RESEARCH



Molecular structure of 3-cyano-4-azido-1,2,5-oxadiazole 2-oxide studied by means of gas electron diffraction and quantum chemical calculations

N. V. Lobanov^{1,2} · A. N. Rykov¹ · A. V. Stepanova¹ · D. A. Kalugin¹ · A. A. Larin³ · L. L. Fershtat³ · I. F. Shishkov¹

Received: 16 September 2024 / Accepted: 17 October 2024 © The Author(s), under exclusive licence to Springer Science+Business Media, LLC, part of Springer Nature 2024

Abstract

For the first time, structure of the 3-cyano-4-azido-1,2,5-oxadiazole 2-oxide (3-cyano-4-azidofuroxan, CAziFO) molecule in the gas phase was studied by means of gas electron diffraction (GED) and quantum chemical calculations. Equilibrium parameters of the molecule were found. The data obtained were compared with those of related compounds studied using gas electron diffraction and X-ray diffraction. It was demonstrated that the best agreement with experiment was obtained at the B3LYP/aug-cc-pVTZ level of theory. The information obtained on the molecular structure of free CAziFO will be useful for structural studies of compounds containing furoxan fragments.

Keywords Equilibrium structure \cdot Molecular structure \cdot 3-Cyano-4-azidofuroxan \cdot Oxadiazoles \cdot Furoxans \cdot Gas electron diffraction \cdot Quantum chemical calculations

Introduction

Furoxans (1,2,5-oxadiazole 2-oxides) are referred to as heterocyclic compounds with a unique set of functional properties [1, 2]. Furoxan derivatives may serve as precursors for creation of high-energy materials [3, 4] and are also of urgent interest in medicinal chemistry. In a latter case, furoxans correspond to a subclass of exogenic nitric oxide (NO) donors. NO plays a crucial role as a necessary link in various physiological processes, cytostatic agent, neurotransmitter, and activator of soluble form of guanylate cyclase. Therefore, in-depth structural studies of furoxan derivatives as NO-donors are of highly importance [5, 6].

At the same time, synthesis and development of new functional organic materials became a hot research topic in recent years with a special emphasis on high-energy density materials (HEDM) [7–9]. Since the theoretical principles for choosing such substances are very vague, their actual testing in practice seems quite logical. However, such an approach faces a number of difficulties: at least tens of kilograms of the proposed substance are needed to conduct bench tests; as a consequence, the connection must be made industrially; for a single promising substance, it is too expensive to create a pilot plant. The way out of this situation is to use methods of statistical thermodynamics to assess the efficiency of proposed fuels, which should initially be based on the physical and chemical characteristics of the substances proposed as potential fuels. Recently, considerable interest has been focused on the development and synthesis of new energetic compounds that are a combination of aromatic nitrogen-oxygen heterocycles and energetic functional groups such as NO₂, N₃, NHNO₂, N=N, and N=N(O) as substituents [10]. In this regard, 1,2,5-oxadiazole (furazan) and its N-oxide (furoxan) have attracted considerable attention due to their high positive enthalpies of formation (196.8) and 198.5 kJ/mol, respectively) and the huge nitrogen-oxygen content within the core. In addition, functionalization of the 1,2,5-oxadiazole ring makes it possible to obtain energetic materials with high density and improved properties [11, 12]. In this regard, 3-cyano-4-azido-1,2,5-oxadiazole 2-oxide (3-cyano-4-azidofuroxan molecule, CAziFO) (Fig. 1) is one of the interesting representatives of furoxan

N. V. Lobanov Lnw94@yandex.ru

¹ Chemistry Department, Lomonosov Moscow State University, Moscow 119991, Russia

² Joint Institute for High Temperatures, Russian Academy of Sciences, Moscow 125412, Russia

³ Zelinsky Institute of Organic Chemistry of Russian Academy of Sciences, Moscow 119991, Russia



Fig.1 Atom numbering in 3-cyano-4-azidofuroxan molecule (CAziFO)

series. Due to its structure, it gives possibilities for perspective syntheses of high-performance energetic materials.

