

Molecular and Crystal Structure of 1,10-Phenanthroline Complex with Nitrosonium Cation*

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Abstract—1,10-Nitroso-1,10-phenanthroline tetrafluoroborate was subjected to X-ray diffraction analysis. A distinctive feature of the complex is the NO group position between two nitrogen atoms of the phenanthroline skeleton, and so the complex may be regarded as belonging to bidentate type. The distance from the N atom of the group to the nitrogens of the skeleton are approximately equal (2.3 Å) and are considerably shorter than the average intermolecular contacts of the pair of nitrogen atoms N...N (3.0 Å). In the crystal two types of cations are present where the NO groups are oriented at angles 54 and 61° with respect to phenanthroline skeleton, and the length of N—O bonds is close to that in NO⁺ cation. The geometrical parameters of cation obtained by ab initio calculations are close to experimental data.

Nitrosonium complexes of organic compounds have been extensively studied for a long time [1], but the X-ray structural data of these complexes are scarce [2-11], and such studies on the complexes of nitrosonium cation with N-bases are lacking [1]. However the evidence on molecular structure of the latter is important for deeper understanding of mechanism of a number of significant organic reactions, for instance, of diazotization [12], nitrosation of amides [1] and heterocyclic compounds [13, 14], of denitrosation of nitrosamines [16] and of the other reactions [10, 17-20]. The data on the structure of nitrosonium complexes of N-heterocyclic compounds are important for understanding of the unique role of NO molecule and NO⁺ cation in biochemical processes [21-29].

The goal of this study was investigation of molecular and crystal structure of 1,10-phenanthroline **I** complex with nitrosonium tetrafluoroborate.

The structure of salt (**I**)-NO⁺BF₄⁻ is built up from cations and tetrahedral anions BF₄⁻ (Figs. 1, 2). In the unit cell are present two crystallographically independent pairs cation-anion with similar values of bond lengths and bond angles (Table 1). Cations in the crystal form stacks with interplanar distance 3.4 Å and anions are localized between them.

The list of shortened interatomic contacts is as follows: N¹¹...F⁴ 2.67, N¹¹...F⁴ (-x, 1-y, 1-z) 2.87, N¹¹...F³ (0.5+x, 1.5-y, -0.5+z) 2.82, H⁵...F¹ (-0.5+x, 1.5-y, -0.5+z) 2.36, H⁷...F³ (-x, 2-y, 1-z) 2.42, H⁵...F¹ 2.47, H⁶...F⁴ (-x, 2-y, 1-z) 2.50, H⁹...F³ (0.5+x, 1.5-y, -0.5+z) 2.51 Å (cf. [30]). A specific feature of the complex consists in

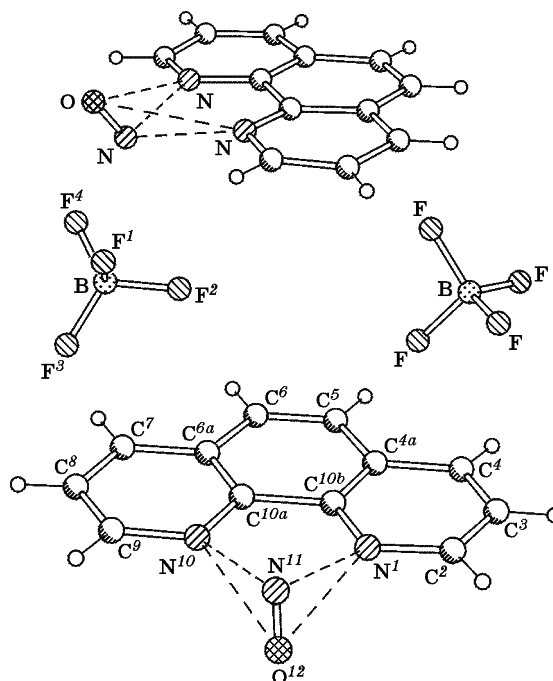


Fig. 1. Molecular structure of phenanthroline complex with NO⁺BF₄⁻.

