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C₈H₆N₂O₂	3-Aminophthalimide Structure by GED/MS and QC <i>N. Vogt, D. S. Savelyev, N. I. Giricheva, and G.V. Girichev</i> <i>Phys. Chem. Chem. Phys.</i> 22 (2020) 27539-27546
C₁₁H₁₂N₂O₂	L-Tryptophan Structure by GED/MS and QC <i>V. V. Dunaeva, G. V. Girichev, and N. I. Giricheva</i> <i>Izv. Vyssh. Uchebn. Zaved. Khim. Khim. Tekhnol.</i> 63 (2020) N 3
	Naphthalenesulfon derivates IR spectra <i>N. I. Giricheva, G. V. Girichev, D. Christen, S. N. Ivanov, V. M. Petrov, and V. N. Petrova</i> <i>Manuscript in progress</i>
C₂₈H₂₈N₄Ni	Nickel octamethylporphyrin Structure by GED/MS and QC <i>A. E. Pogonin, N. V. Tverdova, Yu. V. Minenkov, N. I. Giricheva, and G. V. Girichev</i> <i>Manuscript in preparation</i>
C₃₂H₃₆N₄Ni	Nickel etioporphyrin-II Structure by GED/MS and QC <i>G. V. Girichev, A. E. Pogonin, N. V. Tverdova, and N. I. Giricheva</i> <i>Manuscript in preparation</i>
C₃₂H₃₆CoN₄	Cobalt etioporphyrin-II Structure by GED/MS and QC <i>A. E. Pogonin, A. A. Otyotov, N. V. Tverdova, A. A. Ischenko, V. D. Rumyantseva, O. I. Koifman, and G. V. Girichev</i> <i>J. Mol. Struct.</i> 1216 (2020) 128319
C₁₄H₁₀	Anthracene Structure by GED/MS and QC <i>N. W. Mitzel, Yu. V. Vishnevskiy, N. V. Tverdova, A. A. Otyotov, V. M. Petrov, V. N. Petrova, N. I. Giricheva, and G. V. Girichev</i> <i>Manuscript in preparation</i>

Girichev

C₁₄H₁₄O₂	1,2-Diphenoxymethane Structure by GED/MS and QC <i>J.-H. Weddeling, T. Glodde, I. Yu. Kurochkin, A. A. Otyotov, N. W. Mitzel, and G.V. Girichev</i>
C₁₄H₉F₅O₂	1-Phenoxy-2-pentafluorophenoxyethane Structure by GED/MS and QC <i>J.-H. Weddeling, T. Glodde, I. Yu. Kurochkin, A. A. Otyotov, N. W. Mitzel, and G. V. Girichev</i> <i>Manuscript in preparation</i>
C₁₀H₁₈Si₂ (CH ₃) ₃ Si-C≡C-Si(CH ₃) ₃	1,4-Bis(trimethylsilyl)-1,3-butadiyne Structure by GED/MS and QC <i>A. A. Otyotov, Yu. V. Vishnevskiy, J.-H. Lamm, H.-G. Stammier, N. W. Mitzel, and G.V. Girichev</i> <i>Manuscript in preparation</i>
C₁₂H₁₀	Acenaphthene Structure by GED/MS and QC <i>A. A. Otyotov, Yu. V. Vishnevskiy, J.-H. Lamm, H.-G. Stammier, N. W. Mitzel, and G. V. Girichev</i> <i>Manuscript in preparation</i>
C₃₀H₅₄Co₄O₁₃	Cobalt oxopivalate Structure by GED/MS and QC <i>A. S. Alikhanyan, G. V. Girichev, N. I. Giricheva, and E. A. Morozova</i> <i>Manuscript in preparation</i>
C₄H₁₄OSi₃	1-Methoxy-1,3,5-trisilacyclohexane Structure by GED/MS and QC <i>S. A. Shlykov, I. Arnason, and L. E. Kuzmina</i> <i>Refinement in progress</i>
C₄H₁₄Si₃	1-Methyl-1,3,5-trisilacyclohexane Structure by GED/MS and QC <i>S. A. Shlykov, I. Arnason, and L. E. Kuzmina</i> <i>Refinement in progress</i>
F₅Mo MoF ₅	Molybdenum pentafluoride Structure by GED/MS and QC <i>V. V. Sliznev, O. A. Pimenov, and G. V. Girichev</i> <i>J. Mol. Struct. 1199 (2020) 126884</i>
C₂₀H₄F₂₄KLaO₈ KLa(hfa) ₄	Potassium tetrakis(hexafluoroacetylacetonato)lanthanate(III) Structure by GED/MS and QC <i>G. V. Girichev, N. I. Giricheva, A. E. Khochenkov, N. V. Belova, V. V. Sliznev, and N.W. Mitzel</i> <i>Chem. Eur. J. 27 (2021) 1103–1112</i>
C₂₀H₄F₂₄GdKO₈ KGd(hfa) ₄	Posassium tetrakis(hexafluoroacetylacetonato)gadolinate(III) Structure by GED/MS and QC <i>G. V. Girichev, N. I. Giricheva, A. E. Khochenkov, N. V. Belova, V. V. Sliznev, and N.W. Mitzel</i> <i>Chem. Eur. J. 27 (2021) 1103–1112</i>
C₂₀H₄F₂₄KLuO₈ KLu(hfa) ₄	Potassium tetrakis(hexafluoroacetylacetonato)lutetate(III) Structure by GED/MS and QC <i>G. V. Girichev, N. I. Giricheva, A. E. Khochenkov, N. V. Belova, V. V. Sliznev, and N.W. Mitzel</i> <i>Chem. Eur. J. 27 (2021) 1103–1112</i>
C₁₅H₂₄Si	1-Phenyl-1-tert-butyl-1-silacyclohexane Structure by GED/MS, FT-IR and QC calculations <i>B. A. Shainyan, E. N. Suslova, Tran Dinh Phien, S. A. Shlykov, and L. P. Oznobikhina</i> <i>J. Organomet. Chem. 923 (2020) 121433</i>

