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BeI₂	Beryllium diiodide Structure by GED/MS and QC (CCSD(T)) <i>S. A. Shlykov, Yu. A. Zhabanov, A. V. Zakharov, G. V. Girichev, N. I. Giricheva</i> Manuscript in preparation
Br₃Lu LuBr ₃	Lutetium tribromide Structure by GED/MS and QC <i>N. I. Giricheva, S. A. Shlykov, G. V. Girichev, E. V. Chernova and E. Lapykina</i> Zh. Strukt. Khim. 50 (2) (2009) 243-250
Br₃Y YBr ₃	Yttrium tribromide Structure by GED/MS and QC <i>N. I. Giricheva, S. A. Shlykov, G. V. Girichev, H. Oberhammer</i> Manuscript in preparation
Br₃Yb YbBr ₃	Ytterbium tribromide Structure by GED/MS and QC <i>N. I. Giricheva, S. A. Shlykov, G. V. Girichev, H. Oberhammer, A. V. Bardina, S. N. Ivanov, K. S. Krasnov</i> Manuscript in preparation
Br₄La⁻ LaBr ₄ ⁻	Lanthanum tetrabromide anion Mass-spectrometric study of vapors and structure by DFT calculation <i>M. F. Butman, V. V. Sliznev, L S. Kudin, D. A. Ivanov, V. B. Matalov, K. V. Cramer</i> Zh. Fiz. Khim. 82 (5) (2008) 885-890
CCl₄	Carbon tetrachloride Structure by GED and CCSD(T) calculations <i>A. V. Zakharov, Yu. A. Zhabanov</i> J. Mol. Struct., accepted
CN₂OS₂ S ₂ N ₂ OC	5-Oxo-1,3,2,4-dithiadiazole (Roesky's ketone) Rotational spectrum, rotational constants <i>F. Blockhuys, K. Tersago, S. A. Shlykov, A. Konrad, D. Christen</i> J. Mol. Struct., accepted
C₄Br₄S C ₄ Br ₄ S	Tetrabromothiophene Structure by GED/MS and QC <i>S. A. Shlykov, F. Blockhuys, Yu. Zhabanov</i> Proc. IV All-Russ. School Quant. Chem., Ivanovo, (2009) 288-291
C₄Br₄Se C ₄ Br ₄ Se	Tetrabromoselenophene Structure by GED/MS and QC <i>S. A. Shlykov, F. Blockhuys, Yu. Zhabanov</i> Proc. IV All-Russ. School Quant. Chem., Ivanovo, (2009) 288-291
C₄H₃FN₂O₂	5-Fluorouracil Structure by GED/MS and QC <i>V. A. Naumov, S. A. Shlykov, A. V. Potanin</i> Russ. J. Gen. Chem. 79 (3) (2009) 475-481

C₄H₅ClO₂ C ₄ H ₅ O ₂ Cl	1-Chloro-1,3-butanedione Tautomeric and conformational properties by ab initio study <i>N. V. Belova, H. Oberhammer, G. V. Girichev, S. A. Shlykov</i> <i>J. Phys. Chem. A.</i> 112 (14) (2008) 3209-3214
C₄H₅FO₂ H ₃ C-C(O)-CH ₂ -C(O)-F	Acetoacetyl fluoride Tautomeric and conformational properties by GED, IR(gas), Raman (liquid and solid), NMR spectroscopy and QC study; the geometric structure of the enol tautomer by GED and quantum chemical calculations in the gas phase and by X-ray in the crystal. <i>N. V. Belova, H. Oberhammer, X. Zeng, M. Gerken, H. Willner, R. Berger, S. A. Hayes, and N. W. Mitzel</i> <i>Phys. Chem. Chem. Phys.</i> , submitted