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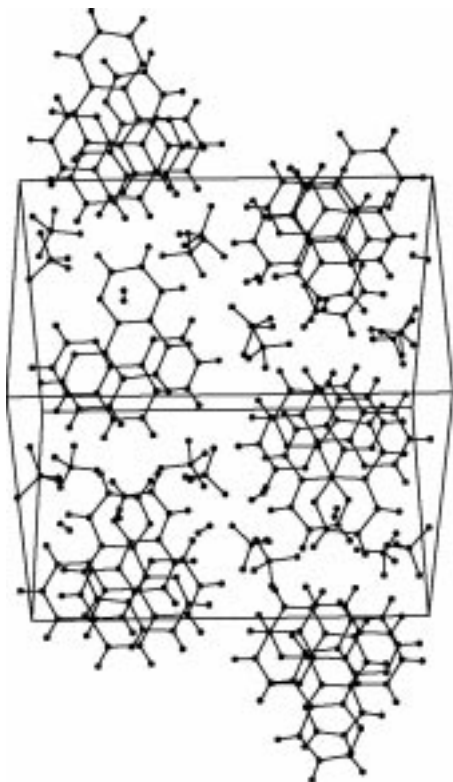


Fig. 2. Spatial position of cations and anions in the crystal of complex (I)-NO⁺ BF₄⁻.

position of the NO groups: Each NO group is located between the nitrogen atoms of the phenanthroline skeleton. The distance from the nitrogen of the group to the nitrogens in the skeleton is approximately equal (Table 1) and considerably smaller than the average intermolecular contact value for the pair of atoms N...N (3.00 Å), whereas the distance from the oxygen of this group is close to the corresponding value for the atoms O...N (2.78 Å) [31]. This fact indicates the presence of a weak covalent bond between the nitrogen in the NO group and the corresponding nitrogens in the skeleton of a bidentate type complex. The NO groups are oriented at angles 54 and 61° with respect to phenanthroline skeleton, and the length of N–O bonds is close to that in NO⁺ cation (0.997 Å) [32], which is also consistent with the assumption that a weak covalent bond N–NO exists in the complex. The atoms of the phenanthroline skeleton are located in the same plane within ±0.02 Å.

The quantum-chemical calculations by AM1 procedure suggest that the most stable is an asymmetrical *p*-complex (I)-NO⁺ (IIA) [33]. Ab initio calculation with the use of 6-31G basis also indicate as preferable an asymmetrical structure (Table 1, 2) that is a local minimum situated by 14.6 kJ mol⁻¹

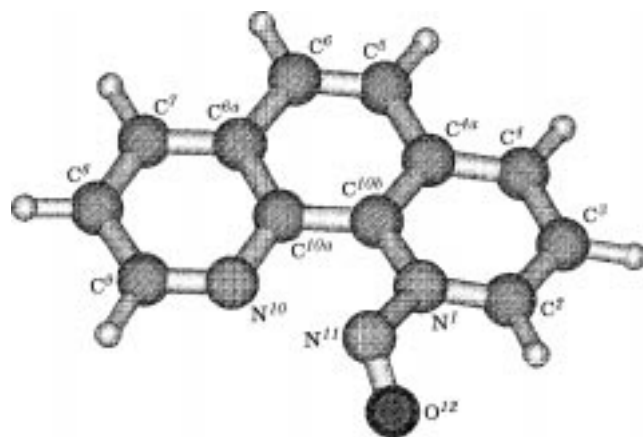


Fig. 3. Structure of asymmetrical complex of phenanthroline with nitronium cation (IIA) according to calculations RHF/6-31G.