The work aims to determine the equilibrium structure of the CAziFO molecule in the absence of intermolecular interactions in the gas phase by gas-phase electron diffraction (GED) and quantum chemical calculations and to compare the GED and single-crystal X-ray diffraction (XRD) results with the reported ones on the molecular structures of a number of related compounds.

Experiment

Table 1 Conditions of GED

experiment

GED

A sample of 3-cyano-4-azidofuroxan used in this work was obtained from the Laboratory of nitrogen compounds of Zelinsky Institute of Organic Chemistry (purity of sample is better than 99%). The spectral data (supplementary materials, Figures S1, S2) are fully consistent with the structure of the target compound. The GED experiment was carried out on an EG-100 M apparatus (Faculty of Chemistry, Moscow State University) for two nozzle-to-plate distances: short (SD) and long (LD). For each distance, a GED pattern was recorded on three plates (an accelerating voltage of 60 kV was used to generate the electron beam with a wavelength λ of about 0.05 Å), and the electron wavelengths were refined by the experiment with the standard substance (CCl₄) conducted at room temperature (25 °C). Full information on the experiment is given in Table 1.

All GED patterns were recorded on MACO EM-FILM EMS films and scanned on an Epson Perfection 4990 scanner. The scanner was calibrated using a Standard IT8 Target (ISO 12641–1 compliant 1997) (Fuji transparency Individually measured Target) on a gray scale. The GED patterns were converted into the intensity curves (Fig. 2) and radial distribution curve (Fig. 3) using UNEX [13].



Fig. 2 Molecular intensity curves sM(s) for the long (LD) and short (SD) nozzle–plate distances for the CAziFO molecule. The experimental values are depicted by circles, and the theoretical sM(s) are shown by solid line. The $\Delta sM(s) = sM(s)_{exp} - sM(s)_{theor}$ differences are also shown

Parameter	Units	Short distance (SD)	Long distance (LD)
"Nozzle-to-plate" distance, D	[mm]	193.9	362.3
Accelerating voltage, U	[kV]	60	60
Electron beam current I	[µA]	1.5	2.0
Wavelength λ , Å	[Å]	0.05621	0.05095
Nozzle temperature T	[K]	318	318
Residual pressure P	[mm Hg]	4.0×10^{-5}	4.0×10^{-5}
Exposition <i>t</i>	[sec]	40, 60, 80	25, 20, 20
Range of scattering intensities ^{ab}	$[Å^{-1}]$	6.6–31.2	3.4–20.0

 ${}^{a}s = 4\pi\lambda^{-1}\sin(\theta/2)$, where θ is the scattering angle; λ is he electron wavelength ${}^{b}A$ step on the scale *s* is 0.2 Å⁻¹



Fig. 3 Experimental (circles) and theoretical (solid line) radial distribution curves f(r) for CAziFO and their differences $\Delta f(r) = f(r)_{exp} - f(r)_{theor}$

QC calculations

Quantum chemical calculations were performed by means of Gaussian 09 [14] using the DFT method with B3LYP density functional [15, 16] and perturbation theory MP2 [17] with basis sets 6-31G(d,p) [18], cc-pVTZ [19], and aug-cc-pVTZ [20] and also using method CCSD [21] with basis set 6-31G(d,p) [22]. For CAZiFO parameter determination, the complete geometry optimization was performed. The numbering of atoms in the molecule studied is shown in Fig. 1.

Cartesian coordinates of atoms for optimized geometry of CAziFO by means of CCSD/6-31G(d,p), B3LYP/cc-pVTZ, and MP2/cc-pVTZ levels of theory are shown in Supplementary Materials (Tables S1, S2, S3).

