several minima were observed on the potential energy surface of ester molecules I and II corresponding to a sofa (S), half-chair (HC-1, HC-2), and also 1,4-, 3,6-, and 2,5-twist (1,4-, 3,6-, and 2,5-T) conformers, with diequatorial (ee, *trans*) or equatorial–axial (ea, *cis*) orientation of substituents.

A. V. Bogatskii Institute of Physics and Chemistry, Ukrainian Academy of Sciences, Odessa 270080, Ukraine; e-mail: physchem@paco.net. Translated from Khimiya Geterotsiklicheskikh Soedinenii, No. 9, pp. 1176-1184, September, 1999. Original article submitted September 10, 1998.

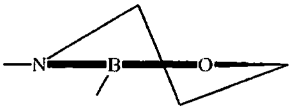
All the forms, apart from S, were obtained with fixed torsion angles $C_{(4)}$NBO and $C_{(6)}$OBN, otherwise they were isomerized into the sofa form. The 2,5-T conformer was converted into a half-chair in the course of minimization by the AM1 approach even under these limitations.



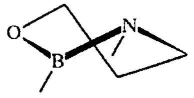
S



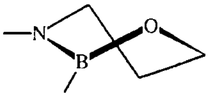
HC-1



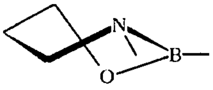
HC-2



1,4-T



3,6-T

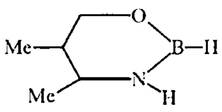


2,5-T

From the values of the endocyclic torsion angles for the most stable conformers of the *cis* and *trans* isomers (ester I as example, Table 1) it follows that the HC-1 and HC-2 forms differ in the degree of distortion of the $C_{(4)}$NBO and $C_{(6)}$OBN fragments. It is also necessary to note the large flattening of the sofa according to AM1 compared with the MM2 results. Calculated values of the bond lengths and valence angles of this form correspond with the experimental data [12,13].

The relative energies for the conformers of esters I and II (Table 2) show that their stability decreases in the series S ≥ HC > 1,4-T > 3,6-T > 2,5-T. For the *trans* isomers, HC-1 (almost degenerate in energy) and HC-2 exist in the neighborhood of the basic minimum (S4e5e or S5e6e). Conformer S4a5e (or S5e6a) are the most stable of the *cis*-isomers, however several local minima (S4e5a, S6e5a, and a group of half-chairs) with differences in

TABLE 1. Endocyclic Torsion Angles (deg) of the Individual Conformers of the Ester I Molecule



Configu-ration	Calculation method	Conformer	1-2-3-4	2-3-4-5	3-4-5-6	4-5-6-1	5-6-1-2	6-1-2-3
cis-	MM2	S 4a5e	4.9	-30.2	55.8	-55.6	27.9	-3.3
		S 4e5a	5.8	-31.2	57.4	-59.1	32.8	-6.4
		HC-1 5e	-2.1	-19.6	50.5	-60.4	37.0	-7.3
		HC-1 5a	-1.4	-21.8	52.9	-62.7	39.0	-7.9
		HC-2 5e	-6.3	32.7	-57.0	54.0	-25.0	1.6
		HC-2 5a	-8.0	37.9	-61.1	54.2	-22.8	-0.6
	AM1	S 4a5e	0.7	-21.2	45.8	-53.6	33.7	-6.7
		S 4e5a	-2.9	-20.3	46.0	-53.2	32.0	-2.8
		HC-1 5e	-2.5	-16.8	43.9	-55.5	37.1	-7.9
		HC-1 5a	-4.2	-16.2	43.6	-55.3	36.9	-6.4
		HC-2 5e	-5.6	28.2	-48.5	-49.6	-27.1	4.1
		HC-2 5a	-5.7	32.3	-50.3	46.1	-20.8	-1.2
trans-	MM2	S 4e5e	-2.3	27.7	-55.5	58.8	-31.9	4.3
		HC-1	-3.5	-18.9	50.7	-61.9	38.6	-7.1
		HC-1	-7.5	37.0	-60.0	53.2	-21.6	-1.5
	AM1	S 4e5e	2.6	19.4	-44.2	51.2	-30.5	2.8
		HC-1	-5.8	-12.5	40.1	-53.6	36.9	-6.8
		HC-1	-5.7	30.9	-48.7	45.5	-21.0	-0.4

TABLE 2. Relative Energies for Conformers of Compounds I-X (kcal/mole)