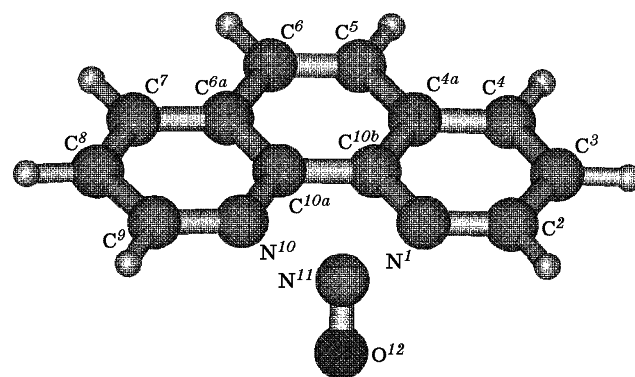


Fig. 4. Structure of symmetrical complex of phenanthroline with nitronium cation (IIC) according to calculations RHF/6-31G.

lower in energy as compared to a symmetrical complex (IIC) (Figs. 3, 4).

Analysis of the Hessian [34] revealed that at constraint by symmetry in the framework of point group C_s in the 6-31G basis the symmetrical complex is a local minimum on the potential energy surface (PES) and is placed by 12.4 kJ mol⁻¹ lower than the asymmetrical structure which is also a local minimum. Optimization with accounting for electron correlation (method MP2/6-31G) of the starting geometry (complex IIA, symmetry C_1) leads to a local minimum with a virtually symmetrical structure (IIC) (Table 1). Apparently the structure of the asymmetrical complex is not a minimum in the framework of MP2/6-31G method. The binding energy between cation NO⁺ and phenanthroline in the symmetrical complex (A_{NO^+}) is fairly large and depends on the chosen approximation (Table 2). All versions of calculations ab initio resulted in close geometrical parameters for symmetrical complex IIC that

Table 1. Values of some bond lengths (Å) and angles (deg) in the complex of 1,10-phenanthroline with nitrosonium cation obtained by X-ray analysis and *ab initio* calculations

Bond or angle	X-ray analysis		<i>Ab initio</i> ^a				
	cation 1	cation 2	IIIC (6-31G)	IIIC (6-31G*)	IIIC(MP2/6-31G)	IIIA (6-31G)	IIIA (6-31G*)
N ^I -C ²	1.301 (14)	1.364 (15)	1.316	1.305	1.356	1.334	1.323
N ^I -C ^{10b}	1.324 (13)	1.351 (13)	1.350	1.347	1.377	1.366	1.365
C ² -C ³	1.355 (16)	1.340 (17)	1.401	1.402	1.421	1.380	1.382
C ³ -C ⁴	1.405 (16)	1.370 (18)	1.371	1.365	1.402	1.380	1.374
C ⁴ -C ^{4a}	1.406 (16)	1.415 (17)	1.410	1.409	1.427	1.405	1.406
C ^{4a} -C ⁵	1.391 (15)	1.434 (16)	1.438	1.439	1.453	1.436	1.437
C ^{4a} -C ^{10b}	1.421 (15)	1.386 (14)	1.397	1.395	1.431	1.402	1.398
C ⁵ -C ⁶	1.361 (16)	1.364 (17)	1.347	1.341	1.382	1.347	1.342
C ⁶ -C ^{6a}	1.455 (15)	1.417 (17)	1.438	1.439	1.452	1.435	1.436
C ^{6a} -C ⁷	1.388 (15)	1.434 (18)	1.410	1.409	1.427	1.412	1.413
C ^{6a} -C ^{10a}	1.396 (14)	1.380 (15)	1.397	1.395	1.431	1.399	1.397
C ⁷ -C ⁸	1.348 (16)	1.330 (20)	1.371	1.365	1.402	1.367	1.361
C ⁸ -C ⁹	1.409 (16)	1.350 (20)	1.401	1.402	1.422	1.409	1.411
C ⁹ -N ¹⁰	1.315 (14)	1.346 (15)	1.316	1.305	1.357	1.310	1.298
N ¹⁰ -C ^{10a}	1.353 (12)	1.325 (13)	1.350	1.347	1.377	1.347	1.341
C ^{10a} -C ^{10b}	1.450 (14)	1.486 (16)	1.436	1.448	1.441	1.433	1.440
N ^I -C ¹¹	2.250 (17)	2.338 (20)	2.184	2.293	2.150	1.532	1.543
N ¹⁰ -N ¹¹	2.284 (17)	2.344 (21)	2.184	2.293	2.153	-	-
N ^I -N ¹²	2.758 (15)	2.727 (20)	2.749	2.820	2.828	-	-
N ¹⁰ -O ¹²	2.810 (15)	2.640 (19)	2.749	2.820	2.831	-	-
N ¹¹ -O ¹²	1.003 (15)	0.895 (14)	1.085	1.058	1.184	1.159	1.131
N ^I -N ¹¹ -O ¹²	110 (1)°	106 (1)°	109.8°	112.8°	112.8°	111.4°	110.8°
C ² -N ^I -C ^{10b}	120 (1)°	117 (1)°	120.6°	119.4°	120.6°	123.3°	123.0°

