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<b>Br<sub>2</sub>Se</b> SeBr <sub>2</sub>	<b>Selenium dibromide</b> S. A. Shlykov, N. I. Giricheva, G. V. Girichev, H. Oberhammer and A. V. Titov Structure from GED/MS and QC , QC for TeX <sub>2</sub> (X=F, Cl, Br, I) Phys. Chem. Chem. Phys. <b>10</b> (2008), 6438–6445.
<b>Br<sub>2</sub>Te</b> TeBr <sub>2</sub>	<b>Tellurium dibromide</b> S. A. Shlykov, N. I. Giricheva, G. V. Girichev, H. Oberhammer and A. V. Titov Structure from GED/MS and QC , QC for SeX <sub>2</sub> (X=F, Cl, Br, I) Eur. J. Inorg. Chem. <b>33</b> (2008), 5220 – 5227
<b>Br<sub>3</sub>La</b> LaBr <sub>3</sub>	<b>Lanthanum tribromide</b> D. A. Ivanov, V. V. Sliznev, L. S. Kudin, M. F. Butman Structure by QC calculation and MS study Chemistry and Chemical Technology Research-Engineering Journal, 2008, accepted
<b>Br<sub>3</sub>Lu</b> LuBr <sub>3</sub>	<b>Lutetium tribromide</b> N. I. Giricheva, S. A. Shlykov, G. V. Girichev, E. V. Chernova and E. Lapykina Structure by GED/MS and QC Zh. Strukt. Khim., submitted
<b>Br<sub>3</sub>Y</b> YBr <sub>3</sub>	<b>Yttrium tribromide</b> N. I. Giricheva, S. A. Shlykov, G. V. Girichev, and H. Oberhammer Structure by GED/MS and QC Manuscript in preparation
<b>Br<sub>3</sub>Yb</b> YbBr <sub>3</sub>	<b>Ytterbium tribromide</b> N. I. Giricheva, S. A. Shlykov, G. V. Girichev, and H. Oberhammer Structure by GED/MS and QC Manuscript in preparation

$\text{Br}_4\text{LaNa}$ $\text{NaLaBr}_4$	<p><b>Sodium tetrabromolanthanum</b>  D. A. Ivanov, V. V. Sliznev, L. S. Kudin, M. F. Butman  structure by QC calculation and MS study  Chemistry and Chemical Technology Research-Engineering Journal,  2008, accepted</p>
$\text{Br}_4\text{La}^-$ $\text{LaBr}_4^-$	<p><b>Lanthanum tetrabromide anion</b>  D. A. Ivanov, V. V. Sliznev, L. S. Kudin, M. F. Butman  Structure by QC calculation and MS study  Chemistry and Chemical Technology Research-Engineering Journal,  2008, accepted</p>
$\text{Br}_4\text{La}^-$ $\text{LaBr}_4^-$	<p><b>Lanthanum tetrabromide anion</b>  M. F. Butman, V. V. Sliznev, L. S. Kudin, D. A. Ivanov, V. B. Motalov,  K. V. Cramer  Structure by QC calculation and MS study  Zh. Fiz. Khim., 2008, accepted</p>
$\text{C}_4\text{Br}_4\text{S}$	<p><b>Tetrabromothiophene</b>  S. A. Shlykov, F. Blockhuys  Structure by GED/MS and QC  Manuscript in preparation</p>