Compound	Conformer	MM2		AM1	
		E	Δ*E*	-*E*	Δ*E*
1	2	3	4	5	6
I	*cis*-				
	S 4a5e	5.4	0.0	1892.8	0.0
	S 4e5a	6.0	0.6	1892.6	0.2
	HC-1 5e	5.7	0.3	1892.7	0.1
	HC-1 5a	6.3	0.9	1892.4	0.4
	HC-2 5e	5.4	0.0	1892.5	0.3
	HC-2 5a	6.4	1.0	1891.8	1.0
	1,4-T 5e	7.7	2.3	1889.9	2.9
	1,4-T 5a	8.5	3.1	1889.9	2.9
	3,6-T 4e	9.2	3.8	1889.3	3.5
	3,6-T 4a	7.9	2.5	1889.0	3.8
	2,5-T	13.1	7.7	—	—
	trans-				
	S 4e5e	4.8	0.0	1893.9	0.1
	HC-1	5.0	0.2	1894.0	0.0
	HC-2	5.2	0.4	1893.0	1.0
	1,4-T	6.5	1.7	1892.4	1.6
	3,6-T	7.8	3.0	1890.5	3.5
	2,5-T	11.8	7.0	—	—
	Δ*E* $C_{(5)}CH_3$*		1.2		1.3
	Δ*E* $C_{(4)}CH_3$*		0.6		1.1
II	*cis*-				
	S 5e6a	3.3	0.0	1892.8	0.0
	S 5a6e	6.0	0.7	1892.0	0.8
	HC-1 5e	5.4	0.1	1892.7	0.1
	HC-1 5a	6.3	1.0	1892.4	0.8
	HC-2 5e	5.5	0.2	1892.4	0.4
	HC-2 5a	6.4	1.1	1891.5	1.8
	1,4-T 5e	7.2	1.9	1890.8	2.3
	1,4-T 5a	8.5	3.2	1898.8	3.0
	3,6-T 4e	8.5	3.2	1888.6	4.2
	3,6-T 4a	9.3	4.0	1887.9	4.9
	2,5-T	13.2	7.9	—	—
	trans-				
	S 5e6e	4.8	0.0	1893.4	0.0
	HC-1	5.1	0.3	1893.3	0.1
	HC-2	5.1	0.3	1892.6	0.8
	1,4-T	7.0	2.2	1891.3	2.1
	3,6-T	7.3	2.5	1890.4	3.0
	2,5-T	11.7	6.9	—	—
	Δ*E* $C_{(5)}CH_3$*		1.2		1.4
	Δ*E* $C_{(6)}CH_3$		0.5		0.6
III	S 5e	3.3	0.0	1614.9	0.0
	S 5a	4.5	1.2	1614.0	0.9
IV	S 4e	3.3	0.0	1614.5	0.0
	S 4a	4.0	0.7	1613.8	0.7
V	S 6e	3.3	0.0	1613.7	0.0
	S 6a	4.0	0.7	1613.4	0.3
VI	C 3e5e	6.1	0.2	1652.6	5.0
	C 3a5e	5.9	0.0	1657.6	0.0
	C 3e5a	7.2	1.3	1651.6	6.0
	C 3a5a	7.1	1.2	1656.9	1.0
	Δ*E* $C_{(5)}CH_3$		1.2		1.0
	Δ*E* N–H		0.1		5.0

TABLE 2 (continued)