^a Calculations *ab initio* for symmetrical complex (IIIC) in versions 6-31G, 6-31G* are carried out under constraint by symmetry C_s.

Table 2. Full energy (*E*, a.u.^a) for phenanthroline (I), complexes (IIIC), (IIIA), and also affinity of phenanthroline to cation NO⁺ (A_{NO⁺}, kJ mol⁻¹)

Molecule	6-31G		6-31G		MP2/6-31G	
	<i>E</i>	A _{NO⁺}	<i>E</i>	A _{NO⁺}	<i>E</i>	A _{NO⁺}
I	-567.76479	-	-567.99518	-	-569.01788	-
IIIC	-696.67187	277.9	-696.98980	223.1	-698.22375	327.5
IIA ^b	-696.67743	292.5	-696.98506	210.7	-	-

^a 1 a.u. = 2625.5437 kJ mol⁻¹.

^b In MP2/6-31G approximation the structure IIIA apparently does not correspond to a minimum on the potential energy surface.

were similar to experimental data obtained by X-ray diffraction study (Table 1).

At accounting for electron correlation the values of bond lengths in the phenanthroline skeleton and NO group somewhat increase. The charge distribution in complexes (IIIC, IIIA) and phenanthroline molecule is presented in Table 3. It follows from the data in

Table 3 that the absolute value of charges in complex (IIIC) depends essentially of the chosen approximation. Both in symmetrical and asymmetrical complexes the NO group bears a significant fraction of the positive charge. In the framework of the RHF/6-31G method the shift of the electron density to the NO group is notably larger in asymmetrical complex (IIIA) than in symmetrical complex (IIIC).

Table 3. Charge distribution according to Mulliken in complexes (**II**C, **II**A) and phenanthroline (**I**) molecule obtained by *ab initio* calculation

Atom no.	II C (6-31G)	II A (6-31G)	II C (6-31G [*])	II A (6-31G [*])	II C (MP2/6-31G)	I (MP2/6-31G)
N ¹	-0.770	-0.983	-0.735	-0.700	-0.479	-0.520
C ²	0.152	0.292	0.120	0.189	0.069	0.062
C ³	-0.259	-0.289	-0.279	-0.300	-0.151	-0.241
C ⁴	-0.099	-0.044	-0.113	-0.064	-0.122	-0.148
C ^{4a}	-0.043	-0.125	-0.026	-0.059	0.049	-0.021
C ⁵	-0.138	-0.147	-0.185	-0.194	-0.125	-0.172
C ⁶	-0.138	-0.123	-0.185	-0.167	-0.124	-0.172
C ^{6a}	-0.043	-0.009	-0.026	-0.003	0.048	-0.021
C ⁷	-0.099	-0.125	-0.113	-0.132	-0.122	-0.148
C ⁸	-0.259	-0.234	-0.279	-0.255	-0.151	-0.241
C ⁹	0.152	0.105	0.120	0.099	0.069	0.062
N ¹⁰	-0.770	-0.591	-0.735	-0.619	-0.480	-0.520
C ^{10a}	0.292	0.184	0.337	0.292	0.191	0.169
C ^{10b}	0.292	0.561	0.368	0.440	0.193	0.169
N ¹¹	0.666	0.513	0.622	0.440	0.335	-
O ¹²	-0.013	-0.223	0.139	-0.163	0.052	-