C₅H₄FNO₄S C ₅ H ₄ SO ₄ NF	2-Nitrobenzenesulfonyl fluoride Structure by GED/MS and QC <i>V. M. Petrov, G. V. Girichev, H. Oberhammer, V. N. Petrova, N. I. Giricheva, A. V. Bardina, S. N. Ivanov</i> <i>J. Mol. Struct.</i> , accepted
C₆H₄CINO₄S 2-NO ₂ -C ₆ H ₄ -SO ₂ Cl	2-Nitrobenzenesulfonyl chloride Structure by GED/MS and QC <i>V. M. Petrov, H. Oberhammer, N. I. Giricheva, G. V. Girichev, V. N. Petrova, S. N. Ivanov</i> Manuscript complete
C₆H₄CINO₄S 4-NO ₂ -C ₆ H ₄ -SO ₂ Cl	4-Nitrobenzenesulfonyl chloride Structure by GED/MS and QC <i>V. M. Petrov, V. N. Petrova, G. V. Girichev, N. I. Giricheva, H. Oberhammer,</i> <i>Zh. Strukt. Khim.</i> 50 (5) (2009) 865-874
C₆H₅NO₅S C ₆ H ₅ SO ₅ N	3-Nitrobenzenesulfonic acid Structure by GED/MS and QC <i>N. I. Giricheva, G. V. Girichev, Yu. S. Medvedeva, A. V. Bardina, V. M. Petrov, S. N. Ivanov</i> Manuscript in preparation
C₆H₅NO₅S C ₆ H ₅ SO ₅ N	2-Nitrobenzenesulfonic acid Structure by GED/MS and QC <i>V. M. Petrov, N. I. Giricheva, V. N. Petrova, G. V. Girichev, S. N. Ivanov</i> <i>Zh. Strukt. Khim.</i> , submitted
C₆H₁₃FSi C ₅ H ₁₀ SiFCH ₃	1-Fluoro-1-methyl-1-silacyclohexane Structure and conformations by GED/MS, NMR and QC calculations <i>S. Y. Wallevik, R. Bjornsson, A. Kvaran, S. Jonsdottir, G. V. Girichev, N. I. Giricheva, K. Hassler, I. Arnason</i> <i>J. Mol. Struct.</i> , accepted
C₇H₅F₃S C ₆ H ₅ SCF ₃	Trifluoromethylphenyl sulfide Structure by GED/MS and QC <i>I. F. Shishkov, L. V. Khristenko, A. N. Rykov, L. V. Vilkov, N. I. Giricheva, S. A. Shlykov, G. V. Girichev, H. Oberhammer</i> <i>J. Mol. Struct.</i> 876 (2008) 147–153
C₇H₁₃F₃Si C ₇ H ₁₃ F ₃ Si	1-Methyl-1-trifluormethyl-1-silacyclohexane Structure and conformations by GED/MS, NMR and QC calculations <i>S. Y. Wallevik, R. Bjornsson, A. Kvaran, S. Jonsdottir, G. V. Girichev, N. I. Giricheva, K. Hassler, I. Arnason</i> <i>J. Mol. Struct.</i> , accepted
C₁₀Cl₁₀Fe C ₁₀ Cl ₁₀ Fe	Decachloroferrocene Structure by GED/MS and QC calculations <i>L. Phillips, M. K. Cooper, A. Haaland, S. Samdal, N. I. Giricheva, G. V. Girichev</i>

	Dalton. Trans., submitted
C₁₀H₁₄O₄Zn ZnO ₄ C ₁₀ H ₁₄	Zinc acetylacetonate Structure by GED and DFT calculations; vibrational frequencies by DFT calculations <i>E. V. Antina, N. V. Belova, M. B. Berezin, G. V. Girichev, N. I. Giricheva, A. V. Zakharov, A. A. Petrova, and S. A. Shlykov</i> Zh. Strukt. Khim. 50 (6) (2009) 1084 – 1094
C₁₀H₁₈Cu₂O₄	Copper pivalate dimer Structure by GED/MS and QC <i>G. V. Girichev, O. A. Pimenov, S. A. Shlykov, A. V. Zakharov</i> Proc. IV All-Russ. School Quant. Chem., Ivanovo, (2009) 302-305