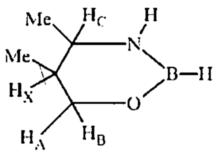
1	2	3	4	5	6
VII	C 3e4e	6.2	0.1	1651.4	5.4
	C 3a4e	6.1	0.0	1656.8	0.0
	C 3e4a	8.1	2.0	1652.0	4.8
	C 3a4a	8.0	1.9	1655.1	1.7
	ΔE $C_{(4)}CH_3$		1.9		1.7
	ΔE N-H		0.1		3.1-5.4
VIII	C 3e6e	6.3	0.2	1651.1	5.0
	C 3a6e	6.1	0.0	1656.1	0.0
	C 3e6a	8.6	2.5	1651.0	5.1
	C 3a6a	8.5	2.4	1655.8	0.3
	ΔE $C_{(6)}CH_3$		2.4		0.3
	ΔE N-H		0.1-0.2		5.0-5.1
IX	*trans-*				
	C 3e4e5e	7.4	0.2	1930.9	5.4
	C 3a4e5e	7.2	0.0	1936.3	0.0
	cis-				
	C 3e4e5a	8.6	0.1	1929..8	5.5
	C 3a4e5a	8.5	0.0	1935.3	0.0
	C 3e4a5e	9.3	0.8	1931.0	4.3
	ΔE $C_{(4)}CH_3$		2.0		2.0
	ΔE $C_{(5)}CH_3$		1.3		1.0
	ΔE N-H		0.1-0.2		3.3-5.5
X	*trans-*				
	C 3e5e6e	7.4	0.1	1930.9	5.0
	C 3a5e6e	7.3	0.0	1935.9	0.0
	cis-				
	C 3e5a6e	8.7	0.1	1929.5	5.8
	C 3a5a6e	8.6	0.0	1934.9	0.4
	C 3e5e6a	9.6	1.0	1930.4	4.9
	C 3a5e6a	9.5	0.9	1935.3	0.0
	ΔE $C_{(5)}CH_3$		1.3		0.0
	ΔE $C_{(6)}CH_3$		2.2		0.6

---

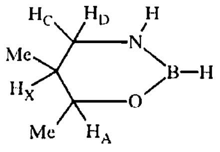
* $\Delta E C_{(5)}CH_3$ = *E* S 4e5a – *E* S 4e5e (or *E* C 3a5a – *E* C 3a5e; or *E* C 3a4e5a – *E* C 3a4e5e); the least of the possible values of Δ are given. Values of ΔE $C_{(4)}CH_3$ and ΔE $C_{(6)}CH_3$ were obtained analogously.

energy from 0.1 to 1.0 kcal/mole are found in the vicinity of these points. The main reason for the existence of such flattened global minima is linked with the decrease in $\Delta E C_{(4)}CH_3$ and $\Delta E C_{(6)}CH_3$ compared with $\Delta E C_{(5)}CH_3$ (compounds I and II, model esters III-V, Table 2), which is characteristic of a system with a flat configuration of the atom in the second position of the ring. The values of $\Delta E C_{(4)}CH_3$ and $\Delta E C_{(6)}CH_3$ were one and a half to two times greater in the molecules of tetrahydro-1,3-oxazines VI-X than $\Delta E C_{(5)}CH_3$ (with the exception of the AM1 results significantly under-estimating the size of $\Delta E C_{(6)}CH_3$ in compounds VIII and X). The experimental values of ΔG^0 for the methyl group at $C_{(4)}$ and $C_{(6)}$ in tetrahydro-1,3-oxazines are unknown, however they must not be significantly different from $\Delta G^0 C_{(4)}CH_3$ in 1,3-dioxanes (2.7-2.9 kcal/mole [14]). At the same time the conformational free energies of the methyl group at $C_{(5)}$ in oxazines and 1,3,2-oxazaborinanes are practically the same [15]. It follows from what has been said that for molecules of the *cis* isomers of oxazines IX and X, according to calculated data, the chair C4e5a (C5a6e) predominates, although the presence of alternative forms is not excluded. For the *trans* isomers the respective C4e5e and C5e6e forms dominate. This is in agreement with the NMR data [16-22]. However it is fairly complicated to single out one preferred conformation for the *cis* and *trans* isomers of the boron esters I and II. It is also necessary to mention that conformers with an axial N–H bond are more stable for oxazines VI-X (Table 2). This has been confirmed experimentally [16-19,23-25]. On the other hand

TABLE 3. Values of the Torsion Angles Between Protons (deg) and Coupling Constants (Hz) for the Most Stable Conformers of Ester Molecules I and II



I



II

Compound	Calculation method	Conformer	φ_{AX}	φ_{BX}	φ_{CX}	φ_{DX}	$^3J_{AX}$	$^3J_{BX}$	$^3J_{CX}$	$^3J_{DX}$	$\Sigma\lvert\Delta J\rvert$ *
1	2	3	4	5	6	7	8	9	10	11	12
cis-I	MM2	S 4e5a	57.2	64.5	57.7	—	3.9	3.0	3.9	—	5.6
		S 4a5e	177.8	56.1	54.0	—	11.4	4.3	4.4	—	5.1
		HC-1 5e	177.3	60.2	49.6	—	11.4	3.5	5.0	—	6.3
		HC-1 5a	60.5	61.6	53.6	—	3.5	3.4	4.4	—	6.1
		HC-2 5e	176.4	54.8	55.0	—	11.3	4.2	4.2	—	4.7
		HC-2 5a	52.8	68.3	61.2	—	4.5	2.7	3.4	—	5.0
	AM1	S 4e5a	48.4	72.8	46.0	—	5.1	2.3	5.5	—	6.7
		S 4a5e	175.6	54.2	45.4	—	11.3	4.3	5.6	—	6.0
		HC-1 5e	177.6	55.9	43.9	—	11.4	4.1	5.8	—	6.5
		HC-1 5a	50.3	71.1	43.8	—	4.8	2.4	5.8	—	7.2
		HC-2 5e	171.6	50.6	47.6	—	11.2	4.8	5.3	—	5.7
		HC-2 5a	41.7	78.9	49.9	—	6.1	1.9	4.9	—	5.5