The molecular model of CAziFO was described by a set of 20 independent geometrical parameters including 11 bond lengths and 9 angles, which are listed in Table 2. The structural parameters discussed were refined during analysis: except O1–N5 and C3–C7, all bond lengths were refined in different groups (Table S4).

To generate a consistent r_e structure from GED research with molecular parameters directly compared with that from QC data, cubic force fields at B3LYP/6-31G(d,p) level of theory were calculated (Table S5) and used to obtain anharmonic vibrational corrections to the internuclear distances [23], as well as vibrational amplitudes by applying VibModule program [24]. Natural bond orbital (NBO) as well as Wiberg bond index calculations for all species were performed within B3LYP/aug-cc-pVTZ level of theory in the frame of NBO 7.0 software [25].

Results and discussion

Table 2 shows the optimized equilibrium parameters of CAziFO obtained from various quantum chemical calculations, which are compared with the values obtained during the electron diffraction experiment. The most significant differences between the experimental and calculated bond lengths were found for the r(O1-N2) and r(O1-N5)bonds (see Table 2). All quantum chemistry methods overestimate the value of the r(O1-N2) bond by approximately 0.03-0.04 Å (except for CCSD/6-31G(d,p), which underestimates the value of the bond by almost 0.01 Å), and the values of the (O1-N5) bonds are exceeded by approximately 0.02-0.06 Å, with the closest results to the experimental those observed for B3LYP/aug-cc-pVTZ and CCSD/6-31G(d,p).

For the values of bond angles and torsion angles, CCSD/6-31G(d,p) gives satisfactory results, almost corresponding to the experimental those within the expected errors of the GED method. However, angles formed by heteroatoms (such as < (O1–N5–C4) and < (O1–N2–O6)) are better reproduced by the MP2/aug-cc-pVTZ level of theory.

A distortion of the five-membered ring, which is often observed in substituted furoxans, was also found for the studied CAziFO molecule.

Herein, we also performed comparison of structural parameters of CAziFO with analogous values closely related and previously investigated by our team furoxan derivatives, 3,4-dicyanofuroxan [26] and 3-cyano-4-aminofuroxan [27], which were obtained using gas electron diffraction, and also with unsubstituted furoxan in solid state. The results are

