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Be₂	Beryllium diiodide Structure by GED/MS and QC (CCSD(T)) <i>S. A. Shlykov, Yu. A. Zhabanov, A. V. Zakharov, G. V. Girichev, and N. I. Giricheva</i> Manuscript completed
C₄N₄S SN ₄ C ₄	1,2,5-Thiadiazole-3,4-dicarbonitrile Structure by GED/MS and QC <i>G. V. Girichev, N. I. Giricheva, and N. V. Tverdova</i> Manuscript ready
C₅H₈O₂ CH ₃ C(O)CH ₂ C(O)CH ₃	Acetylacetone Structure by GED/MS and QC <i>N. V. Belova, N. H. Trang, G. V. Girichev, and H. Oberhammer</i> J.Org.Chem., 79 (12) (2014), 5412
C₅H₉O₂Tl C ₄ H ₉ -COOTl	Thallium(I) pivalate Structure by GED/MS and QC <i>G. V. Girichev, Yu. A. Zhabanov, A. E. Pogonin, and O. A. Pimenov</i> VI International Conference of Young Scientists "ORGANIC CHEMISTRY TODAY". Saint Petersburg, Russia, 23-25 September, 2014
C₅H₁₀O C ₅ H ₁₀ O	Tetrahydropyran QC <i>S. A. Shlykov and D. Yu. Osadchiy</i> Calculations completed
C₅H₁₂OSi	3-Methyl-1-oxa-silacyclohexane Structure by QC

$C_4H_8OSi(CH_3)H$	S. A. Shlykov and D. Yu. Osadchiy Calculations completed
$C_5H_{12}SSi$ $C_4H_8SSi(CH_3)H$	3-Methyl-1-thia-silacyclohexane GED/MS, NMR and QC B. A. Shainyan, S. V. Kirpichenko, E. Kleinpeter, S. A. Shlykov, and D. Yu. Osadchiy Manuscript in preparation
$C_5H_{12}SSi$ $C_4H_8SSi(CH_3)H$	3-Methyl-1-thia-silacyclohexane QC D. Yu. Osadchiy Festival of Students and Young Scientists ISU " Young science at classical university ", ISU , 21-25 April 2014
$C_6H_{13}N$ $C_5H_{10}N-CH_3$	N-Methylpiperidine Structure and vibrational spectra by QC calculations T. D. Phien, S. A. Shlykov, Y. Shang, and P. M. Weber Manuscript in preparation
$C_7H_7NO_5S$	4-Nitrobenzenesulfonic acid methyl ester Structure by GED/MS and QC M. S. Fedorov, N. I. Giricheva, G. V. Girichev, and S. N. Ivanov J. Mol. Struct., in press
$C_7H_7NO_5S$	2-Nitrobenzenesulfonic acid methyl ester Structure by GED/MS and QC M. S. Fedorov, N. I. Giricheva, G. V. Girichev, and S. N. Ivanov J. Struct. Chem., in press
$C_7H_7NO_5S$ $4-NO_2-C_6H_4-SO_2OCH_3$	4-Nitrobenzenesulfonic acid methyl ester (4-nitrobenzenesulfonate) Structure by GED/MS and QC M. S. Fedorov, N. I. Giricheva, G. V. Girichev, and S. N. Ivanov Manuscript is ready
$C_7H_7NO_5S$ $2-NO_2-C_6H_4-SO_2OCH_3$	2-Nitrobenzenesulfonic acid methyl ester (2-nitrobenzenesulfonate) Structure by GED/MS and QC M. S. Fedorov, N. I. Giricheva, G. V. Girichev, and S. N. Ivanov Manuscript is ready
$C_7H_7NO_5S$ $NO_2-C_6H_4-SO_2-OCH_3$	ortho-Nitromethylbenzenesulfonate Structure by GED/MS and QC N. I. Giricheva, M. S. Fedorov, S. N. Ivanov, and G. V. Girichev J. Mol. Struct., 1085 (2015), 191
$C_7H_7NO_5$ $4-NO_2-C_6H_4-SO_2-OCH_3$	Methylbenzenesulfonate Conformational properties determination by GED and IR N. I. Giricheva, M. S. Fedorov, and G. V. Girichev Manuscript is ready
$C_7H_{15}N$ $C_5H_{10}N-C_2H_5$	N-Ethylpiperidine Structure and vibrational spectra by QC calculations T. D. Phien, S. A. Shlykov, Y. Shang, and P. M. Weber Manuscript in preparation