TABLE 3 (continued)

1	2	3	4	5	6	7	8	9	10	11	12
trans-I	MM2	S 4e5e	179.7	58.1	179.8	—	11.4	3.8	11.4	—	3.6
		HC-1	176.6	60.6	178.3	—	11.4	3.5	11.4	—	3.9
		HC-2	175.3	53.7	175.9	—	11.3	4.4	11.4	—	2.9
	AM1	S 4e5e	171.4	50.5	167.7	—	11.2	4.8	11.0	—	2.4
		HC-1	173.7	52.4	163.8	—	11.3	4.6	10.7	—	2.0
		HC-2	166.0	45.6	172.0	—	10.8	5.5	11.3	—	3.8
cis-II	MM2	S 4e6a	59.9	—	54.4	65.3	3.4	—	4.5	3.1	6.0
		S 4a6e	54.8	—	175.1	55.2	4.0	—	12.0	4.4	3.8
		HC-1 5e	57.0	—	172.1	52.4	3.7	—	11.8	4.8	3.3
		HC-1 5a	63.0	—	50.7	68.7	3.0	—	5.1	2.8	6.1
		HC-2 5e	52.0	—	178.1	57.8	4.4	—	12.0	4.0	4.6
		HC-2 5a	55.2	—	58.1	62.2	4.0	—	4.0	3.5	6.3
	AM1	S 4e6a	52.4	—	39.9	76.8	4.3	—	6.7	2.1	5.3
		S 4a6e	48.5	—	165.1	48.4	4.8	—	11.4	5.4	4.6
		HC-1 5e	49.4	—	163.5	46.8	4.7	—	11.2	5.6	4.5
		HC-1 5a	53.3	—	38.4	78.2	4.2	—	6.9	2.1	4.6
		HC-2 5e	45.3	—	169.0	52.1	5.3	—	11.7	4.9	4.9
		HC-2 5a	45.8	—	45.1	71.9	5.2	—	5.9	2.5	6.6
trans-II	MM2	S 5e6e	178.0	—	177.3	57.0	10.8	—	12.0	4.2	3.7
		HC-1	174.1	—	173.6	53.6	10.7	—	11.9	4.6	3.9
		HC-2	176.5	—	179.3	59.8	10.8	—	12.0	3.8	3.3
	AM1	S 5e6e	174.9	—	164.2	47.6	10.7	—	11.3	5.5	4.2
		HC-1	176.5	—	162.4	45.9	10.8	—	11.1	5.8	4.2
		HC-2	166.0	—	167.8	50.9	10.3	—	11.6	5.0	3.6

---

* $\Sigma \Delta J| = |\Sigma(J_{\mathrm{exp}} - J_{\mathrm{calc}})|$. Experimental coupling constants [3]: *cis* I $^3J_{AX} = 7.6$ Hz, $^3J_{BX} = 4.5$ Hz, $^3J_{CX} = 3.5$ Hz; *trans* I $^3J_{AX} = 11.2$ Hz, $^3J_{BX} = 4.6$ Hz, $^3J_{CX} = 8.8$ Hz; *cis* II $^3J_{AX} = 3.6$ Hz, $^3J_{CX} = 8.8$ Hz, $^3J_{DX} = 4.6$ Hz; *trans* II $^3J_{AX} = 9.1$ Hz, $^3J_{CX} = 10.6$ Hz, $^3J_{DX} = 3.6$ Hz.