C₁₂H₁₈CuN₂O₂ C ₁₂ H ₁₈ N ₂ O ₂ Cu	N,N'-Ethylene-bis(acetylacetoneiminato)copper(II) Structure and conformations by GED/MS and QC calculations <i>G. V. Girichev, N. I. Giricheva, N. P. Kuzmina, Yu. S. Medvedeva, A. Yu. Rogachev</i> Zh. Strukt. Khim. 49 (5) (2008) 871 – 882
C₁₂H₁₈N₂NiO₂ C ₁₂ H ₁₈ N ₂ O ₂ Ni	N,N'-Ethylene-bis(acetylacetoneiminato)nickel(II) Structure and conformations by GED/MS and QC calculations <i>G. V. Girichev, N. I. Giricheva, N. P. Kuzmina, Yu. S. Medvedeva, A. Yu. Rogachev</i> Zh. Strukt. Khim. 49 (5) (2008) 871 – 882
C₁₂H₁₈N₂O₂Zn ZnC ₁₂ H ₁₈ N ₂ O ₂	N,N'-Ethylene-bis(acetylacetoneiminato)zinc Structure by GED/MS and QC <i>G. V. Girichev, N. I. Giricheva, E. D. Pelevina, N. V. Tverdova, N. P. Kuz'mina, O. V. Kotova</i> Zh. Strukt. Khim. 51 (1) (2010) 29-37
C₁₂H₁₈N₂O₂Zn ZnO ₂ N ₂ C ₁₂ H ₁₈	N,N'-Ethylene-bis(acetylacetoneiminato)zinc Structure by GED/MS and QC <i>G. V. Girichev, N. I. Giricheva, E. D. Pelevina, N. V. Tverdova, N. P. Kuz'mina, O. V. Kotova,</i> Zh. Strukt. Khim. 51 (1) (2010) 29-37
C₁₄H₁₆N₂O₂Zn ZnC ₁₄ H ₁₆ N ₂ O ₂	N,N-Bis(salicylidene)ethylenediaminozinc Structure by GED/MS and QC <i>G. V. Girichev, N. I. Giricheva, A. O. Symakov, N. V. Tverdova, N. P. Kuz'mina, O. V. Kotova</i> Zh. Strukt. Khim. 51 (2) (2010) 38 – 46
C₁₅H₃F₈O₆Sm SmC ₁₅ F ₁₈ O ₆ H ₃	Tris(hexafluoroacetylacetonato)samarium Structure by GED/MS and QC <i>N. V. Tverdova, G. V. Girichev, S. A. Shlykov, V. V. Rybkin, N. P. Kuz'mina, O. V. Kotova</i> Manuscript complete
C₁₅H₃F₁₈LaO₆ LaC ₁₅ F ₁₈ O ₆ H ₃	Tris(hexafluoroacetylacetonato)lanthanum Structure by GED/MS and QC <i>N. V. Tverdova, G. V. Girichev, S. A. Shlykov, V. V. Rybkin, N. P. Kuz'mina, O. V. Kotova</i> Manuscript complete
C₁₅H₃F₁₈NdO₆ NdC ₁₅ F ₁₈ O ₆ H ₃	Tris(hexafluoroacetylacetonato)neodymium Structure by GED/MS and QC <i>N. V. Tverdova, G. V. Girichev, S. A. Shlykov, V. V. Rybkin, N. P. Kuz'mina, O. V. Kotova</i> Manuscript complete
C₁₅H₁₂O₂ C ₆ H ₅ -C(O)-CH ₂ -C(O)-C ₆ H ₅	Dibenzoylmethane Tautomeric and conformational properties by GED and QC study - <i>N.V. Belova, H. Oberhammer, G. V. Girichev</i> Manuscript complete
	N,N-Bis(salicylidene)ethylenediamincopper(II)

C₁₆H₁₄CuN₂O₂ CuC ₁₆ H ₁₄ N ₂ O ₂	Structure and conformations by GED/MS and QC calculations <i>N. I. Giricheva, G. V. Girichev, N. P. Kuzmina, Yu. S. Medvedeva, A. Yu. Rogachev.</i> Zh. Strukt. Khim. 50 (1) (2009) 58-65
C₁₆H₁₆N₂O₂ C ₁₆ H ₁₆ N ₂ O ₂	N,N-Bis(salicylidene)ethylenediamine Structure by DFT calculations <i>V. V. Sliznev, G. V. Girichev</i> Zh. Strukt. Khim. , submitted