A small energy difference between symmetrical and asymmetrical complexes as calculated by RHF/6-31G, RHF/6-31G^{*} and MP2/6-31G methods suggests that any of these complexes may prevail depending on the state of aggregation of the system. For instance, according to the data of ¹H, ¹³C, and IR spectroscopy in a liquid phase (solution in MeCN) the more stable is asymmetrical complex **II**A that undergoes fast in the NMR scale degenerate rearrangement by transfer of NO group from one nitrogen in the phenanthroline skeleton to another [33]. In the crystalline state symmetrical complex **II**C turned out to be more feasible, and the dynamic process apparently is frozen out [4, 35–38].

EXPERIMENTAL

In the study were used the following reagents: 1,10-phenanthroline of “pure for analysis” grade sublimed in a vacuum at 110–115°C, nitrosonium tetrafluoroborate Fluka of purum grade sublimed in a vacuum at 215–220°C, acetonitrile purified as in [39], thrice distilled over P₂O₅ and then over calcium hydride (water content <0.004%).

Salt **I**-NO⁺BF₄⁻ crystals were obtained by reaction of 1,10-phenanthroline (0.098 g, 0.55 mmol) with a salt NO⁺BF₄⁻ (0.065 g, 0.55 mmol) in MeCN (2 ml) at 20°C in dry box under argon with subsequent keeping in a sealed ampule at -15°C for 10 days.

The X-ray diffraction analysis was carried out on diffractometer Bruker P4 (MoK_α radiation, graphite monochromator, $\theta/2\theta$ -scanning, $2\theta < 45^\circ$ at temperature -35°C). Crystals of salt (**I**)-NO⁺BF₄⁻ monoclinic, space group *P*2₁/*n*, *a* 11.137 (1), *b* 18.608 (2), *c* 13.355 (5) Å, β 112.62 (2)°, *V* 2555 (1) Å³, [C₁₂H₈N₃O]⁺BF₄⁻ *M* 297.02, *Z* 8, *D*_c 1.544 g cm⁻³, μ 0.14 mm⁻¹, crystal habit 0.9×0.3×0.2 mm. Corrections were done on decrease in up to 93.9% of the intensity of control reflections and on absorption by integration procedure (transmission 0.94–0.98). The structure was solved using software Bruker-XTL, SHELXS-97 and was refined by the least-squares method in anisotropic approximation with the program SHELXL-97 till *wR*₂ 0.4802, *S* 1.568 for all independent 3158 reflections [*R*₁ 0.1619 for *F*_o > 4 σ (*F*)].*

The parameters of hydrogen atoms were taken into account in each refining cycle. The atom coordinates are given in Table 4 and are deposited in the Cambridge Structural Database.

The *ab initio* calculations were performed along restricted Hartree-Fock method (RHF) along GAMESS software [40]. After full optimization of structural geometry (up till gradient value 2×10^{-5} Hartree/Bohr) we calculated Hessian [34] to

* Large *R*₁ and *wR*₂ values are apparently due to insufficiently high quality of the crystal (the presence of a satellite, probable twinning).

