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<b>Be<sub>2</sub></b> Be <sub>2</sub>	<b>Beryllium diiodide</b> Structure by GED/MS and QC (CCSD(T)) S. A. Shlykov, Yu. A. Zhabanov, N. I. Giricheva, A. G. Girichev, and G. V. Girichev Struct. Chem., <b>26</b> (2015) 1451
<b>C<sub>4</sub>N<sub>4</sub>S</b> SN <sub>4</sub> C <sub>4</sub>	<b>1,2,5-Thiadiazole-3,4-dicarbonitrile</b> Structure by GED/MS and QC G. V. Girichev, N. I. Giricheva, and N. V. Tverdova Manuscript ready
<b>C<sub>5</sub>H<sub>9</sub>O<sub>2</sub>Tl</b> TlC <sub>5</sub> H <sub>9</sub> O <sub>2</sub>	<b>Thallium(I) pivalate</b> Structure by GED/MS and QC Yu. A. Zhabanov, O. A. Pimenov, S. Blomeyer, and G. V. Girichev 16th European symposium on gas-phase electron diffraction, Frauenchiemsee, Germany, June 21-26, 2015, Book of abstracts, page 48.
<b>C<sub>5</sub>H<sub>12</sub>OSi</b> C <sub>4</sub> H <sub>8</sub> OSiH(CH <sub>3</sub> )	<b>3-Methyl-3-silatetrahydropyran</b> Synthesis and conformational analysis by GED/MS, IR, NMR and QC B. A. Shainyan, S. V. Kirpichenko, N. N. Chipanina, L. P. Oznobikhina, E. Kleinpeter, S. A. Shlykov, and D. Yu. Osadchiy J. Org. Chem., <b>80</b> (21) (2015) 12492
<b>C<sub>5</sub>H<sub>12</sub>SSi</b> C <sub>4</sub> H <sub>8</sub> SSiH(CH <sub>3</sub> )	<b>3-Methyl-3-silathiane</b> Structure by GED/MS, IR and QC S. A. Shlykov, D. Yu. Osadchiy, N. N. Chipanina, L. P. Oznobikhina, and B. A. Shainyan J. Mol. Struct., <b>1100</b> (2015) 555

<b>C<sub>6</sub>H<sub>10</sub>N<sub>2</sub></b> C <sub>5</sub> H <sub>10</sub> N-CN	<b>N-Cyanopiperidine</b> Structure by GED/MS and QC <i>Tran Dinh Phien, S. A. Shlykov, Y. Gao, and P. M. Weber</i> Manuscript in preparation
<b>C<sub>7</sub>H<sub>7</sub>NO<sub>5</sub>S</b>	<b>2-Nitrobenzenesulfonic acid methyl ester (2-nitrobenzenesulfonate)</b> Structure by GED/MS and QC <i>M. S. Fedorov, N. I. Giricheva, G. V. Girichev, and S. N. Ivanov</i> J. Mol. Struct., <b>1085</b> (2015) 191
<b>C<sub>7</sub>H<sub>7</sub>NO<sub>5</sub>S</b>	<b>4-Nitrobenzenesulfonic acid methyl ester (4-nitrobenzenesulfonate)</b> Structure by GED/MS and QC <i>N. I. Giricheva, M. S. Fedorov, and G. V. Girichev</i> Struct. Chem., <b>26</b> (2015) 1543
<b>C<sub>8</sub>H<sub>5</sub>N<sub>3</sub></b>	<b>3-Aminophthalonitrile</b> Structure by GED/MS and QC <i>D. S. Savelyev, N. I. Giricheva, N. Vogt, M. K. Islyaikin, and G. V. Girichev</i> Manuscript in preparation
<b>C<sub>8</sub>H<sub>5</sub>N<sub>3</sub></b>	<b>3-Aminophthalonitrile</b> IR spectrum <i>D. S. Savelyev, M. K. Islyaikin, and G. V. Girichev</i> submitted in February