C₁₈H₁₈N₂O₄Zn H ₁₈ C ₁₈ O ₄ N ₂ Zn	N,N-Bis(3-methoxysalicylidene)ethylenediaminozinc Structure, IR spectra by QC <i>N. V. Tverdova, G. V. Girichev, N. P. Kuzmina, O. V. Kotova</i> Manuscript complete
C₂₀H₁₄CuN₂O₂ CuH ₁₄ C ₂₀ O ₂ N ₂	N,N-(o-Phenylen)-bis(salicylidenediamino)copper Structure by GED/MS and QC <i>G. V. Girichev, N. I. Giricheva, E. D. Pelevina, N. V. Tverdova, N. P. Kuz'mina, O. V. Kotova</i> Manuscript in preparation
C₂₀H₁₄N₂NiO₂ NiH ₁₄ C ₂₀ O ₂ N ₂	N,N-(o-Phenylen)-bis(salicylidenediamino)nickel Structure by GED/MS and QC <i>G. V. Girichev, N. I. Giricheva, E. D. Pelevina, N. V. Tverdova, N. P. Kuz'mina, O. V. Kotova</i> Manuscript in preparation
C₂₀H₁₄N₂O₂Zn ZnH ₁₄ C ₂₀ O ₂ N ₂	N,N-(o-Phenylen)-bis(salicylidenediamino)zinc Structure by GED/MS and QC <i>G. V. Girichev, N. I. Giricheva, N. V. Tverdova, E. D. Pelevina, N. P. Kuzmina, O. V. Kotova</i> J. Mol. Struct. (2010), doi:10.1016/j.molstruc.2010.02.023.
C₂₂H₁₈N₂O₄Zn H ₁₈ C ₂₂ O ₄ N ₂ Zn	N,N-(o-Phenylen)-bis(3-methoxysalicylidenediamino)zinc Structure, IR spectra by QC <i>N. V. Tverdova, G. V. Girichev, N. P. Kuzmina, O. V. Kotova</i> Manuscript complete
C₂₈H₂₈CuN₄ C ₂₈ H ₂₈ N ₄ Cu	Octamethylporphyrin copper(II) Structure by GED/MS and QC <i>G. V. Girichev, N. I. Giricheva, O. A. Golubchikov, Y. V. Minenkov, A. S. Semeikin, S. A. Shlykov</i> J. Mol. Struct. accepted
C₂₈H₂₈N₄Ni C ₂₈ H ₂₈ N ₄ Ni	Nickeloctamethylporphyrine Structure, ruffling effect and conformations by GED/MS and QC calculations <i>G. V. Girichev, N. I. Giricheva, O. A. Golubchikov, Yu. V. Minenkov, A. S. Semeikin, S. A. Shlykov.</i> Manuscript in preparation
C₃₂H₁₆CuN₈ C ₃₂ H ₁₆ CuN ₈	Copperphthalocyanine Structure by GED/MS and QC calculations <i>G. V. Girichev, N. I. Giricheva, O. A. Golubchikov, Yu. V. Minenkov, A. S. Semeikin, S. A. Shlykov</i> Manuscript in preparation
C₃₂H₁₆N₈OTi TiOC ₃₂ H ₁₆ N ₈	Oxotitaniumphthalocyanine Structure by GED/MS and QC <i>A. V. Zakharov, S. A. Shlykov, Yu. A. Zhabanov, G. V. Girichev</i> Phys. Chem. Chem. Phys. (2009) 3472-3477
C₄₂H₃₉N₁₅S₃	Trithiadiazoletri(5-tert-butylisoindole)macrocycle Structures by GED experiment and DFT calculations <i>A. V. Zakharov, S. A. Shlykov, E. A. Danilova, A. V. Krasnov, M. K. Islyaikin, G. V. Girichev</i>

	Phys. Chem. Chem. Phys. 11 (2009) 8570-8579
C₄₂H₃₉N₁₅S₃ S ₃ C ₄₂ H ₃₉ N ₁₅	Structure by GED/MS and QC <i>V. Zakharov, S. A. Shlykov, E. A. Danilova, A. V. Krasnov, M. K. Islyaikin, G. V. Girichev</i> Phys. Chem. Chem. Phys. 11 (2009) 8570 - 8579
Cl₃Er ErCl ₃	Erbium trichloride Structure by GED/MS and QC <i>N. I. Giricheva, S. A. Shlykov, G. V. Girichev, E. V. Chernova and E. Lapykina</i> Zh. Strukt. Khim. 50 (2) (2009) 251-261