$C_8H_6N_2O_2$	3-Aminophthalimide Structure by GED/MS and QC G. V. Girichev, N. I. Giricheva, M. K. Islyaikin, and D. S. Savelyev Manuscript in preparation
$C_8H_6O_2N_2$	3-Aminophthalimide Structure by GED/MS and QC G. V. Girichev, N. I. Giricheva, M. K. Islyaikin, and D. S. Savelyev Manuscript is ready

$C_9H_{11}NO_2$	L-Phenylalanine Thermodynamics of sublimation by Knudsen method <i>V. V. Tyunina, A. V. Krasnov, E. Yu. Tyunina, V. G. Badelin, and G. V. Girichev</i> J. Chem. Thermodyn., 74 (2014), 221
$C_9H_{11}NO_3$	L-Tyrosine Thermodynamics of sublimation by Knudsen method <i>V. V. Tyunina, A. V. Krasnov, E. Yu. Tyunina, V. G. Badelin, and G. V. Girichev</i> J. Chem. Thermodyn., 74 (2014), 221
$C_{10}H_6Cl_2O_4S_2$	1,5-Naphthalene disulfonyl dichloride IR spectrum <i>N. I. Giricheva, G. V. Girichev, D. Christen, S. N. Ivanov, V. M. Petrov, and V. N. Petrova</i> Manuscript in preparation
$C_{10}H_6Cl_2O_4S_2$	1,5-Naphthalene disulfonyl dichloride MS study <i>N. I. Giricheva, G. V. Girichev, H. Oberhammer, V. M. Petrov, and V. N. Petrova</i> Manuscript in preparation
$C_{10}H_6Cl_2O_4S_2$	1,5-Naphthalene disulfonyl dichloride Structure by GED/MS and QC <i>N. I. Giricheva, G. V. Girichev, M. Dakkouri, S. N. Ivanov, V. M. Petrov, and V. N. Petrova</i> Manuscript in preparation
$C_{10}H_7ClO_2S$	β-Naphthalene sulfonyl chloride IR spectrum <i>N. I. Giricheva, G. V. Girichev, D. Christen, S. N. Ivanov, V. M. Petrov, and V. N. Petrova</i> Manuscript in preparation
$C_{10}H_7ClO_2S$	α-Naphthalene sulfonyl chloride IR spectrum <i>N. I. Giricheva, G. V. Girichev, D. Christen, S. N. Ivanov, V. M. Petrov, and V. N. Petrova</i> Manuscript in preparation
$C_{10}H_7ClO_2S$	β-Naphthalene sulfonyl chloride MS study <i>N. I. Giricheva, G. V. Girichev, H. Oberhammer, V. M. Petrov, and V. N. Petrova</i> Manuscript in preparation
$C_{10}H_7ClO_2S$	α-Naphthalene sulfonyl chloride MS study <i>N. I. Giricheva, G. V. Girichev, H. Oberhammer, V. M. Petrov, and V. N. Petrova</i> Manuscript in preparation
$C_{10}H_9NO_2S$	α-Naphthalene sulfonamide IR spectrum <i>N. I. Giricheva, G. V. Girichev, D. Christen, S. N. Ivanov, V. M. Petrov, and V. N. Petrova</i> Manuscript in preparation
$C_{10}H_9NO_2S$	β-Naphthalene sulfonamide IR spectrum <i>N. I. Giricheva, G. V. Girichev, D. Christen, S. N. Ivanov, V. M. Petrov, and V. N. Petrova</i> Manuscript in preparation
	α-Naphthalene sulfonamide

C₁₀H₉NO₂S	MS study <i>N. I. Giricheva, G. V. Girichev, H. Oberhammer, V. M. Petrov, and V. N. Petrova</i> Manuscript in preparation
C₁₀H₉NO₂S	β-Naphthalene sulfonamide MS study <i>N. I. Giricheva, G. V. Girichev, H. Oberhammer, V. M. Petrov, and V. N. Petrova</i> Manuscript in preparation
C₁₀H₉NO₂S α-C ₁₀ H ₇ SO ₂ NH ₂	α-Naphthalenesulfonamide Structure by GED/MS and QC <i>V. N. Petrova, S. A. Shlykov, S. N. Ivanov, and G. V. Girichev</i> J. Phys. Chem DOI: 10.1021/jp5067617
C₁₀H₉NO₂S β-C ₁₀ H ₇ SO ₂ NH ₂	β-Naphthalenesulfonamide Structure by GED/MS and QC <i>V. N. Petrova, S. A. Shlykov, S. N. Ivanov, and G. V. Girichev</i> J. Phys. Chem DOI: 10.1021/jp5067617