<b>C<sub>8</sub>H<sub>6</sub>N<sub>2</sub>O<sub>2</sub></b>	<b>3-Aminophthalimide</b> IR spectrum <i>D. S. Savelyev, M. K. Islyaikin, and G. V. Girichev</i> submitted in January
<b>C<sub>8</sub>H<sub>6</sub>N<sub>2</sub>O<sub>2</sub></b>	<b>3-Aminophthalimide</b> Structure by GED/MS and QC <i>D. S. Savelyev, M. K. Islyaikin, N. I. Giricheva, N. Vogt, and G. V. Girichev</i> Manuscript in preparation
<b>C<sub>9</sub>H<sub>20</sub>SSi</b>	<b>1-tert-Butyl-1-silacyclohexane</b> Structure by GED/MS, Raman spectrum and QC <i>A. V. Belyakov, Yu. Sigolaev, S. A. Shlykov, S. Wallevik, N. R. Jonsdottir, R. Bjornsson, S. Jonsdottir, A. Kvaran, T. Kern, K. Hassler, and I. Arnason</i> Struct. Chem., <b>26</b> (2) 2015 445
<b>C<sub>10</sub>H<sub>6</sub>Cl<sub>2</sub>O<sub>4</sub>S<sub>2</sub></b>	<b>1,5-Naphthalene disulfonyl dichloride</b> 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 ready
<b>C<sub>10</sub>H<sub>9</sub>NO<sub>2</sub>S</b>	<b>α-Naphthalene sulfonamide</b> Structure by GED/MS and QC <i>V. N. Petrova, S. A. Shlykov, S. N. Ivanov, and G. V. Girichev</i> J. Phys. Chem. A, <b>119</b> (9) (2015) 1502
<b>C<sub>10</sub>H<sub>9</sub>NO<sub>2</sub>S</b>	<b>β-Naphthalene sulfonamide</b> Structure by GED/MS and QC <i>V. N. Petrova, S. A. Shlykov, S. N. Ivanov, and G. V. Girichev</i> J. Phys. Chem. A, <b>119</b> (9) (2015) 1502
<b>C<sub>10</sub>H<sub>18</sub>Si<sub>2</sub></b> (CH <sub>3</sub> ) <sub>3</sub> Si-C≡C-C≡C-Si(CH <sub>3</sub> ) <sub>3</sub>	<b>1,4-Bis(trimethylsilyl)-1,3-butadiyne</b> Structure by GED/MS and QC <i>N. V. Tverdova, A. A. Otyotov, N. I. Giricheva, G. V. Girichev, and N. W. Mitzel</i> Manuscript in preparation

<b>C<sub>10</sub>H<sub>8</sub></b> C <sub>10</sub> H <sub>8</sub>	<b>Naphthalene</b> 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
<b>C<sub>11</sub>H<sub>12</sub>N<sub>2</sub>O<sub>2</sub></b>	<b>L-Tryptophan</b> Structure by GED/MS and QC <i>V. V. Tyunina, N. I. Giricheva, and G. V. Girichev</i> Manuscript in preparation
<b>C<sub>11</sub>H<sub>15</sub>N</b> C <sub>5</sub> H <sub>10</sub> N-C <sub>6</sub> H <sub>5</sub>	<b>N-Phenylpiperidine</b> Structure by GED/MS and QC <i>Tran Dinh Phien, S. A. Shlykov, Y. Gao, and P. M. Weber</i> Manuscript in preparation
<b>C<sub>11</sub>H<sub>16</sub>OSi</b>	<b>3-Methyl-3-phenyl-3-silatetrahydropyran</b> Structure by GED/MS, NMR and QC <i>B. A. Shainyan, S. V. Kirpichenko, E. Kleinpeter, S. A. Shlykov, and D. Yu. Osadchiy</i> Tetrahedron, <b>71</b> (2015) 3810
<b>C<sub>11</sub>H<sub>21</sub>N</b> C <sub>5</sub> H <sub>10</sub> N-C <sub>6</sub> H <sub>11</sub>	<b>N-Cyclohexylpiperidine</b> Structure by GED/MS and QC calculations, IR spectrum <i>Tran Dinh Phien, S. A. Shlykov, Y. Gao, and P. M. Weber</i> Struct. Chem., <b>26</b> (5) (2015) 1501