$\text{C}_4\text{H}_5\text{ClO}_2$ $\text{C}_4\text{H}_5\text{O}_2\text{Cl}$	<p><b>1-Chloro-1,3-butanedion</b>  N. V. Belova, H. Oberhammer, G. V. Girichev, S. A. Shlykov  Tautomeric and conformational properties by ab initio study  J. Chem. Phys. A., in press</p>
$\text{C}_4\text{H}_7\text{NO}_3$	<p><b>Malonamic acid methyl ester</b>  N. V. Belova, H. Oberhammer, S. A. Shlykov  Tautomeric and conformational properties by GED and QC study  J. Phys. Chem. A. <b>112</b> (18) (2008), 4355-4359</p>
$\text{C}_5\text{H}_4\text{FNO}_4\text{S}$ $\text{C}_5\text{H}_4\text{SO}_4\text{NF}$	<p><b>2-Nitrobenzenesulphonyl fluoride</b>  V. M. Petrov, G. V. Girichev, H. Oberhammer, V. N. Petrova, N. I.  Giricheva, A. V. Bardina, S. N. Ivanov  Conformation analysis, ra, rh1 structure by GED and quantum chemical  calculations, vapour composition by GED and MS.  J. Phys. Chem. A, in press.</p>
$\text{C}_5\text{H}_7\text{ClO}_2$	<p><b>3-Chloro-2,4-pentanedione</b>  N. V. Belova, H. Oberhammer, G. V. Girichev, S. A. Shlykov  Tautomeric and conformational properties by GED and QC study</p>

	J. Phys. Chem. A. <b>112</b> (14) (2008), 3209-3214
<b>C<sub>6</sub>H<sub>4</sub>ClNO<sub>4</sub>S</b> C <sub>6</sub> H <sub>4</sub> SO <sub>4</sub> NCl	<b>4-Nitrobenzenesulphonyl chloride</b> V. M. Petrov, V. N. Petrova, G. V. Girichev, N. I. Giricheva, H. Oberhammer, A. V. Bardina, S. N. Ivanov, A. V. Krasnov Molecular structure by GED, DFT, MP2 calculations Zh. Strukt. Khim., in press.
<b>C<sub>6</sub>H<sub>4</sub>ClNO<sub>4</sub>S</b> C <sub>6</sub> H <sub>4</sub> SO <sub>4</sub> NCl	<b>2-Nitrobenzenesulphonyl chloride</b> V. M. Petrov, H. Oberhammer, N. I. Giricheva, G. V. Girichev, V. N. Petrova, S. N. Ivanov Molecular structure by GED, DFT calculations, conformation composition. in progress
<b>C<sub>6</sub>H<sub>4</sub>Cl<sub>2</sub>O<sub>2</sub>S</b> C <sub>6</sub> H <sub>4</sub> SO <sub>2</sub> Cl <sub>2</sub>	<b>2-Chlorobenzenesulphonyl chloride</b> V. N. Petrova, V. M. Petrov, G. V. Girichev, H. Oberhammer, S. N. Ivanov Molecular structure by GED, DFT, MP2 calculations Zh. Strukt. Khim. <b>49</b> (5) (2008), 883-890.
<b>C<sub>6</sub>H<sub>4</sub>NO<sub>5</sub>S</b> C <sub>6</sub> H <sub>4</sub> SO <sub>5</sub> N	<b>2-Nitrobenzene sulphoacid</b> V. M. Petrov, N. I. Giricheva, V. N. Petrova, G. V. Girichev, S. N. Ivanov Molecular structure by GED, DFT calculations, conformation composition Zh. Strukt. Khim.