C₁₀H₈ C ₁₀ H ₈	Naphthalene Structure by GED/MS and QC <i>N. I. Giricheva, G. V. Girichev, M. Dakkouri, S. N. Ivanov, V. M. Petrov, and V. N. Petrova</i> Manuscript in preparation
C₁₁H₁₂N₂O₂ C ₁₁ H ₁₂ N ₂ O ₂	L-Tryptophan Thermodynamics of sublimation by Knudsen method <i>V. V. Tyunina, A. V. Krasnov, E. Yu. Tyunina, V. G. Badelin, and G. V. Girichev</i> J. Chem. Thermodyn., 74 (2014), 221
C₁₁H₁₂O₂N₂ COOHCH(NH ₂)CH ₂ C ₈ H ₆ N	L-Tryptophan Structure by GED/MS and QC <i>V. V. Tyunina, N. I. Giricheva, and G. V. Girichev</i> Manuscript in preparation
C₁₁H₁₆OSi C ₄ H ₈ OSi(C ₆ H ₅)CH ₃	3-Methyl-3-phenyl-3-silatetrahydropyran GED/MS, NMR and QC <i>B. A. Shainyan, S. V. Kirpichenko, E. Kleinpeter, S. A. Shlykov, and D. Yu. Osadchiy</i> Manuscript submitted
C₁₁H₁₆Si C ₅ H ₁₀ Si(C ₆ H ₅)H	1-Phenyl-1-silacyclohexane Structure by GED/MS, QC, NMR <i>B. A. Shainyan, S. V. Kirpichenko, S. A. Shlykov, E. Kleinpeter, and D. Yu. Osadchiy</i> Struct. Chem., 25 (2014), 1677
C₁₁H₂₁N C ₅ H ₁₀ N-C ₆ H ₁₁	N-Cyclohexylpiperidine Structure by GED/MS and QC calculations, IR spectrum <i>T. D. Phien, S. A. Shlykov, Y. Shang, and P. M. Weber</i> Manuscript in preparation
C₁₂H₁₄N₂O₂S (CH ₃) ₂ N-C ₁₀ H ₆ -SO ₂ NH ₂	Dansylamide Conformations in gas and crystal <i>N. I. Giricheva, E. A. Lapykina, M. S. Fedorov, and D. A. Petrova</i> J. Struct. Chem., (2015), accepted
C₁₂H₁₆ C ₆ H ₁₀ (C ₆ H ₅)H	1-Phenylcyclohexane QC <i>S. A. Shlykov and D. Yu. Osadchiy</i> Calculations completed
C₁₂H₁₈Si	1-Methyl-1-phenyl-1-silacyclohexane QC

$C_5H_{10}Si(C_6H_5)CH_3$	S. A. Shlykov and D. Yu. Osadchiy Calculations completed
$C_{15}H_{21}FeO_6$ $Fe(C_5H_7O_2)_3$	Iron tris-acetylacetonate molecular and electronic structure by GED/MS and QC A. A. Petrova, G. V. Girichev, N. I. Giricheva, and N. P. Kuzmina Manuscript in preparation
$C_{15}H_{27}AlO_2$ $(C_4H_9COO)_3Al$	Aluminum(III) pivalate Structure by QC Yu. A. Zhabanov, A. E. Pogonin, and O. A. Pimenov VI. International Conference of Young Scientists "ORGANIC CHEMISTRY TODAY". Saint Petersburg, Russia, 23-25 September, 2014
$C_{15}H_{27}GaO_2$ $(C_4H_9COO)_3Ga$	Gallium(III) pivalate Structure by QC G. V. Girichev, Yu. A. Zhabanov, A. E. Pogonin, O. A. Pimenov, and B. V. Puchkov XXV. Austin symposium on molecular structure and dynamics. Dallas, Texas U.S.A., 1-4 March, 2014
$C_{15}H_{27}InO_2$ $(C_4H_9COO)_3In$	Indium(III) pivalate Structure by GED/MS and QC G. V. Girichev, Yu. A. Zhabanov, A. E. Pogonin, O. A. Pimenov, and B. V. Puchkov XXV. Austin symposium on molecular structure and dynamics. Dallas, Texas U.S.A., 1-4 March, 2014
$C_{15}H_{27}O_2Ti$ $(C_4H_9COO)_3Ti$	Thallium(III) pivalate Structure by QC Yu. A. Zhabanov, A. E. Pogonin, and O. A. Pimenov VI. International Conference of Young Scientists "ORGANIC CHEMISTRY TODAY". Saint Petersburg, Russia, 23-25 September, 2014
$C_{16}N_{16}S_4Zn$ $ZnS_4N_{16}C_{16}$	Zinc tetrakis-(thiadiazole)porphyrin Structure by GED/MS and QC G. V. Girichev, N. I. Giricheva, and N. V. Tverdova Manuscript is ready
