

Prof. Dr. Igor F. Shishkov

Prof. Dr. Leonid S. Khaikin

Prof. Dr. Natalja Vogt

Dr. Lyudmila V. Khristenko

Dr. N. M. Karasev

Dr. I. N. Kolesnikova

Dr. I. I. Marochkin

Dr. A. N. Rykov

Dr. E. P. Altova

N. F. Moiseeva

A. L. Vilkova

Department of Chemistry

Moscow State University

119992 GSP-2, Leninskiye gori 1, Moscow

Russia

Telephone: (+7) (95)939-26-37
 Telefax: (+7) (95)932-88-46
 E-Mail: IFShishkov@phys.chem.msu.ru
 khrist@phys.chem.msu.ru
 Iskhaikine@rambler.ru

Homepage:

C₃H₇NO₂	α-Alanine (2-aminopropanoic acid) The equilibrium structure by ED and QC <i>E. P. Altova, A. N. Rykov, L. V. Khristenko, E. Yu. L'vova, and I. F. Shishkov</i> Manuscript in preparation
C₃H₉SiNCSe	Silyl- and alkyl-pseudohalides X₃YNCZ (X = H or CH₃; Y = C or Si; Z = O, S, or Se) Quantum-chemical calculations for silyl- and alkyl-pseudohalides X ₃ YNCZ (X = H or CH ₃ ; Y = C or Si; Z = O, S, or Se) and electron diffraction study of the equilibrium molecular structure of (CH ₃) ₃ SiNCSe <i>L. S. Khaikin, O. E. Grikina, I. V. Kochikov, and N. F. Stepanov</i> Russ. J. Phys. Chem. A 88 (4) (2014), 657
C₄H₄O₃	Dihydro-2,5-furandione (succinic anhydride) Molecular structure and conformations by ED and QC <i>N. Vogt, E. P. Altova, D. N. Ksenafontov, and A. N. Rykov</i> Work in progress
C₄H₉NO₃	Threonine (2-amino-3-hydroxybutanoic acid) The equilibrium structure by ED and QC <i>D. S. Tikhonov, L. S. Khaikin, O. E. Grikina, and A. N. Rykov</i> Work in progress
C₄H₉NSeSi (CH ₃) ₃ Si-N=C=Se	Trimethylsilyl isoselenocyanate Calculated regularities for structure of pseudohalides X ₃ YNCZ (X = H, CH ₃ ; Y = C, Si; Z = O, S, Se) and equilibrium molecular structure of (CH ₃) ₃ SiNCSe by GED <i>L. S. Khaikin, O. E. Grikina, I. V. Kochikov, and N. F. Stepanov</i> Russ. J. Phys. Chem. A, 88 (4) (2014), 657
C₅H₄N₂O₄	Orotic acid (1,2,3,6-Tetrahydro-2,6-dioxo-4-pyrimidinecarboxylic acid) Molecular structure and conformations by ED and QC <i>N. Vogt, E. P. Altova, A. N. Rykov, and I. F. Shishkov</i> Work in progress
	Histamine (2-(1H-imidazol-4-yl)ethanamine)

C₅H₉N₃	The equilibrium structure by ED and QC <i>D. S. Tikhonov, L. S. Khaikin, O. E. Grikina, and A. N. Rykov</i> Work in progress
C₅H₁₀N₂O (CH ₃) ₂ NCH(CN)OCH ₃	(Cyanomethoxy)(dimethylamino)methane Molecular structure from GED data and quantum chemical calculations <i>E. P. Altova, R. G. Kostyanovsky, and I. F. Shishkov</i> Russ. J. Phys. Chem. A, 88 (4) (2014), 667
C₆H₃N₃O₆	1,3,5-Trinitrobenzene Analysis of electron diffraction data for several symmetric coordinates of large amplitude motion in the case of 1,3,5-trinitrobenzene molecule. <i>L. S. Khaikin, I. V. Kochikov, D. S. Tikhonov, and O. E. Grikina</i> Russ. J. Phys. Chem. A, in press
C₆H₇NO	Benzamide Equilibrium molecular structure from gas-phase electron diffraction and theoretical calculations <i>I. N. Kolesnikova, I. F. Shishkov, and I. Hargittai</i> Struct. Chem., in press
C₆H₁₂N₂ (CH ₂) ₆ N ₄	Urotropine Interpreting the vibrational spectra of -d ₀ and -d ₁₂ isotopomers by scaling the quantum-chemical force field <i>L. S. Khaikin, O. E. Grikina, I. V. Kochikov, and N. F. Stepanov</i> Russ. J. Phys. Chem. A, 88 (3) (2014), 450
C₆H₁₂N₂ (CH ₂) ₆ N ₄	Urotropine Equilibrium molecular structure by GED using data from quantum chemistry and vibrational spectroscopy <i>L. S. Khaikin, O. E. Grikina, N. M. Karasev, D. M. Kovtun, and I. V. Kochikov</i> Russ. J. Phys. Chem. A, 88 (4) (2014), 652
C₈H₁₁NO₃	4-[(1R)-2-amino-1-hydroxyethyl]benzene-1,2-diol (noradrenaline) Molecular structure and conformations by ED and QC <i>E. P. Altova, N. Vogt, A. N. Rykov, M. V. Popik, and I. F. Shishkov</i> Work in progress
C₉H₃F₉ C ₆ H ₃ (CF ₃) ₃	1,3,5-Tris(trifluoromethyl)benzene Molecular structure and conformation by ED and QC <i>I. N. Kolesnikova, O. V. Dorofeeva, N. M. Karasev, H. Oberhammer, and I. F. Shishkov</i> J. Mol. Struct., 1074 (2014), 196
C₉H₉Cl₂N₃	Clonidine (N-(2,6-dichlorophenyl)-4,5-dihydro-1H-imidazol-2-amine) Molecular structure and conformations by ED and QC <i>I. N. Kolesnikova, A. N. Rykov, L. V. Khristenko, and I. F. Shishkov</i> Work in progress
C₉H₁₃NO₃	(R)-4-(1-Hydroxy-2-(methylamino)ethyl)benzene-1,2-diol (adrenaline) Molecular structure and conformations by ED and QC <i>E. P. Altova, N. Vogt, A. N. Rykov, M. V. Popik, and I. F. Shishkov</i> Work in progress
C₁₁H₈O₂ CH ₃ -C ₁₀ H ₅ O ₂	Vitamin K3 (menadione) Quantum chemical calculations and electron diffraction study of equilibrium molecular structure (preliminary results) <i>L. S. Khaikin, D. S. Tikhonov, O. E. Grikina, A. N. Rykov, and N. F. Stepanov</i> Russ. J. Phys. Chem. A, 88 (5) (2014), 886