Table 4. Coordinates of atoms ($\times 10^4$, Å) and equivalent isotropic factors ($\times 10^3$, Å²) for complex (I)-NO⁺BF₄⁻

Atom no.	x	y	z	U
N ¹	949 (9)	6950 (5)	6419 (7)	52 (3)
C ²	1656 (12)	7228 (7)	5936 (10)	61 (3)
C ³	1763 (12)	7947 (7)	5829 (10)	61 (3)
C ⁴	1131 (12)	8423 (8)	6283 (9)	68 (4)
C ^{4a}	349 (11)	8133 (6)	6796 (9)	52 (3)
C ⁵	-340 (11)	8555 (6)	7252 (9)	58 (3)
C ⁶	-1106 (11)	8259 (6)	7728 (9)	59 (3)
C ^{6a}	-1197 (10)	7482 (6)	7802 (8)	43 (3)
C ⁷	1981 (11)	7145 (8)	8255 (9)	63 (4)
C ⁸	-2038 (12)	6422 (7)	8270 (9)	59 (3)
C ⁹	-1315 (12)	6034 (6)	7786 (9)	56 (3)
N ¹⁰	-561 (8)	6328 (4)	7346 (7)	45 (2)
C ^{10a}	-504 (10)	7054 (5)	7352 (8)	43 (3)
C ^{10b}	284 (11)	7371 (6)	6820 (9)	47 (3)
N ¹¹	435 (15)	5777 (8)	6344 (12)	91 (4)
O ¹²	1213 (12)	5493 (7)	6815 (12)	104 (4)
B ¹	739 (19)	5928 (7)	3567 (13)	136 (12)
F ¹	2045 (17)	5973 (14)	3830 (2)	372 (17)
F ²	300 (2)	5572 (6)	2671 (11)	237 (10)
F ³	500 (2)	6615 (5)	3486 (10)	232 (9)
F ⁴	626 (10)	5617 (5)	4423 (7)	124 (14)
N ^{1'}	2504 (9)	6700 (5)	-458 (7)	59 (3)
C ^{2'}	2532 (13)	5968 (7)	-382 (10)	69 (4)
C ^{3'}	1868 (14)	5603 (8)	102 (11)	78 (4)
C ^{4'}	1131 (12)	5954 (8)	566 (10)	72 (4)
C ^{4a1}	1057 (11)	6712 (6)	504 (8)	47 (3)
C ^{5'}	303 (11)	7119 (8)	966 (10)	65 (4)
C ^{6'}	302 (13)	7851 (8)	912 (10)	71 (4)
C ^{6a'}	1028 (11)	8212 (6)	397 (9)	55 (3)
C ^{7'}	1046 (14)	8982 (8)	331 (11)	75 (4)
C ^{8'}	1786 (17)	9267 (9)	-144 (13)	94 (5)
C ^{9'}	2483 (13)	8874 (8)	-575 (10)	70 (4)
N ^{10'}	2469 (9)	8150 (5)	-555 (7)	55 (3)
C ^{10a'}	1760 (11)	7848 (6)	-69 (8)	49 (3)
C ^{10b'}	1778 (11)	7050 (6)	-4 (8)	48 (3)
N ^{11'}	3935 (18)	7405 (7)	-938 (13)	96 (5)
O ^{12'}	3595 (15)	7434 (8)	-1663 (12)	117 (5)
B ^{1'}	-431 (14)	9389 (7)	2840 (12)	71 (5)
F ^{1'}	-1238 (12)	8912 (7)	2123 (12)	201 (7)
F ^{2'}	227 (13)	9011 (9)	3740 (11)	212 (8)
F ^{3'}	-1203 (9)	9900 (4)	2995 (8)	119 (3)
F ^{4'}	382 (9)	9629 (4)	2414 (7)	109 (3)

determine the type of critical points on the potential energy surface. In the calculations were used bases 6-31G and 6-31G*. The electron correlation was accounted for in the framework of MP2 procedure.