TABLE 4. Values of the Torsion Angles (deg) Corresponding to the Experimental Coupling Constants for Esters I and II

Comfiguration	I			II		
	φ_{AX}	φ_{BX}	$\varphi_{AX} \pm \varphi_{BX}$	φ_{CX}	φ_{DX}	$\varphi_{CX} \pm \varphi_{DX}$
*Cis**	140.5 (31)	53 (122)	87.5 (91)	145 (25)	54 (95)	91 (95)
Trans	172.0	52.0	120	157.5	61.0	96.5

* Two alternative sets of angles were determined for the *cis* isomers.

the distinguishing special feature of 1,3,2-oxazaborinanes is the planar configuration of the nitrogen atom, permitting maximum p–π-electron exchange along the B–N bond [1-5]. Consequently conformers with an axial N–H bond are absent (in the course of minimization such forms undergo rapid isomerization into a sofa form with the N–H bond coplanar with five atoms of the ring). This indicates objectively a reduction of the transition barrier between the different conformers, compared with oxazines IX and X, and an increase in the conformational variety for both *cis* and *trans* isomers of esters I and II.

A preferred sofa conformation was assigned previously to the *trans* isomers of 1,3,2-oxazaborinanes I and II and a 2,5-T conformation to the *cis* isomers on the basis of ^{1}H and ^{13}C NMR data [3]. The low probability for the existence of significant quantities of the latter (the most unstable form), which was evident after carrying out the calculations, makes it necessary to compare the optimum geometric parameters with the actual structure of the molecules of cyclic esters I and II. For this purpose calculated values of the coupling constants $^3J_{AX}$, $^3J_{BX}$, $^3J_{CX}$, and $^3J_{DX}$ were determined in the present work based on the torsion angles φ between the appropriate protons (optimal geometry data) using the equation from [26] and values of the electronegativity of the substituent groups from [27] (Table 3). Comparison with the experimental coupling constants [3] indicates the impossibility of choosing unequivocally one conformer either for the *cis* or the *trans* isomers. Not one of the sets of calculated constants, as $\Sigma|\Delta J|$ values show, correspond completely with the ^{1}H NMR data. This is mainly explained not by errors in the parametrization of the equation [26] and not by the absence of a correction for the effect of the medium (in each case calculations were for an isolated molecule in vacuum), but by the impossibility of realizing the torsion angles corresponding to the experimental coupling constants. In reality an empirical relationship exists for all values of φ for any conformer (Table 3), *viz.* $\varphi_{AX} + \varphi_{BX}$ (or $\varphi_{AX} - \varphi_{BX}$) and $\varphi_{CX} + \varphi_{DX}$ (or $\varphi_{CX} - \varphi_{DX}$) = 116.0-121.6°.

It is not difficult to see (Table 4) that angles established according to the equation from [26] and satisfying the experimental coupling constants, differ from those developed by the empirical relationship by 20-30° (with the exception of *trans* I). It therefore follows that the actual state of the ester molecules I and II corresponds to not one but several conformers in complete agreement with the calculated data. For the *trans* isomers the sofa S4e5e (S5e6e) predominates with a possible contribution of HC-1 and HC-2, but the *cis* isomers, in contrast to the results of [3], are characterized by a multicomponent equilibrium with the participation of the S4a5e (S5e6a), S4e5a (S5a6e), and a family of half-chair forms.

The investigated compounds therefore belong to a conformationally flexible system presuming the existence of significant quantities of geometrically nonequivalent forms in the vicinity of the minimum point [28,29]. The results obtained supplement the data base on the stereochemistry of 1,3,2-oxazaborinanes and afford the possibility to predict the conformational composition of molecules for these compounds with several chiral centers.

REFERENCES

1. A. R. Kalyuskii, V. V. Kuznetsov, Yu. E. Shapiro, S. A. Bochkor, and A. I. Gren', *Khim. Geterotsikl. Soedin.*, No. 10, p. 1424 (1990).
2. A. R. Kalyuskii, Authors summary of dissertation for candidate of chemical sciences, Odessa (1990).
3. A. R. Kalyuskii, V. V. Kuznetsov, O. S. Timofeev, and A. I. Gren', *Zh. Obshch. Khim.*, **60**, 2093 (1990).