$C_{24}H_{26}Si_2$ $C_{24}H_{26}Si_2$	1,8-Bis(trimethylsilylethynyl)anthracene Structure by GED/MS and QC calculations N. V. Tverdova, Yu. A. Zhabanov, V. V. Rybkin, A. A. Otlyotov, N. I. Giricheva, and G. V. Girichev Manuscript in preparation
$C_{28}H_{28}N_4Ni$	Nickel octamethylporphyrin Structure by GED/MS and QC G. V. Girichev, A. E. Pogonin, and Yu. V. Minenkov Manuscript in preparation
$C_{30}H_{18}$ $C_{30}H_{18}$	1,8-Bis(phenylethynyl)anthracene Structure by GED/MS, XRD and QC calculations J.-H. Lamm, J. Horstmann, H.-G. Stammler, N. W. Mitzel, Yu. A. Zhabanov, N. V. Tverdova, A. A. Otlyotov, N. I. Giricheva, and G. V. Girichev Manuscript in preparation
$C_{32}H_{36}CoN_4$	Cobalt etioporphyrin-II Structure by GED/MS and QC G. V. Girichev, A. E. Pogonin, and N. V. Tverdova Manuscript in preparation
$C_{32}H_{36}CuN_4$	Copper etioporphyrin-II Structure by GED/MS and QC

$\text{CuN}_4\text{C}_{32}\text{H}_{36}$	A. E. Pogonin, N. V. Tverdova, A. A. Ischenko, V. D. Rumyantseva, O. I. Koifman, N. I. Giricheva, and G. V. Girichev J. Mol. Struct., 1085 (2015), 276
$\text{C}_{32}\text{H}_{36}\text{N}_4\text{Ni}$	Nickel etioporphyrin-II Structure by GED/MS and QC G. V. Girichev, A. E. Pogonin, and N. V. Tverdova Manuscript in preparation
$\text{C}_{32}\text{H}_{36}\text{N}_4\text{Ni}$	Nickel-etio porphyrin-II Structure by GED/MS and QC G. V. Girichev, A. E. Pogonin, and Yu. V. Minenkov Manuscript in preparation
$\text{C}_{32}\text{H}_{36}\text{N}_4\text{Zn}$ $\text{ZnN}_4\text{C}_{32}\text{H}_{36}$	Zinc-etio porphyrin-II Structure by GED/MS and QC G. V. Girichev, A. E. Pogonin, and N. V. Tverdova Manuscript in preparation
$\text{C}_{42}\text{H}_{45}\text{N}_6\text{NdO}_6$	Tris-(1-phenyl-3-methyl-4-isobutyryl-pirasil-5-onato)neodymium Thermodynamics of sublimation by Knudsen method N. M. Lazarev, Yu. A. Bessonova, B. I. Petrov, G. A. Abakumov, L. N. Bochkarev, A. V. Safronova, A. V. Arapova, A. V. Krasnov, and G. V. Girichev Coord.Chem., 40 (2014), 1
$\text{C}_{42}\text{H}_{45}\text{N}_6\text{NdO}_6$ $\text{Nd}(\text{C}_{14}\text{H}_{15}\text{N}_2\text{O}_2)_3$	Tris-(1-phenyl-3-methyl-4-isobutyryl-pirasil-5-onato)neodymium Thermodynamics of sublimation by Knudsen method N. M. Lazarev, Yu. A. Bessonova, B. I. Petrov, G. A. Abakumov, L. N. Bochkarev, A. V. Safronova, A. V. Arapova, A. V. Krasnov, and G. V. Girichev Russ. J. Coord. Chem., 40 (3) (2014), 179
$\text{C}_{42}\text{H}_{45}\text{N}_6\text{O}_6\text{Tb}$	Tris-(1-phenyl-3-methyl-4-isobutyryl-pirasil-5-onato)terbium Thermodynamics of sublimation by Knudsen method N. M. Lazarev, Yu. A. Bessonova, B. I. Petrov, G. A. Abakumov, L. N. Bochkarev, A. V. Safronova, A. V. Arapova, A. V. Krasnov, and G. V. Girichev Coord.Chem., 40 (2014), 1
$\text{C}_{42}\text{H}_{45}\text{N}_6\text{O}_6\text{Tb}$ $\text{Tb}(\text{C}_{14}\text{H}_{15}\text{N}_2\text{O}_2)_3$	Tris-(1-phenyl-3-methyl-4-isobutyryl-pirasil-5-onato)terbium Thermodynamics of sublimation by Knudsen method N. M. Lazarev, Yu. A. Bessonova, B. I. Petrov, G. A. Abakumov, L. N. Bochkarev, A. V. Safronova, A. V. Arapova, A. V. Krasnov, and G. V. Girichev Russ. J. Coord. Chem., 40 (3) (2014), 179