Girichev

$C_5H_4N_2O_3$	4-Nitropyridine N-oxide
	Structure by GED/MS and QC calculations
	N. V. Belova, O. A. Pimenov, G. V. Girichev, V. E. Kotova, and G. V. Girichev
	<i>J. Mol. Struct.</i> 1217 (2020) 128476
$C_{44}H_{29}N_3S$	5,10,15,20-Tetraphenyl-21-thia-porphyrin
	Structure by GED/MS and QC calculations
	I. A. Kuzmin and S. A. Shlykov
	Refinement in progress
$C_{44}H_{26}F_4N_4$	5,10,15,20-Tetrakis(4'-fluorophenyl)porphyrin
	Structure by GED/MS and QC calculations, enthalpy of sublimation by MS, IR spectrum
	I. Yu. Kurochkin, A. E. Pogonin, A. A. Otyotov, A. N. Kiselev, A. V. Krasnov, S. A. Shlykov, and G. V. Girichev
	<i>J. Mol. Struct.</i> 1221 (2020) 128662
$C_{44}H_{26}F_4N_4$	5,10,15,20-Tetrakis(4'-fluorophenyl)porphyrin
	Structure by QC calculations
	I. Yu. Kurochkin, A. E. Pogonin, A. A. Otyotov, A. N. Kiselev, and G. V. Girichev
	<i>Izv. Vyssh. Uchebn. Zaved. Khim. Khim. Tekhnol.</i> 63 (2020) 51-57
$C_{44}H_{26}Cl_4N_4$	5,10,15,20-Tetrakis(4'chlorophenyl)porphyrin
	Structure by GED/MS and QC calculations, enthalpy of sublimation by
	A. E. Pogonin, I. Yu. Kurochkin, A. A. Otyotov, A. N. Kiselev, S. A. Shlykov, and G. V. Girichev
	<i>Izv. Vyssh. Uchebn. Zaved. Khim. Khim. Tekhnol.</i> 63 (2020) N 1
$C_{44}H_{26}Br_4N_4$	5,10,15,20-Tetrakis(4'-bromophenyl)porphyrin
	Structure by GED/MS and QC calculations, enthalpy of sublimation by
	A. E. Pogonin, I. Yu. Kurochkin, A. A. Otyotov, A. N. Kiselev, S. A. Shlykov, and G. V. Girichev
	<i>Izv. Vyssh. Uchebn. Zaved. Khim. Khim. Tekhnol.</i> 63 (2020) N 1
	o-Substituted benzenesulfonic acids
	Effect of intramolecular hydrogen bond type
	N. I. Giricheva, S. N. Ivanov, A. V. Ignatova, M. S. Fedorov, and G. V. Girichev
	<i>Molecules</i> 25 (2020) 5806
$C_5H_5N_3O$	Pyrazinamide
	Structure by GED and QC calculations
	A. A. Otyotov, G. V. Girichev, A. N. Rykov, T. Glodde, and Yu. V. Vishnevskiy
	<i>J. Phys. Chem. A</i> 124 (2020) 5204-5211
$C_5H_{17}NSi_3$	N,N-Dimethylamino-1,3,5-trisilacyclohexane
	Structure by GED/MS, IR and QC calculations
	Tran Dinh Phien, L. E. Kuzmina, I. Arnason, N. R. Jonsdottir, and S. A. Shlykov
	<i>J. Mol. Struct.</i> 1224 (2021) 129046
	1,7-Diphenyl-3,5-bis(2-thiophenyl)-aza-BODIPY
	Structure by QC calculations
	A. E. Pogonin, A. Y. Shagurin, M. A. Savenkova, F. Yu. Telegin, Yu. S. Marfin, and A. S. Vashurin
	<i>Molecules</i> 25 (2020) 5361
	Aluminum trisdipivaloylmethanate
	Structure of ions and energy of the processes of their formation in saturated vapor
	G. V. Girichev and N. I. Giricheva
	<i>J. Struct. Chem.</i> 61 (2020) 1958-1970