Table 2Structural parametersof CAziFO

Parameter	GED ^a	B3LYP		MP2		CCSD	
		/cc-pVTZ	/aug-cc-pVTZ	/cc-pVTZ	/aug-cc-pVTZ	/6-31G(d,p)	
Independent parameters							
$r_{\rm e}({\rm O1-N2})$	1.416(6) ¹	1.441	1.440	1.439	1.464	1.408	
$r_{\rm e}({\rm N2}={\rm C3})$	$1.345(16)^2$	1.342	1.341	1.326	1.350	1.339	
$r_{\rm e}(\rm C3-C4)$	$1.418(11)^3$	1.424	1.424	1.393	1.406	1.433	
$r_{\rm e}({\rm C4}{=}{\rm N5})$	$1.319(8)^4$	1.302	1.302	1.332	1.321	1.308	
$r_{\rm e}({\rm O1-N5})$	1.343(3) ⁵	1.375	1.376	1.397	1.347	1.390	
$r_{\rm e}({\rm N2-O6})$	$1.224(4)^{6}$	1.200	1.201	1.250	1.210	1.218	
$r_{\rm e}(\rm C3-C7)$	1.399(3) ⁵	1.404	1.405	1.407	1.407	1.421	
$r_{\rm e}({\rm C7}\equiv{\rm N8})$	$1.158(16)^7$	1.152	1.152	1.159	1.174	1.168	
$r_{\rm e}({\rm C4-N9})$	1.429(8)8	1.381	1.381	1.396	1.386	1.397	
$r_{\rm e}({\rm N9}{=}{\rm N10})$	1.227(12) ⁹	1.244	1.244	1.246	1.244	1.264	
$r_{\rm e}({\rm N10} = {\rm N11})$	$1.148(3)^{10}$	1.120	1.119	1.140	1.146	1.135	
<(O1–N2–C3)	108.7(6) ¹¹	106.3	106.4	107.9	104.8	107.3	
<(N2–C3–C4)	104.4(12) ¹²	106.5	106.5	106.7	107.5	106.1	
<(C3–C4–N5)	111.8(4) ¹³	111.8	111.7	112.6	111.3	111.3	
<(O1–N5–C4)	$107.1(7)^{14}$	106.8	106.8	105.3	107.2	106.1	
<(N2–O1–N5)	108.0(6)15	108.7	108.7	107.5	109.2	109.1	
<(O1–N2–O6)	120.5(9) ¹⁶	118.9	118.9	116.5	119.2	118.8	
<(C3–N2–O6)	130.8(15) ¹⁷	134.8	134.8	135.6	136.0	133.8	
<(N2–C3–C7)	123.3(6)18	122.6	122.7	123.0	121.5	121.7	
<(C4–C3–C7)	132.1(8) ¹⁹	130.9	130.8	130.3	131.1	132.2	
Dependent parameters							
<(C3–C7–N8)	180.0(12)	178.9	178.9	179.1	179.2	177.8	
<(C4–N9–N10)	116.5(8)	116.6	116.5	115.2	114.6	115.0	
<(N9–N10–N11)	176.3(6)	171.9	171.9	178.4	172.2	170.5	
D(O1-N2-C3-C4)	$0.9(4)^{b}$	0.0	0.0	0.0	0.0	-0.4	
D(N2-O1-N5-C4)	$-0.9(2)^{b}$	0.0	0.0	0.0	0.0	-0.3	
D(C3-C4-N5-O1)	$0.7(4)^{b}$	0.0	0.0	0.0	0.0	-0.3	
D(C4-N9-N10-N11)	179.2(5) ^b	180.0	180.0	179.8	180.0	179.1	
R _f LD	7.1						
R _f SD	7.3						
R _f total	7.2						

Bond lengths in Å, bond angles in degrees, R_f in percent. Parameters with the same numerical superscript were refined in one group

^aErrors were determined as 3σ -LSM; i.e., they are equal to the triple standard deviation by LSM.

^bInitial approximation was determined at the B3LYP/6-31G(d,p) level of theory

shown in Table 3. Thus, the angle < (O1–N2–C3), corrected due to the electron-withdrawing cyano group, is approximately 1.5° greater, and the angle < (O1–N5–C4) near electron-withdrawing azido group is approximately 0.5° greater than that of the unsubstituted furoxan molecule. Thus, ring distortion in the CAziFO molecule directly correlates with the donor–acceptor properties of its substituents [28].

NBO analysis based on the B3LYP/aug-cc-pVTZ method showed that the substituents on the furoxan ring contribute to the overall conjugation of the π -electron system. If we compare CAziFO with

3-cyano-4-aminofuroxan, we can see that the values of the Wiberg indices decrease for all bonds by an average of 2–5%, with the exception of the index of the bond connecting the nitrogen of the azide group with the carbon in the oxadiazole ring, which increased by 2% (Fig. 4). The distribution of effective charges on the atoms is similar to the case of 3-cyano-4-aminofuroxan, although to a somewhat lesser extent due to increased electron delocalization. This suggests that the $-N_3$ functional group exhibits more pronounced electron-withdrawing properties compared to the amino group.