<b>C<sub>12</sub>H<sub>10</sub></b> C <sub>12</sub> H <sub>10</sub>	<b>Acenaphthene</b>  Manuscript in preparation
<b>C<sub>12</sub>H<sub>14</sub>N<sub>2</sub>O<sub>2</sub>S</b>	<b>Dansylamide</b> Conformations in gas and crystal <i>N. I. Giricheva, E. A. Lapykina, M. S. Fedorov, and D. A. Petrova</i> J. Struct. Chem., <b>56</b> (4) (2015) 619
<b>C<sub>12</sub>H<sub>18</sub>Si</b> C <sub>5</sub> H <sub>10</sub> Si(C <sub>6</sub> H <sub>5</sub> )CH <sub>3</sub>	<b>1-Methyl-1-phenyl-1-silacyclohexane</b> GED/MS and QC <i>S. A. Shlykova and D. Yu. Osadchiy</i> Refinement in progress
<b>C<sub>12</sub>H<sub>8</sub></b> C <sub>12</sub> H <sub>8</sub>	<b>Acenaphthylene</b> Structure by QC
<b>C<sub>14</sub>H<sub>10</sub></b> C <sub>14</sub> H <sub>10</sub>	<b>Anthracene</b> Structure by GED/MS and QC <i>N. V. Tverdova, A. A. Otlyotov, V. M. Petrov, V. N. Petrova, N. I. Giricheva, and G. V. Girichev</i> Manuscript in preparation
<b>C<sub>15</sub>H<sub>21</sub>FeO<sub>6</sub></b> Fe(C <sub>5</sub> H <sub>7</sub> O <sub>2</sub> ) <sub>3</sub>	<b>Iron trisacetylacetonate</b> Molecular and electronic structure by GED/MS and QC <i>A. A. Petrova, G. V. Girichev, N. I. Giricheva, and N. P. Kuzmina</i> Manuscript in preparation
<b>C<sub>16</sub>N<sub>16</sub>S<sub>4</sub>Zn</b> ZnS <sub>4</sub> N <sub>16</sub> C <sub>16</sub>	<b>Zinc tetrakis(thiadiazole)porphyrazine</b> Structure by GED/MS and QC <i>N. V. Tverdova, N. I. Giricheva, D. S. Savelyev, and G. V. Girichev</i> Manuscript ready
	<b>Potassium lanthanum tetrakisacetylacetonates</b>

$C_{20}H_4F_{24}KLaO_8$	Structure by QC  <i>N. V. Belova, A. E. Khochenkov, V. V. Sliznev, and G. V. Girichev</i> VI. All-Russian youth school-conference "Quantum chemical calculation: structure and reactivity of organic and inorganic molecules" Ivanovo, 2015, Book of articles, p. 353-357
$C_{24}H_{26}Si_2$ $C_{24}H_{26}Si_2$	<b>1,8-Bis(trimethylsilylethynyl)anthracene</b> Structure by GED/MS and QC calculations <i>N. V. Tverdova, Yu. A. Zhabanov, V. V. Rybkin, A. A. Otlyotov, N. I. Giricheva, and G. V. Girichev</i> Manuscript in preparation
$C_{28}H_{28}N_4Ni$ $NiN_4C_{28}H_{28}$	<b>Nickel octamethylporphyrin</b> Structure by GED/MS and QC <i>A. E. Pogonin, N. V. Tverdova, Yu. V. Minenkov, N. I. Giricheva, and G. V. Girichev</i> Manuscript in preparation
$C_{28}H_{28}N_4Ni$ $NiN_4C_{28}H_{28}$	<b>Nickel octamethylporphyrin</b> Structure by GED/MS and QC <i>G. V. Girichev, A. E. Pogonin, and N. V. Tverdova</i> School-Conference «Atomistic Simulation of Functional Materials (ASFM 2014)» <a href="http://atomisticmodel.ru/ASFM2014%20Book%20of%20abstracts.pdf">http://atomisticmodel.ru/ASFM2014%20Book%20of%20abstracts.pdf</a>
