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$C_2H_5NO_2$ $O_2NCH_2CH_2OH$	**2-Nitroethanol** Intramolecular dynamics and equilibrium structure *D. M. Kovtun , I. V. Kochikov , A. A. Ivanov , and Yu. I. Tarasov* 15-th Eur. Symp. on GED, Germany, 2013, Abstracts, P. 24
$C_3H_7NO_2$ $CH_3CH(NH_2)COOH$	**α-Alanine** Molecular structure by GED and quantum chemical calculation. *E. P. Altova, A. N. Rykov, L. V. Khristenko, and I. F. Shishkov* 15-th Eur. Symp. on GED, Germany, 2013, Abstracts, P. 43
$C_3H_8N_4$ $(CH_3)_2NCH_2N_3$	**N-Azidomethyl-N,N-dimethylamine** Molecular structure from GED data and quantum chemical calculations. *E. O. Altova, O. G. Nabiev, N. M. Karasev, R. G. Kostyanovsky, L. S. Khaikin, and I. F. Shishkov* Mendeleev Commun., **23** (2013), 166
$C_4H_3FN_2O_2$	**5-Fluorouracil** Molecular structure by ED and QC *D. N. Ksenafontov, N. Vogt, and A. N. Rykov* Work in progress
$C_4H_4N_2O_2$ $C_4H_4N_2O_2$	**Uracil** Equilibrium molecular structure from GED data and coupled-cluster calculations. *N. Vogt, L. S. Khaikin, O. E. Grikina, and A. N. Rykov* J. Mol. Struct., **1050** (2013), 114
$C_4H_4O_3$	**Dihydro-2,5-furandione (succinic anhydride)** Molecular structure and conformations by ED and QC *N. Vogt, E. P. Altova, D. N. Ksenafontov, and A. N. Rykov* Work in progress
$C_4H_4O_5$	**Oxobutanedioic acid** Molecular structure and conformations by ED and QC *L. S. Khaikin, O. E. Grikina, and A. N. Rykov* Work in progress
$C_4H_9NO_2$	**4-Aminobutanoic acid** Molecular structure and conformations by ED and QC

$H_2N(CH_2)_3COOH$	*D. N. Ksenafontov, N. F. Moiseeva, A. N. Rykov, I. F. Shishkov, and H. Oberhammer* Work in progress
C_4H_9NSeSi $(CH_3)_3Si\text{-}N{=}C{=}Se$	**Trimethylsilyl isoselenocyanate** Calculated regularities for structure of pseudohalides X3YNCZ (X = H,CH3; Y = C,Si; Z = O,S,Se) and equilibrium molecular structure of (CH3)3SiNCSe by GED *L. S. Khaikin, O. E. Grikina, I. V. Kochikov, and N. F. Stepanov* Russ. J. Phys. Chem. A, **88** (2014), 663, in press
$C_5H_6N_2O_2$ $CH_3\text{-}C_4H_3N_2O_2$	**1-Methyluracil** r_a, r_e^{se}, r_e (best ab initio) structure by ED and quantum chemical calculations *N. Vogt, I. I. Marochkin, and O. V. Dorofeeva* J. Phys. Chem. A, **117** (2013), 11374
$C_5H_6O_2$	**Methoxyfuran** Structure of by GED and quantum-chemical calculations *I. F. Shishkov* 15-th Eur. Symp. on GED, Germany, 2013, Abstracts, P.9
C_5H_9NSe $(CH_3)_3CNCSe$	**tert-Butyl isoselenocyanate** Molecular structure by ED and QC *L. S. Khaikin, O. E. Grikina, and I. Hargittai* Work in progress
$C_5H_{10}N_2O$ $(CH_3)_2NCH(CN)OCH_3$	**(Cyanomethoxy)(dimethylamino)methane** Molecular structure from GED data and quantum chemical calculations *E. P. Altova, R. G. Kostyanovsky, and I. F. Shishkov* Russ. J. Phys. Chem. A, **88** (2014), 673, in press
$C_6H_3N_3O_6$ $C_6H_3(NO_2)_3$	**1,3,5-Trinitrobenzene** Some peculiarities of analysis for GED data with consideration of equivalence of large amplitude motion coordinates *I. V. Kochikov, L. S. Khaikin, D. S. Tikhonov, and O. E. Grikina* 15-th Eur. Symp. on GED, Germany, 2013, Abstracts, P. 55
$C_6H_5NO_2$ C_5H_4NCOOH	**Pyridine-3-carboxylic acid (nicotinic acid)** Molecular structure and conformations by ED and QC *I .I. Marochkin, N. Vogt, and A. N. Rykov* Work in progress
$C_6H_5NO_2$ C_5H_4NCOOH	**Pyridine-2-carboxylic acid (picolinic acid)** Molecular structure and conformations by ED and QC *I. N. Kolesnikova, N. Vogt, A. N. Rykov, and J. Vogt* Work in progress
$C_6H_8N_2O_2$	**1-Methylthymine** ra, rese, re (best ab initio) structure by ED and quantum chemical calculations *N. Vogt, I. I. Marochkin, I. F. Shishkov, and A. N. Rykov* Manuscript in preperation
$C_6H_{12}N_2$ $(CH_2)_6N_4$	**Urotropine** Interpreting the vibrational cpectra of –d0 and –d12 isotopomers by scaling the quantum-chemical force field *L. S. Khaikin, O. E. Grikina, I. V. Kochikov, and N. F. Stepanov* Russ. J. Phys. Chem. A, **88** (2014), 450, in press
$C_6H_{12}N_2$ $(CH_2)_6N_4$	**Urotropine** Equilibrium molecular structure by GED using data from quantum chemistry and vibrational spectroscopy *L. S. Khaikin, O. E. Grikina, N. M. Karasev, D. M. Kovtun, and I. V. Kochikov* Russ. J. Phys. Chem. A, **88** (2014), 658, in press