Cl₃Yb YbCl ₃	Ytterbium trichloride Structure by GED/MS and QC <i>N. I. Giricheva, S. A. Shlykov, G. V. Girichev, E. V. Chernova and E. Lapykina</i> Zh. Strukt. Khim. 50 (2) (2009) 251-261
Cl₄Te TeCl ₄	Tellurium tetrachloride Structure by GED/MS and QC <i>S. A. Shlykov, N. I. Giricheva, A. V. Titov, M. Szwak, D. Lentz G. V. Girichev</i> Dalton Trans. 39 (2010) 3245–3255
DyI₃ DyI ₃	Dysprosium triiodide Structure and nuclear dynamics by GED/MS and QC <i>S. A. Shlykov, N. I. Giricheva, E. A. Lapykina, G. V. Girichev, H. Oberhammer</i> J. Mol. Struct., accepted
Erl₃ Erl ₃	Erbium triiodide Structure and nuclear dynamics by GED/MS and QC <i>S. A. Shlykov, N. I. Giricheva, E. A. Lapykina, G. V. Girichev, H. Oberhammer</i> J. Mol. Struct., accepted
F₄Te TeF ₄	Tellurium tetrafluoride Structure by GED/MS and QC <i>S. A. Shlykov, N. I. Giricheva, A. V. Titov, M. Szwak, D. Lentz G. V. Girichev</i> Dalton Trans. 39 (2010) 3245–3255
GdI₃ GdI ₃	Gadolinium triiodide Structure and nuclear dynamics by GED/MS and QC <i>S. A. Shlykov, N. I. Giricheva, E. A. Lapykina, G. V. Girichev, H. Oberhammer</i> Manuscript in preparation
Hol₃ Hol ₃	Holmium triiodide Structure and nuclear dynamics by GED/MS and QC <i>S. A. Shlykov, N. I. Giricheva, E. A. Lapykina, G. V. Girichev, H. Oberhammer</i> J. Mol. Struct., accepted
I₂Te Tel ₂	Tellurium diiodide Structure by GED/MS and QC <i>S. A. Shlykov, N. I. Giricheva, G. V. Girichev, H. Oberhammer and A. V. Titov</i> Eur. J. Inorg. Chem. 33 (2008) 5220 – 5227
I₃Pr PrI ₃	Praseodymium triiodide Structure and nuclear dynamics by GED/MS and QC <i>S. A. Shlykov, N. I. Giricheva, E. A. Lapykina, G. V. Girichev, H. Oberhammer</i> Manuscript in preparation
	Terbium triiodide

I₃Tb TbI ₃	Structure and nuclear dynamics by GED/MS and QC <i>S. A. Shlykov, N. I. Giricheva, E. A. Lapykina, G. V. Girichev, H. Oberhammer</i> J. Mol. Struct., accepted
O₆Sb₄ Sb ₄ O ₆	Antimony(III) oxide Structure by GED/MS and QC <i>S. L. Masters, G. V. Girichev, S. A. Shylkov</i> Dalton.Trans., submitted
	Dihalogenated porphyrins and phthalocyanines of titanium Structures by DFT calculations <i>A. V. Zakharov</i> Mol. Phys. 107 (2009) 2493-2501
	Hemiporphyrazines Structres, vibrational spectra and electronic spectra by DFT calculations <i>A. V. Zakharov, M. G. Stryapan, M. K. Islyaikin</i> J. Mol. Struct.: THEOCHEM 906 (2009) 56-62
	Thiadiazole-containing expanded heteroazaporphyrinoids Structures by DFT calculations <i>A. V. Zakharov, S. A. Shlykov, E. A. Danilova, A. V. Krasnov, M. K. Islyaikin, G. V. Girichev</i> Phys. Chem. Chem. Phys. 11 (2009) 8570-8579