<b>C<sub>6</sub>H<sub>4</sub>NO<sub>5</sub>S</b> C <sub>6</sub> H <sub>4</sub> SO <sub>5</sub> N	<b>3-Nitrobenzene sulphoacid</b> V. M. Petrov, N. I. Giricheva, G. V. Girichev, V. N. Petrova, S. N. Ivanov Molecular structure by GED, DFT calculations, conformation composition in progress
<b>C<sub>6</sub>H<sub>13</sub>FSi</b> C <sub>5</sub> H <sub>10</sub> SiFCH <sub>3</sub>	<b>1-Flouro-1-methyl-1-silacyclohexane</b> I. Arnason, N. I. Giricheva, G. V. Girichev Structure and conformations by GED and QC calculations Manuscript in preparation
<b>C<sub>7</sub>H<sub>5</sub>F<sub>3</sub>S</b> C <sub>6</sub> H <sub>5</sub> SCF <sub>3</sub>	<b>Trifluoromethylphenyl sulfide</b> H. Oberhammer, G. V. Girichev, N. I. Giricheva, S. A. Shlykov, Moscow GED

	<p>The molecular structure, GED/MS, MP2 J. Mol. Struct., in press</p>
<p><b>C<sub>7</sub>H<sub>5</sub>F<sub>3</sub>S</b> C<sub>6</sub>H<sub>5</sub>SCF<sub>3</sub></p>	<p><b>(Trifluoromethyl)thiobenzene</b> N. I. Giricheva, S. A. Shlykov, G. V. Girichev, and H. Oberhammer Structure of the “overheated molecule” by GED/MS and QC Manuscript in preparation</p>
<p><b>C<sub>7</sub>H<sub>5</sub>F<sub>3</sub>S</b> C<sub>6</sub>H<sub>5</sub>SCF<sub>3</sub></p>	<p><b>(Trifluoromethyl)thiobenzene</b> I. F. Shishkov, L. V. Khristenko, A. N. Rykov, L. V. Vilkov, N. I. Giricheva, S. A. Shlykov, G. V. Girichev, H. Oberhammer r<sub>h1</sub> and r<sub>g</sub> structures by GED and <i>ab initio</i> calculations J. Mol. Struct. <b>876</b> (2008), 147–153</p>
<p><b>C<sub>7</sub>H<sub>9</sub>NO<sub>2</sub>S</b> C<sub>7</sub>H<sub>7</sub>SO<sub>2</sub>NH<sub>2</sub></p>	<p><b>p-Methylbenzenesulphonamide</b> V. M. Petrov, G. V. Girichev, H. Oberhammer, V. N. Petrova, N. I. Giricheva, A. V. Bardina Molecular structure by GED, DFT, MP2 calculations conformation composition J. Phys. Chem. A <b>112</b> (113) (2008), 2969-2976</p>
<p><b>C<sub>7</sub>H<sub>9</sub>NO<sub>2</sub>S</b> C<sub>7</sub>H<sub>7</sub>SO<sub>2</sub>NH<sub>2</sub></p>	<p><b>o-Methylbenzenesulphonamide</b> V. M. Petrov, G. V. Girichev, H. Oberhammer, V. N. Petrova, N. I. Giricheva, A. V. Bardina Molecular structure by GED, DFT, MP2 calculations conformation composition J. Phys. Chem. A <b>112</b> (113) (2008), 2969-2976</p>
<p><b>C<sub>7</sub>H<sub>13</sub>F<sub>3</sub>Si</b></p>	<p><b>1-Methyl-1-trifluormethyl-1-silacyclohexane</b> I. Arnason, N. I. Giricheva, G. V. Girichev Structure and conformations by GED and QC calculations Manuscript in preparation</p>
<p><b>C<sub>10</sub>H<sub>2</sub>CaF<sub>12</sub>O<sub>4</sub></b> C<sub>10</sub>H<sub>2</sub>O<sub>4</sub>F<sub>12</sub>Ca</p>	<p><b>Calcium hexafluoroacetylacetonate</b> N. V. Belova, G. V. Girichev, H. Oberhammer Internal rotation of CH<sub>3</sub> groups by DFT calculations Zh. Strukt. Khim., manuscript in preparation</p>