$C_7H_4F_4O$ $C_6H_4(OCF_3)F$	**m-Fluoro(trifluoromethoxy)benzene** Conformational composition by vibrational spectroscopy *L. V. Khristenko, V. M. Senyavin, B. V. Lokshin, A L. Vilkova, and I. F. Shishkov* Struct. Chem., (2013), in press
$C_7H_4F_4O$ $C_6H_4(OCF_3)F$	**o-Fluoro(trifluoromethoxy)benzene** Determination of conformational composition by vibrational spectroscopy *L. V. Khristenko, V. M. Senyavin, B. V. Lokshin, A. L. Vilkova, and I. F. Shishkov* Struct. Chem., (2013), in press
C_7H_7NO C_6H_5-NH-CHO	**Formanilide** Molecular structure and relative stability of trans and cis conformers from GED data and quantum chemical calculations *I. I. Marochkin and O. V. Dorofeeva* Struct. Chem., **24** (2013), 233
$C_8H_{11}NO_3$	**Noradrenaline** Structure by GED and quantum-chemical calculations *I. F. Shishkov* 15-th Eur. Symp. on GED, Germany, 2013, Abstracts, P.9
$C_8H_{11}NO_3$	**l-1-(3,4-Dihydroxyphenyl)-2-aminoethanol (noradrenaline)** Molecular structure and conformations by ED and QC *M. A. Abaev, A. N. Rykov, M. V. Popik, and I. F. Shishkov* Manuscript in preparation
$C_9H_3F_9$ $C_6H_3(CF_3)_3$	**1,3,5-Tris(trifluoromethyl)benzene** Molecular structure and conformation by ED and QC *O. V. Dorofeeva, I. N. Kolesnikova, I. F. Shishkov, and H. Oberhammer* Manuscript in preparation
$C_9H_{13}NO_3$	**(R)-4-(1-Hydroxy-2-(methylamino)ethyl)benzene-1,2-diol (adrenaline)** Molecular structure and conformations by ED and QC *E. P. Altova, N. Vogt, A. N. Rykov, M .V. Popik, and I. F. Shishkov* Work in progress
$C_{11}H_8O_2$ CH_3-$C_{10}H_5O_2$	**Vitamin K3 (menadione)** Quantum chemical calculations and electron diffraction study of equilibrium molecular structure (preliminary results) *L. S. Khaikin, D. S. Tikhonov, O. E. Grikina, A. N. Rykov, and N. F. Stepanov* Russ. J. Phys. Chem. A, **88** (2014), in press
$C_{12}H_{14}N_2O_2$ C_6H_5-C_4H_5ON-CH_2CONH_2	**Carphedon (Phenylpiracetam)** Molecular structure from GED data and quantum chemical calculations *D. N. Ksenafontov, N. F. Moiseeva, A. N. Rykov, I. F. Shishkov, and H. Oberhammer* Struct. Chem., **24** (2013), 171
	Development of iterative methods Iterative methods for calculations of extreme eigenvalues of large symmetric matrices *A. V. Mitin* Mathematical Modelling and Geometry, submitted
	Basis sets for atoms Ga through Kr Polarization functions for the modified m6-31G basis sets for atoms Ga through Kr *A. V. Mitin* J. Comput. Chem., **34** (2013), 2014
	Methyl derivatives of uracil

	Molecular structure study of some methyl derivatives of uracil by electron diffraction method and high-level ab initio calculations. *I. I. Marochkin, N. Vogt, A. N. Rykov, O. V. Dorofeeva, J. Vogt, and I. F. Shishkov* 15-th Eur. Symp. on GED, Germany, 2013, Abstracts, P. 59