$\text{C}_{48}\text{H}_{48}\text{CuN}_8$ $\text{CuN}_8\text{C}_{48}\text{H}_{48}$	Copper(II) 2,9,16,23-tetra-tert-butyl phthalocyanine Structure by GED/MS and QC G. V. Girichev, N. I. Giricheva, O. A. Pimenov, S. Blomeyer, and V. E. Mayzlish Manuscript completed
$\text{C}_{72}\text{H}_{32}\text{F}_{24}\text{MgN}_8$	Magnesium octa(trifluoromethylphenyl)porphyrzine Structure by GED/MS and QC A. V. Zakharov, Yu. A. Zhabanov, S. A. Shlykov, and G. V. Girichev Manuscript completed
$\text{C}_{72}\text{H}_{32}\text{F}_{24}\text{N}_8\text{Mg}$ $\text{MgC}_{72}\text{N}_8\text{F}_{24}\text{H}_{32}$	Magnesium octa(trifluoromethylphenyl)porphyrzine Structure by GED/MS and QC A. V. Zakharov, Yu. A. Zhabanov, S. A. Shlykov, and G. V. Girichev J. Mol. Struct., submitted
	α-Acetylacetone derivatives Structures by QC N. H. Trang, N. V. Belova, H. Oberhammer, and G. V. Girichev

	25th Austin Symposium on Molecular Structure and Dynamics, March 2014, Dallas, USA.- p.246.
	<p>Methane hydrates Structure and electron energy characteristics of methane hydrates by quantum chemical calculations <i>N. I. Giricheva, A. A. Ischenko, V. I. Yusupov, V. N. Bagratashvili, and G. V. Girichev</i> Chem. Techn., 57(9) (2014), 3</p>
	<p>Methane hydrates Electronic structure of methane hydrates <i>N. I. Giricheva, A. A. Ischenko, V. I. Yusupov, V. N. Bagratashvili, and G. V. Girichev</i> Chem. Techn., 57(10) (2014), 13</p>
	<p>Methane hydrates Vibrational Spectra of methane hydrates <i>N. I. Giricheva, A. A. Ischenko, V. I. Yusupov, V. N. Bagratashvili, and G. V. Girichev</i> Chem. Techn., 57(12) (2014), 17</p>
	<p>α- and β-Naphthalenesulfonyl derivatives MS <i>N. I. Giricheva, G. V. Girichev, H. Oberhammer, V. M. Petrov, and V. N. Petrova</i> J. Struct. Chem., (2015), in press</p>
	<p>Benzenesulfonic acid and benzoic acid derivatives QC (Energies of the Gas Phase Deprotonation) <i>S. N. Ivanov, N. I. Giricheva, T. V. Nurkevich, and M. S. Fedorov</i> Zh. Fiz. Khimii, 88(4) (2014), 647 / Russ. J. Phys. Chem. A, 88(4) (2014), 667</p>
	<p>Benzenesulfonic acid derivatives QC (energies of the gas phase deprotonation) <i>S. N. Ivanov, N. I. Giricheva, T. V. Nurkevich, and M. S. Fedorov</i> Zh. Fiz. Khimii, 88(4) (2014), 647 / Russ. J. Phys. Chem. A, 88(4) (2014), 667</p>
	<p>Cobalt, nickel, copper and zinc etioporphyrin-II Structure and vibrational spectra by QC calculations experimental IR spectra <i>V. V. Sliznev, A. E. Pogonin, A. A. Ischenko, and G. V. Girichev</i> Macroheterocycles, 7(1) (2014), 60</p>
	<p>Tris-2,2,6,6-tetramethylheptan-3,5-dionato complexes of rare earth elements Structures by QC <i>V. V. Sliznev, N. V. Belova, and G. V. Girichev</i> Comput. Theor. Chem., 1055 (2015), 78</p>
	<p>Mg-tetra(1,2,5-oxadiazolo)porphyrazine and their S, Se and Te analogs Structure by QC <i>Yu. A. Zhabanov, N. V. Tverdova, and G. V. Girichev</i> Manuscript in preparation</p>