Table 3Comparison ofstructural parameters of furoxan,3-cyano-4-azidofuroxan(CAziFO), 3-cyano-4-aminofuroxan (CAFO) and3,4-dicyanofuroxan (DCFO)

Parameter ^a	Furoxan (XRD) [28]	CAziFO (GED)	CAFO (GED) [27]	DCFO (GED) [26]
$r_{\rm e}({\rm O1-N2})$	1.441	1.416(12)	1.415(12)	1.459(5)
$r_{\rm e}({\rm N2}={\rm C3})$	1.302	1.345(6)	1.340(3)	1.331(3)
$r_{\rm e}(\rm C3-C4)$	1.401	1.418(6)	1.430(6)	1.419(2)
$r_{\rm e}({\rm C4}{=}{\rm N5})$	1.292	1.319(12)	1.306(2)	1.299(3)
$r_{\rm e}({\rm O1-N5})$	1.379	1.343(12)	1.390(3)	1.367(5)
$r_{\rm e}({\rm N2-O6})$	1.240	1.224(15)	1.207(3)	1.199(4)
$r_{\rm e}(\rm C3-C7)$	_	1.399(5)	1.403(2)	1.399(2)
<(O1–N2–C3)	107.2	108.7(6)	106.7(3)	105.0(4)
<(N2–C3–C4)	107.2	104.4(12)	106.9(3)	107.1(6)
<(C3–C4–N5)	111.9	111.8(4)	110.9(2)	111.7(3)
<(O1–N5–C4)	106.6	107.1(7)	106.7(2)	107.9(3)
<(N2–O1–N5)	_	108.0(6)	108.8(3)	108.8(3)
<(O1–N2–O6)	116.4	120.5(9)	119.2(3)	119.3(6)
<(N2–C3–C7)	_	123.3(6)	123.4(5)	122.6(3)



Fig. 4 Wiberg indices and the effective atomic charges in the molecules of furoxan (a), DCFO (b), CAFO (c), and CAziFO (d)

Conclusion

In summary, using gas electron diffraction and quantum chemical calculations, the structure of the CAziFO molecule in the gas phase was studied and the equilibrium parameters of the target molecule were found for the first time. The obtained data were compared with similar parameters for related compounds studied using gas electron diffraction and X-ray diffraction. It was demonstrated that the best agreement with experiment was obtained at the CCSD/6-31G(d,p) and B3LYP/aug-cc-pVTZ level of theory. It has been shown that the presence of an azide group as a substituent, compared to 3-cyano-4-aminofuroxan, causes a distortion of the geometry of the target molecule, which is expressed in the shortening of the r(O1-N5) bond by 0.05 Å, as well as an increase in the valence angle < (O1–N2–C3) by 2.0°. The NBO analysis carried out at the B3LYP/aug-cc-pVTZ level of theory showed that the azide group is an acceptor of electron density and, as a result, concentrates part of the electron cloud on itself. Unlike 3-cyano-4-aminofuroxan, CAziFO is to a greater extent a conjugated π -electron system, since each substituent of the five-membered ring makes a significant contribution to the overall delocalization of the electron cloud.

Supplementary Information The online version contains supplementary material available at https://doi.org/10.1007/s11224-024-02403-4.

Author contribution N.V. Lobanov: conceptualization, investigation, GED experiment, methodology, software, and writing original draft. A.N. Rykov: GED experiment and resources. A.V. Stepanova: investigation, conceptualization, writing, review, and editing. D.A. Kalugin: writing original draft. A.A. Larin: resources. L.L. Fershtat: resources, writing, review, and editing. I.F. Shishkov: conceptualization, writing, review, editing, and supervision.

Funding N.V. Lobanov, A.N. Rykov, A.V. Stepanova, D.A. Kalugin, and I.F. Shishkov are grateful for the support of the work within the State Task "The molecular structure and supramolecular organization of individual substances, hybrid and functional materials" (CITIS number: 121031300090–2); N.V. Lobanov is grateful and also notes that the work was supported by the State Task for the Joint Institute for High Temperatures, Russian Academy of Sciences, 2024 (No. 075–00270-24–00, 27.12.2023). A.A. Larin and L.L. Fershtat are grateful to the Russian Science Foundation (project 23–43-00090) for the financial support of the synthetic part of this work.

Data availability No datasets were generated or analysed during the current study.

Declarations

Competing interests The authors declare no competing interests.