REFERENCES

- Borodkin, G.I. and Shubin, V.G., *Usp. Khim.*, 2001, vol. 70, no. 3, pp. 241–261.
- Mamatyuk, V.I., Detsina, A.N., Nagi, Sh.M., Gatilov, Yu.V., Borodkin, G.I., and Mudrakovskii, I.L., Abstracts of Papers, *III Vsesoyuznoe soveshchanie "Spektroskopiya koordinatsionnykh soedinenii"* (3rd All-Union Meeting on Spectroscopy of Coordinated Compounds), Krasnodar, 1984.
- Brownstein, S., Gabe, E., Lee, F., and Tan, L.A., *Chem. Commun.*, 1984, no. 23, pp. 1566–1568.
- Borodkin, G.I., Nagi, Sh.M., Gatilov, Yu.V., Mamatyuk, V.I., Mudrakovskii, I.L., and Shubin, V.G., *Dokl. Akad. Nauk SSSR*, 1986, vol. 288, no. 6, pp. 1364–1369.
- Brownstein, S., Gabe, E., Lee, F., and Piotrowski, A., *Canad. J. Chem.*, 1986, vol. 64, no. 8, pp. 1661–1667.
- Kim, E.K. and Kochi, J.K., *J. Am. Chem. Soc.*, 1991, vol. 113, no. 13, pp. 4962–4980.
- Kim, E.K. and Kochi, J.K., *J. Org. Chem.*, 1993, vol. 58, no. 3, pp. 786–792.
- Rathore, R., Lindeman, S.V., and Kochi, J.K., *J. Am. Chem. Soc.*, 1997, vol. 119, no. 40, pp. 9393–9404.
- Rathore, R. and Kochi, J.K., *J. Org. Chem.*, 1998, vol. 63, no. 24, pp. 8630–8631.
- Rathore, R., Lindeman, S.V., Rao, K.S.S.P., Sun, D., and Kochi, J.K., *Angew. Chem.*, 2001, vol. 112, no. 12, pp. 2207–2211.
- Lindeman, S.V., Bosch, E., and Kochi, J.K., *J. Chem. Soc., Perkin Trans. II*, 2001, no. 9, pp. 1919–1923.
- Williams, D.L.H., *Nitrosation*, Cambridge: Cambridge University Press, 1988, pp. 77–149.
- Castro, A., Iglesias, E., Leis, J.R., Pena, M.E., Tato, J.V., and Williams, D.L.H., *J. Chem. Soc., Perkin Trans. II*, 1986, no. 8, pp. 1165–1168.
- Loeppky, R.N. and Cui, W., *Tetrahedron Lett.*, 1998, vol. 39, no. 14, pp. 1845–1848.
- Loeppky, R.N., Bao, Y.T., Bae, J., Yu, L., and Shevlin, G., *Nitrosamines and Related N-Nitroso Compounds. Chemistry and Biochemistry*, Loeppky, R.N. and Michejda, C.J., Eds., Washington: American Chemical Society, 1994, pp. 52–65.
- Williams, D.L.H., *Nitrosamines and Related N-Nitroso Compounds. Chemistry and Biochemistry*, Loeppky, R.N. and Michejda, C.J., Eds., Washington: American Chemical Society, 1994, pp. 66–73.
- Freitas, M.A., O'Hair, R.A.J., Schmidt, J.A.R., Tichy, S.E., Plashko, B.E., and Williams, T.D., *J. Mass Spectrom.*, 1996, vol. 31, no. 10,