Girichev

	Interaction of somolecular dipeptides with sodium dodecyl sulfate micelles Quantum chemical and molecular dynamics modeling of interaction of isomolecular dipeptides of α -L-alanyl- α -L-alanine and β -alanyl- β -alanine with sodium dodecyl sulfate micelles <i>V. P. Barannikov, M. S. Kurbatova, D. L. Gurina, N. I. Giricheva</i> <i>Comput. Theoret. Chem.</i> 1182 (2020) 112844
	Structural dynamics of free molecules and condensed matter Structural dynamics of free molecules and condensed matter <i>S. A. Aseyev, A. S. Akhmanov, G. V. Girichev, A. A. Ischenko, I. V. Kochikov, V. Ya. Panchenko, and E. A. Ryabov</i> <i>Phys. Uspekhi</i> 63 (2020) 103-122
	Electronic absorption spectra and intermolecular hydrogen bonds in mzoen - nemesogen systems <i>N. I. Giricheva, K. E. Bubnova, E. M. Chernova, M. S. Fedorov, S. A. Syrbu, and G. V. Girichev</i> <i>J. Struct. Chem.</i> 61 (2020) 1595-1605
	Calcium and zinc porphyrazines Structures and electronic absorption spectra by QC calculations <i>A. A. Otyotov, I. V. Ryzhov, I. A. Kuzmin, Yu. A. Zhabanov, M. S. Mikhailov, and P. A. Stuzhin</i> <i>Internat. J. Mol. Sci.</i> 21 (2020) 2923
	Iron and cobalt porphyrazines Structures by QC calculations <i>Yu. A. Zhabanov, V. V. Sliznev, I. V. Ryzhov, and P. A. Stuzhin</i> <i>J. Porphyrins Phthalocyanines</i> 2020; 24
	Yttrium, lanthanum and lutetium porphyrazines Structures, electronic and vibrational absorption spectra by QC calculations <i>Yu. A. Zhabanov, I. V. Ryzhov, I. A. Kuzmin, A. V. Eroshin, and P. A. Stuzhin</i> <i>Molecules</i> 26 (2021) 113
	Ca(II), Ni(II) and Zn(II) with hemi- and dicarbahemiporphyrazines Structures and electronic absorption spectra by QC calculations <i>A. V. Eroshin, A. A. Otyotov, Yu. A. Zhabanov, V. V. Veretennikov, and M. K. Islyaikin</i> <i>Makroheterocycles</i> 2021
$C_{16}N_{16}NiS_4$	Nickel tetrakis(1,2,5-thiadiazole)porphyrazine Structure by GED and QC calculations <i>A. A. Otyotov, Yu. A. Zhabanov, I. A. Kuzmin, and S. A. Shlykov</i> <i>Manuscript in preparation</i>
$C_7H_{15}NO_3Si$	1-Methylsiltrane Structure by GED and QC calculations <i>E. F. Belogolova, S. A. Shlykov, A. V. Eroshin, E. P. Doronina, and V. F. Sidorkin</i> <i>Phys. Chem. Chem. Phys.</i> , accepted
$C_{11}H_{13}NO$	1-Phenyl-piperidin-4-one Structure by GED and QC calculations <i>A. V. Eroshin and S. A. Shlykov</i> <i>Refinement in progress</i>
$C_{15}H_{21}O_6Sc$	Trisacetylacetonatoscandium Structure by GED/MS and QC calculations <i>N. I. Giricheva, N. V. Tverdova, S. A. Shlykov, and G. V. Girichev</i> <i>Manuscript in preparation</i>
	Bisacetylacetonatoscandium

Girichev

C₁₀H₁₄O₄Sc	Structure by GED/MS and QC calculations <i>N. I. Giricheva, N. V. Tverdova, S. A. Shlykov, and G. V. Girichev</i> <i>Manuscript in preparation</i>
C₄₄H₂₈N₄Pt	5,10,15,20-Tetraphenylporphyrinatoplatinum(II) Structure by GED/MS and QC calculations <i>I. Yu. Kurochkin, N. V. Tverdova, N. I. Giricheva, V. A. Olshevskaya, N. W. Mitzel, and G. V. Girichev</i> <i>Refinement finished</i>