References

- Larin AA et al (2020) Pushing the energy-sensitivity balance with high-performance bifuroxans. ACS Appl Energy Mater 3(8):7764–7771. https://doi.org/10.1021/acsaem.0c01162
- 2. Larin AA, Fershtat LL (2022) Mendeleev Commun 32:703–713. https://doi.org/10.1016/j.mencom.2022.11.001
- Larin AA, Ananyev IV, Dubasova EV, Teslenko FE, Monogarov KA, Khakimov DV, He Chun-lin, Pang Si-ping, Gazieva GA, Fershtat LL (2022) Simple and energetic: novel combination of furoxan and 1,2,4-triazole rings in the synthesis of energetic materials. Energ Mater Front 3(3):146–153. https://doi.org/10.1016/j.enmf. 2022.08.002
- Larin AA, Degtyarev DD, Ananyev IV, Pivkina AN, Fershtat LL (2023) Linear furoxan assemblies incorporating nitrobifuroxan scaffold: en route to new high-performance energetic materials. Chem Eng J 470:144144. https://doi.org/10.1016/j.cej.2023. 144144
- Stevens J, Schweizer M, Rauhut G (2001) Toward an understanding of the furoxandinitrosoethylene equilibrium. J Am Chem Soc 123(30):7326–7333. https://doi.org/10.1021/ja010792c
- Fershtat LL, Zhilin ES (2021) Recent advances in the synthesis and biomedical applications of heterocyclic NO-donors. Molecules 26:5705. https://doi.org/10.3390/molecules26185705
- Barton LM, Edwards JT, Johnson EC, Eric J, Bukowski EJ, Rosario C, Sausa RC, Byrd EFC, Orlicki JA, Sabatini JJ, Baran PS (2019) Impact of stereo- and regiochemistry on energetic materials. J Am Chem Soc 141(32):12531–12535. https://doi.org/10. 1021/jacs.9b06961
- Zhao G, He C, Yin P, Imler GH, Parrish DA, Shreeve JM (2018) Efficient construction of energetic materials via nonmetallic catalytic carbon-carbon cleavage/oxime-release-coupling reactions. J Am Chem Soc 140(10):3560–3563. https://doi.org/10.1021/jacs. 8b01260
- Shaferov AV, Fershtat LL (2024) Energetic 1,2,4-oxadiazoles: synthesis and properties. Russ. Chem. Rev 93(2). https://doi.org/ 10.59761/RCR5109
- Gao H, Shreeve JM (2011) Azole-based energetic salts. Chem Rev 111(11):7377–7436. https://doi.org/10.1021/cr200039c
- Fershtat LL, Makhova NN (2020) 1,2,5-Oxadiazole-based highenergy-density materials: synthesis and performance. ChemPlusChem 85(1):13–42. https://doi.org/10.1002/cplu.201900542
- Larin AA, Muravyev NV, Pivkina AN, Suponitsky KYu, Ananyev IV, Khalimov DV, Fershtat LL, Makhova NN (2019) Assembly of tetrazolylfuroxan organic salts: multipurpose green energetic materials with high enthalpies of formation and excellent detonation performance. Chem - A Eur J 25(16):4225–4233. https://doi. org/10.1002/chem.201806378
- Vishnevskiy YV (2023) UNEX 1.7-56-gf0aacc7. https://unex. vishnevskiy.group. Accessed 21 Oct 2024
- Gaussian 09, Revision A.02, Frisch MJ, Trucks GW, Schlegel HB, Scuseria GE, Robb MA, Cheeseman JR, Scalmani G, Barone V, Petersson GA, Nakatsuji H, Li X, Caricato M, Marenich A, Bloino