4. A. P. Kalyuskii, V. V. Kuznetsov, and A. I. Gren', *Zh. Obshch. Khim.*, **61**, 1351 (1991).
5. A. R. Kalyuskii, V. V. Kuznetsov, Yu. E. Brusilovskii, V. Ya. Gorbatyuk, M. G. Glukhova, and A. I. Gren', *Zh. Org. Khim.*, **26**, 2498 (1990).
6. A. R. Kalyuskii, V. V. Kuznetsov, N. E. Kruglyak, I. V. Yudanova, L. P. Trigub, and A. I. Gren', Deposition in VINITI No. 1113-V90; *Ref. Zh. Khim.*, No. 11, B1095 (1990).
7. R. C. Bingham, M. J. S. Dewar, and D. H. Lo, *J. Am. Chem. Soc.*, **97**, 1294 (1975).
8. P. Birner and H. Hofmann, *Int. J. Quant. Chem.*, **21**, 833 (1982).
9. N. L. Allinger, *J. Am. Chem. Soc.*, **99**, 8127 (1977).
10. M. J. S. Dewar, E. G. Zoebisch, E. P. Healy, and J. J. P. Stewart, *J. Am. Chem. Soc.*, **107**, 3902 (1985).
11. M. J. S. Dewar, C. Jie, and E. G. Zoebisch, *Organometallics*, **7**, 513 (1988).
12. A. I. Gren' and V. V. Kuznetsov, *Chemistry of Cyclic Esters of Boric Acids* [in Russian], Naukova Dumka, Kiev (1988).
13. R. Seip and H. Seip, *J. Mol. Struct.*, **28**, 441 (1975).
14. W. J. Orville-Thomas (editor), *Internal Rotation in Molecules*, cited in [Russian translation], Mir, Moscow (1977), p. 373.
15. V. V. Kuznetsov, A. R. Kalyuskii, and A. I. Gren', *Khim. Geterotsikl. Soedin.*, No. 1, 106 (1996).
16. Yu. Yu. Samitov, B. V. Unkovskii, I. P. Boiko, O. I. Zhuk, and Yu. F. Malina, *Zh. Org. Khim.*, **9**, 193 (1973).
17. Yu. Yu. Samitov, O. I. Zhuk, B. V. Unkovskii, I. P. Boiko, and Yu. F. Malina, *Zh. Org. Khim.*, **9**, 201, (1973).
18. O. I. Danilova, Yu. Yu. Samitov, I. P. Boiko, T. O. Bordyukova, and B. V. Unkovskii, Deposition in ONIITEKhIM, No. 1056khp-D80; *Ref. Zh. Khim.*, No. 9, B329 (1981).
19. F. N. Latypova, V. V. Zorin, S. S. Zlotskii, D. L. Rakhmankulov, R. A. Karakhanov, M. Bartok, and A. Molnar, *Acta Phys. Chem.*, **27**, 87 (1981).
20. F. A. Alimirzoev, A. U. Stepanyants, F. N. Latypova, and B. V. Unkovskii, Deposition in ONIITEKhIM, No. 3093/79 dep; *Ref. Zh. Khim.*, No. 3, B325 (1980).
21. O. I. Danilova, Yu. Yu. Samitov, I. P. Boiko, T. O. Bordyukova, and B. V. Unkovskii, Deposition in ONIITEKhIM, No. 1055khp-D80; *Ref. Zh. Khim.*, No. 9, B330 (1981).
22. O. I. Danilova, Yu. Yu. Samitov, I. P. Boiko, T. O. Bordyukova, and B. V. Unkovskii, Deposition in ONIITEKhIM, No. 539, khp-D81; *Ref. Zh. Khim.*, No. 24, B392 (1981).
23. O. I. Danilova, Yu. Yu. Samitov, I. P. Boiko, and B. V. Unkovskii, Deposition in ONIITEKhIM, No. 1058 khp-D80; *Ref. Zh. Khim.*, No. 9, B328 (1981).
24. H. Booth and R. U. Lemieux, *Can. J. Chem.*, **49**, 777 (1971).
25. M. J. Cook, R. A. Y. Jones, A. R. Katritzky, M. M. Monas, A. C. Richards, A. J. Sparrow, and D. L. Trepanier, *J. Chem. Soc., Perkin Trans. 2*, No. 4, 325 (1973).
26. P. L. Durette and D. Horton, *Org. Magn. Res.*, **3**, 417 (1971).
27. M. L. Huggins, *J. Am. Chem. Soc.*, **75**, 4123 (1953).
28. O. V. Shishkin, A. S. Polyakova, Yu. T. Struchkov, and S. M. Desenko, *Mendeleev Commun.*, No. 5, 182 (1994).
29. O. V. Shishkin, *Izv. Russ. Akad. Sci., Ser. Khim.*, No. 12, 2095 (1997).