- pp. 1086–1092.
18. Morkovnik, A.S., Dobaeva, L.N., and Okhlobystin, O.Yu., *Zh. Obshch. Khim.*, 1988, vol. 58, no. 9, pp. 2174–2175.
 19. York, C., Prakash, G.K.S., Wang, Q., and Olah, G.A., *Synlett.*, 1994, no. 6, pp. 425–426.
 20. Cai, H. and Fishbein, J.C., *J. Am. Chem. Soc.*, 1999, vol. 121, no. 9, pp. 1826–1833.
 21. Butler, A.R., *Chem. Ind.*, 1995, pp. 828–830.
 22. Stamler, J.S. and Feelisch, M., *Methods in Nitric Oxide Research*, Feelisch, M., and Stamler, J.C., Chichester: John Wiley and Sons, 1996, pp. 19–27.
 23. Murad, F., *Angew. Chem., Int. Ed.*, 1999, vol. 38, no. 13/14, pp. 1857–1868.
 24. Furchgott, R.F., *Angew. Chem., Int. Ed.*, 1999, vol. 38, no. 13/14, pp. 1871–1880.
 25. Ignarro, L.J., *Angew. Chem., Int. Ed.*, 1999, vol. 38, no. 13/14, pp. 1883–1892.
 26. Lipton, S.A., Chol, Y.-B., Pan, Z.-H., Lel, S.Z., Chen, H.-S.V., Sucher, N.J., Loscalzo, J., Singel, D.J., and Stamler, J.S., *Nature*, 1993, vol. 364, no. 6438, pp. 626–632.
 27. Stamler, J.S., Singel, D.J., and Loscalzo, J., *Science*, 1992, vol. 258, no. 5090, pp. 1898–1902.
 28. Kirchner, J.J., Sigurdsson, S.T., and Hopkins, P.B., *J. Am. Chem. Soc.*, 1992, vol. 114, no. 11, pp. 4021–4027.
 29. Elcock, A.H., Lyne, P.D., Mulholland, A.J., Nandra, A., Richards, W.G., *J. Am. Chem. Soc.*, 1995, vol. 117, no. 16, pp. 4706–4707.
 30. Zefirov, Yu.V. and Zorkii, P.M., *Zh. Strukt. Khim.*, 1980, vol. 21, no. 4, pp. 150–155.
 31. Zefirov Yu.V., Zorkii P.M., *Zh. Strukt. Kh.*, 1976, vol. 17, no. 6, pp. 994–998.
 32. Barbier, P., Mairesse, G., Wignacourt, J.P., and Baert, F., *Cryst. Struct. Commun.*, 1976, vol. 5, pp. 633–637.
 33. Andreev, R.V., Borodkin, G.I., and Shubin, V.G., *Zh. Org. Khim.*, 2001, vol. 37, no. 1, pp. 151–153.
 34. Minkin, V.I., Simkin, B.Ya., Minyaev, R.M., *Kvantovaya khimiya organicheskikh soedinenii. Mekhanizmy reaktsii* (Quantum Chemistry of Organic Compounds Reaction Mechanisms), Moscow: Khimiya, 1986, pp. 10–60.
 35. Borodkin, G.I., Nagy, S.M., Mamatyuk, V.I., Shukirov, M.M., and Shubin, V.G., *Chem. Commun.*, 1983, no. 24. 1533–1535.
 36. Borodkin, G.I., Nagi, Sh.M., Gatilov, Yu.V., and Shubin, V.G., *Dokl. Akad. Nauk SSSR*, 1985, vol. 280, no. 4, pp. 881–884.
 37. Mefed, A.E., Nagi, Sh.M., Borodkin, G.I., Mamatyuk, V.I., and Shubin, V.G., *Dokl. Akad. Nauk SSSR*, 1987, vol. 297, no. 1, pp. 133–136.
 38. Borodkin, G.I., Nagi, Sh.M., Gatilov, Yu.V., Shukirov, M.M., Rybalova, T.V., and Shubin, V.G., *Zh. Org. Khim.*, 1992, vol. 28, no. 9, pp. 1806–1826.
 39. Gordon, A.J. and Ford, R.A., *Chemist's Companion: A Handbook of Practical Data, Techniques, and References*, New York: John Wiley & Sons, 1973.
 40. Schmidt, M.W., Baldrige, K.K., Boatz, J.A., Elbert, S.T., Gordon, M.S., Jensen, J.H., Koseki, S., Matsunaga, N., Ngugen, K.A., Su, S.J., Widus, T.L., Dupuis, M., and Montgomery, J.A., *J. Comput. Chem.*, 1993, vol. 14, no. 11, pp. 1347–1363.