	Lanthanum bromine system Mass-spectrometric study of vapors and structure by DFT calculation <i>D. A. Ivanov, V. V. Sliznev, L. S. Kudin, M. F. Butman</i> Izv. Vys. Uch. Zav. Khim. Khim. Tekhnol. 51 (3) (2008) 23-26
	Neodymium, erbium, ytterbium and lutetium dipivaloylmethanates Mass-spectrometric study of overheated vapors <i>G. V. Girichev, N. V. Belova, N. K. Chang, S. A. Shlykov, N. P. Kuzmina</i> Zh. Neorg. Khim. , submitted
	N,N'-Ethylene-bis(acetylacetoneiminato)complexes of copper, nickel and zinc Mass-spectrometric study of vapors <i>G. V. Girichev, N. V. Tverdova, N. P. Kuz'mina, A. O. Symakov, O. V. Kotova</i> Russ. J. Inorg. Chem. 54 (12) (2009) 1–6
	Tris(hexafluoroacetylacetonato)ytterbium Mass-spectrometric study of vapors <i>G. V. Girichev, V. V. Rybkin, V.V. Tunina, A.V. Krasnov, N. V. Tverdova, N. P. Kuz'mina, I. G. Zaitseva</i> Russ. J. Inorg. Chem., submitted
	Chalcogen tetrahalides Structure and conformations by QC <i>H. Oberhammer, S. A. Shlykov</i> Dalton Trans. 39 (2010) 2838 - 2841
	Copper and scandium acetylacetone derivatives Internal rotation of CX ₃ substituents by QC study <i>N. V. Belova, G. V.Girichev, H. Oberhammer</i> Zh. Strukt. Khim. , submitted
	Aluminium, gallium and indium dipivaloylmethanates Structure by DFT calculations <i>N. V. Belova, T. A. Zhukova, G. V. Girichev</i> Materials of IV Seminar for young scientists "Quantum-chemical calculations: structure and reactivity of organic and inorganic molecules", Ivanovo, (2009) 115-117

	Cobalt, iron and manganese dipivaloylmethanates Molecular structure and electronic states by QC <i>N. V. Belova, V. V. Sliznev, G. V. Girichev</i> Zh. Strukt. Khim., accepted
	N,N-Bis(salicylidene)ethylenediamino complexes of copper, nickel and zinc Mass-spectrometric study of vapors <i>N. V. Tverdova, G. V. Girichev, S. A. Shlykov, V. V. Rybkin, N. P. Kuz'mina, O. V. Kotova</i> Russ. J. Inorg. Chem., submitted
	N,N'-Ethylene-bis(acetylacetoinato) and N,N-bis(salicylidene)ethylenediamino complexes with copper, nickel and zinc Structure, IR spectra by QC <i>N. V. Tverdova, N. I. Giricheva, G. V. Girichev, N. P. Kuz'mina, O. V. Kotova, A. V. Zakharov</i> Russ. J. Phys. Chem. A 83 (13) (2009) 61–71
	Carbonyl compounds Tautomeric and conformational properties by DFT calculation (NBO analysis). <i>N. V. Belova, V. V. Sliznev, H. Oberhammer, G. V. Girichev</i> J. Mol. Struct., doi:10.1016/j.molstruc.2010.02.070
	Diselenium dichloride and dibromide Structure by QC <i>S. A. Shlykov</i> Proc. IV All-Russ. School Quant. Chem., Ivanovo, (2009) 291-295