J, Janesko BJ, Gomperts R, Mennucci B, Hratchian HR, Ortiz JV, Izmaylov AF, Sonnenberg JL, Williams-Young D, Ding F, Lipparini F, Egidi F, Goings J, Peng B, Petrone A, Henderson T, Ranasinghe D, Zakrzewski VG, Gao J, Rega N, Zheng G, Liang W, Hada M, Ehara M, Toyota K, Fukuda R, Hasegawa J, Ishida M, Nakajima T, Honda Y, Kitao O, Nakai H, Vreven T, Throssell J, Montgomery JA, Peralta JE Jr., Ogliaro F, Bearpark M, Heyd JJ, Brothers E, Kudin KN, Staroverov VN, Keith T, Kobayashi R, Normand J, Raghavachari K, Rendell A, Burant JC, Iyengar SS, Tomasi J, Cossi M, Millam JM, Klene M, Adamo C, Cammi R, Ochterski JW, Martin RL, Morokuma K, Farkas O, Foresman JB, Fox DJ, Gaussian, Inc., Wallingford CT (2016). https://gaussian. com/g09citation/

- Becke AD (1988) Density-functional exchange-energy approximation with correct asymptotic behavior. Phys Rev A 38(6):3098– 3100. https://doi.org/10.1103/physreva.38.3098
- Lee C, Yang W, Parr RG (1988) Development of the Colle-Salvetti correlation-energy formula into a functional of the electron density. Phys Rev B 37:785. https://doi.org/10.1103/PhysRevB.37.785
- Møller C, Plesset MS (1934) Note on an approximation treatment for many-electron systems. Physical Review 46:618. https://doi. org/10.1103/PhysRev.46.618
- 18 Petersson A, Bennett A, Tensfeldt TG, Al-Laham MA, Shirley WA, Mantzaris J (1988) A complete basis set model chemistry. I. The total energies of closed-shell atoms and hydrides of the first-row elements. J Chem Phys 89(4):2193–2218. https://doi.org/10. 1063/1.455064
- 19 Dunning TH (1989) Gaussian basis sets for use in correlated molecular calculations. I. The atoms boron through neon and hydrogen. J Chem Phys 90:1007–1023. https://doi.org/10.1063/1.456153
- 20 Kendall RA Jr, Dunning TH, Harrison RJ (1992) Electron affinities of the first-row atoms revisited. Systematic basis sets and wave functions. J Chem Phys 96:6796–6806. https://doi.org/10. 1063/1.462569
- Scuseria GE, Janssen CL, Schaefer HF (1988) An efficient reformulation of the closed-shell coupled cluster single and double excitation (CCSD) equations. J Chem Phys 89(12):7382–7387. https://doi.org/10.1063/1.455269
- Petersson A, Bennett A, Tensfeldt TG, Al-Laham MA, Shirley WA, Mantzaris J (1988) J Chem Phys 89(4):2193–2218. https:// doi.org/10.1063/1.455064
- Sipachev VA (2000) Anharmonic corrections to structural experiment data. Struct Chem 11:167–172. https://doi.org/10.1023/A: 1009217826943
- Vishnevskiy YV, Zhabanov YA (2015) New implementation of the first-order perturbation theory for calculation of interatomic vibrational amplitudes and corrections in gas electron diffraction. J Phys: Conf Ser 633:012076. https://doi.org/10.1088/1742-6596/ 633/1/012076
- 25 Glendening ED, Landis CR, Weinhold F (2019) NBO 7.0: new vistas in localized and delocalized chemical bonding theory. J Comput Chem 40(25):2234–2241. https://doi.org/10.1002/jcc.25873
- 26 Kolesnikova IN, Kolesnikov SV, Lobanov NV, Sharanov PY, Larin AA, Teslenko FE, Fershtat LL, Shishkov IF (2023) Molecular structure of 3,4-dicyanofuroxan studied by gas electron diffraction. Application of DFT theory and coupled cluster computations. Chem Phys Lett 829:140770. https://doi.org/10.1016/j. cplett.2023.140770
- Lobanov NV, Rykov AN, Stepanova AV, Larin AA, Fershtat LL, Shishkov IF (2024) Equilibrium molecular structure of 3-cyano-4-amino-1,2,5-oxadiazole-2-oxide in the gas phase. J Struct Chem 65(8):1603–1611. https://doi.org/10.1134/S0022476624080110
- 28 Pasinszki Tibor, Havasi Balázs, Hajgató Balázs, Westwood Nicholas P. C (2009) Synthesis, spectroscopy and structure of the parent furoxan (HCNO)₂. J Phys Chem A 113(1):170–176. https://doi. org/10.1021/jp810066r