$C_{30}H_{18}$ $C_{30}H_{18}$	<b>1,8-Bis(phenylethynyl)anthracene</b> Structure by GED/MS, XRD and QC calculations <i>J.-H. Lamm, J. Horstmann, H.-G. Stammer, N. W. Mitzel, Yu. A. Zhabanov, N. V. Tverdova, A. A. Otlyotov, N. I. Giricheva, and G. V. Girichev</i> Org. Biomol. Chem., <b>13</b> (2015) 8893
$C_{32}H_{36}CoN_4$ $CoN_4C_{32}H_{36}$	<b>Cobalt etioporphyrin-II</b> Structure by GED/MS and QC <i>G. V. Girichev, A. E. Pogonin, and N. V. Tverdova</i> VII All-Russian youth school-conference "Quantum chemical calculation: structure and reactivity of organic and inorganic molecules" Ivanovo, 2015, Book of articles, p.240-244
$C_{32}H_{36}CoN_4$ $CoN_4C_{32}H_{36}$	<b>Cobalt etioporphyrin-II</b> Structure by GED/MS and QC <i>G. V. Girichev, A. E. Pogonin, N. V. Tverdova, and N. I. Giricheva</i> Manuscript in preparation
$C_{32}H_{36}CuN_4$ $CuN_4C_{32}H_{36}$	<b>Copper etioporphyrin-II</b> Structure by GED/MS and QC <i>A. E. Pogonin, N. V. Tverdova, A. A. Ischenko, V. D. Rumyantseva, O. I. Koifman, N. I. Giricheva, and G. V. Girichev</i> J. Mol. Struct., <b>1085</b> (2015) 276
$C_{32}H_{36}N_4Ni$ $NiN_4C_{32}H_{36}$	<b>Nickel-etioporphyrin-II</b> Structure by GED/MS and QC <i>G. V. Girichev, A. E. Pogonin, and N. V. Tverdova</i> School-Conference «Atomistic Simulation of Functional Materials (ASFM 2014)» <a href="http://atomisticmodel.ru/ASFM2014%20Book%20of%20abstracts.pdf">http://atomisticmodel.ru/ASFM2014%20Book%20of%20abstracts.pdf</a>
$C_{32}H_{36}N_4Ni$	<b>Nickel-etioporphyrin-II</b> Structure by GED/MS and QC

$\text{NiN}_4\text{C}_{32}\text{H}_{36}$	<i>G. V. Girichev, A. E. Pogonin, N. V. Tverdova, and N. I. Giricheva</i> Manuscript in preparation
$\text{C}_{32}\text{H}_{36}\text{N}_4\text{Zn}$ $\text{ZnN}_4\text{C}_{32}\text{H}_{36}$	<b>Zinc-etioporphyrin-II</b> Structure by GED/MS and QC <i>N. V. Tverdova, A. E. Pogonin, A. A. Ischenko, V. D. Rumyantseva, O. I. Koifman, N. I. Giricheva, and G. V. Girichev</i> Struct. Chem., <b>26</b> (5) (2015) 1521
$\text{C}_{44}\text{H}_{28}\text{N}_4\text{Pd}$ $\text{PdN}_4\text{C}_{20}\text{H}_8\text{C}_{24}\text{H}_{20}$	<b>Palladium tetraphenylporphyrin</b> Structure by GED/MS and QC, IR spectrum <i>D. S. Savelyev, N. V. Tverdova, N. I. Giricheva, V. A. Ol'shevckaya, and G. V. Girichev</i> Manuscript ready
$\text{C}_{44}\text{H}_{28}\text{N}_4\text{Zn}$ $\text{ZnN}_4\text{C}_{20}\text{H}_8\text{C}_{24}\text{H}_{20}$	<b>Zinc tetraphenylporphyrin</b> Structure by GED/MS and QC, IR spectrum <i>D. S. Savelyev, N. V. Tverdova, N. I. Giricheva, and G. V. Girichev</i> Manuscript is ready