Publisher's Note Springer Nature remains neutral with regard to jurisdictional claims in published maps and institutional affiliations.

Springer Nature or its licensor (e.g. a society or other partner) holds exclusive rights to this article under a publishing agreement with the author(s) or other rightsholder(s); author self-archiving of the accepted manuscript version of this article is solely governed by the terms of such publishing agreement and applicable law.

Lobanov Nikolay Valerievich engineer and junior researcher of Gas Electron Diffraction Scientific Laboratory of Lomonosov Moscow State University (Department of Chemistry) (119992, Russia, Moscow, Leninskie Gory, 1); junior researcher of Thermophysical Databases Laboratory (V.P. Glushko Thermocenter), Joint Institute for High Temperatures (JIHT) RAS (125412, Russia, Moscow, Izhorskaya str., 13). E-mail: lnw94@yandex.ru, ResearcherID: JCE-1800-2023, Scopus Author ID: 58312740100, ORCID: https://orcid.org/0000-0001-5172-746X

Rykov Anatoly Nikolaevich PhD (chemistry), leading researcher of Gas Electron Diffraction Scientific Laboratory of Lomonosov Moscow State University (Department of Chemistry) (119992, Russia, Moscow, Leninskie Gory, 1). E-mail: Rykovanatolii@gmail.com, Scopus Author ID: 7005825583

Stepanova Anna Valer'evna PhD (Phys.-Math.), researcher of Gas Electron Diffraction Scientific Laboratory of Lomonosov Moscow State University (Department of Chemistry) (119992, Russia, Moscow,

Leninskie Gory, 1). E-mail: avstepanova73@mail.ru, ORCID: https://orcid.org/0009-0004-2802-5362

Kalugin Danila Alekseevich student of Lomonosov Moscow State University (Department of Chemistry) (119992, Russia, Moscow, Leninskie Gory, 1). E-mail: den16009@yandex.ru, ORCID: https://orcid. org/0000-0002-7670-3648

Larin Alexander Alexandrovich PhD (Chemistry), senior researcher at the Laboratory of Nitrogen Compounds at N.D. Zelinsky Institute of Organic Chemistry, Russian Academy of Sciences (ZIOC RAS) (119991, Russia, Moscow, Leninsky prosp., 47). E-mail: roby3@mail. ru, ResearcherID: F-8368-2017, Scopus Author ID: 57188655453, ORCID: https://orcid.org/0000-0001-7862-2895

Fershtat Leonid Leonidovich D.Sc. (Chemistry), leading researcher, head of the Laboratory of Nitrogen Compounds at N.D. Zelinsky Institute of Organic Chemistry, Russian Academy of Sciences (ZIOC RAS) (119991, Russia, Moscow, Leninsky prosp., 47). E-mail: fershtat@bk.ru, ResearcherID: M-9653-2016, Scopus Author ID: 36457430400, ORCID: https://orcid.org/0000-0002-0203-1025

Shishkov Igor Fedorovich D.Sc. (Chemistry), leading researcher, head of the Gas Electron Diffraction Laboratory of Lomonosov Moscow State University (Department of Chemistry) (119992, Russia, Moscow, Leninskie Gory, 1). E-mail: igormg@mail.ru, ResearcherID: B-2578-2015, Scopus Author ID: 6701850450, ORCID: https://orcid.org/0000-0002-1132-1905