$\text{C}_{48}\text{H}_{48}\text{CuN}_8$ $\text{CuN}_8\text{C}_{48}\text{H}_{48}$	<b>Copper(II) 2,9,16,23-tetra-tert-butylphthalocyanine</b> Structure by GED/MS and QC <i>O. A. Pimenov, N. I. Giricheva, S. Blomeyer, V. E. Mayzlish, N. W. Mitzel, and G. V. Girichev</i> Struct. Chem., <b>26</b> (5) (2015) 1531
$\text{C}_{72}\text{H}_{32}\text{F}_{24}\text{MgN}_8$ $\text{MgC}_{72}\text{N}_8\text{F}_{24}\text{H}_{32}$	<b>Magnesium octa(trifluoromethylphenyl)porphyrazine</b> Structure by GED/MS and QC <i>Yu. A. Zhabanov, A. V. Zakharov, N. I. Giricheva, S. A. Shlykov, O. I. Koifman, and G. V. Girichev.</i> J. Mol. Struct., <b>1092</b> (2015) 104
	<b>Napthalenesulfonyl derivatives</b> 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
	<b>Napthalensulfonyl derivatives</b> mass spectra and electron ionization <i>N. I. Giricheva, G. V. Girichev, H. Oberhammer, V. M. Petrov, and V. N. Petrova</i> J. Struct. Chem., (2016) in press
	<b>Pyridine N-oxides</b> Structure by QC calculations <i>N. V. Belova, N. I. Giricheva, and M. S. Fedorov</i> Struct. Chem., <b>26</b> (2015) 1459
	<b>Rare earth trisdipivaloylmethanates</b> Structure and vibrational spectra by QC calculations, experimental IR and Raman spectra <i>N. V. Belova, V. V. Sliznev, D. Christen, and G. V. Girichev</i> Manuscript in preparation
	<b>Aluminum(III), gallium(III), indium(III) and thallium(III) pivalate</b> Structure and vibrational spectra by QC calculations <i>O. A. Pimenov, Yu. A. Zhabanov, A. E. Pogonin, S. Blomeyer, and B. V. Puchkov</i> Struct. Chem., <b>26</b> (5) (2015) 1443
	<b>N-Piperidine derivatives</b> Structure by QC <i>Tran Dinh Phien and S. A. Shlykov</i> submitted
	<b>Tris-2,2,6,6-tetramethyl-heptane-3,5-dionato complexes of rare earth elements</b> Structure by QC

	<p><i>V. V. Sliznev, N. V. Belova, and G. V. Girichev</i>  Comput. Theor. Chem., <b>1055</b> (2015) 78</p>
	<p><b>Molybdenum and tungsten tri- and tetrachlorides and tri- and tetrafluorides</b>  Geometrical and electronic structure by QC calculations  Jahn-Teller effect and spin-orbit coupling  <i>V. V. Sliznev</i>  16th European symposium on gas-phase electron diffraction,  Frauenchiemsee, Germany, June 21-26, 2015, Book of abstracts, page  11.</p>
	<p><b>Magnesium tetra(1,2,5-oxadiazolo)-, tetra(1,2,5-sulfuradiazolo)-, tetra(1,2,5-selenadiazolo)-, and tetra(1,2,5-telluradiazolo)porphyrazines and their monohydrates</b>  Structure by QC  <i>Yu. A. Zhabanov, N. V. Tverdova, and G. V. Girichev</i>  Manuscript in preparation</p>