<p><b>C<sub>10</sub>H<sub>14</sub>CaO<sub>4</sub></b></p>	<p><b>Calcium acetylacetonate</b> N. V. Belova, G. V. Girichev, H. Oberhammer Internal rotation of CH<sub>3</sub> groups by DFT calculations Zh. Strukt. Khim., manuscript in preparation</p>

<p><b>C<sub>10</sub>H<sub>14</sub>O<sub>4</sub>Zn</b> ZnO<sub>4</sub>C<sub>10</sub>H<sub>14</sub></p>	<p><b>Zinc acetylacetonate</b> 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 Structure by GED and DFT calculations; vibrational frequencies by DFT calculations Zh. Strukt. Khim., in press</p>
<p><b>C<sub>11</sub>H<sub>12</sub>AuNO</b> AuC<sub>11</sub>H<sub>12</sub>NO</p>	<p><b>Dimethylgold oxinate</b> V. V. Rybkin, A. A. Besonov Structure and vibrational frequencies by DFT, electronic spectrum by TD-DFT and MCQDPT; experimental IR- and UV-visual-spectra Manuscript in preparation</p>
<p><b>C<sub>11</sub>H<sub>12</sub>AuNS</b> AuC<sub>11</sub>H<sub>12</sub>NS</p>	<p><b>Dimethylgold thiooxinate</b> V. V. Rybkin, A. A. Bessonov Structure and vibrational frequencies by DFT, electronic spectrum by TD-DFT and MCQDPT; experimental IR- and UV-visual-spectra Manuscript in preparation</p>
<p><b>C<sub>12</sub>H<sub>18</sub>CuN<sub>2</sub>O<sub>2</sub></b> C<sub>12</sub>H<sub>18</sub>N<sub>2</sub>O<sub>2</sub>Cu</p>	<p><b>N,N'-Ethylene-bis(acetylacetonateiminato)copper</b> G. V. Girichev, N. V. Tverdova, A. V. Zakharov, N. P. Kuzmina, O. V. Kotova Structure, IR spectra by Qc and experimental study Manuscript in preparation</p>
<p><b>C<sub>12</sub>H<sub>18</sub>CuN<sub>2</sub>O<sub>2</sub></b> C<sub>12</sub>H<sub>18</sub>N<sub>2</sub>O<sub>2</sub>Cu</p>	<p><b>N,N'-ethylene-bis(acetylacetonateiminato)copper(II)</b> N. I. Giricheva, G. V. Girichev, Yu. S. Medvedeva, N. P. Kuzmina, O. V. Kotova Structure by GED and QC calculations Zh. Strukt. Khim., submitted</p>
<p><b>C<sub>12</sub>H<sub>18</sub>N<sub>2</sub>NiO<sub>2</sub></b> C<sub>12</sub>H<sub>18</sub>N<sub>2</sub>O<sub>2</sub>Ni</p>	<p><b>N,N'-Ethylene-bis(acetylacetonateiminato)nickel</b> N. V. Tverdova, G. V. Girichev, A. V. Zakharov, N. P. Kuzmina, O. V. Kotova Structure, IR spectra by QC Zh. Fiz. Khim., accepted</p>
<p><b>C<sub>12</sub>H<sub>18</sub>N<sub>2</sub>O<sub>2</sub>Zn</b></p>	<p><b>N,N'-Ethylene-bis(acetylacetonateiminato)zinc</b> N. V. Tverdova, G. V. Girichev, A. V. Zakharov, N. P. Kuzmina, O. V. Kotova Structure, IR spectra by QC Zh. Fiz. Khim., accepted</p>

<p><b>C<sub>15</sub>H<sub>3</sub>DyF<sub>18</sub>O<sub>6</sub></b> DyC<sub>15</sub>F<sub>18</sub>O<sub>6</sub>H<sub>3</sub></p>	<p><b>Tris(hexafluoroacetylacetonato)dysprosium</b> G. V. Girichev, V. V. Rybkin, N. V. Tverdova, S. A. Shlykov, N. P. Kuzmina, I. G. Zaitseva Vapour composition by MS, r<sub>h1</sub> and r<sub>g</sub> structures by GED, <i>ab initio</i> calculations Zh. Strukt. Khim. <b>49</b> (6) (2008), 1041-1051</p>
<p><b>C<sub>15</sub>H<sub>3</sub>ErF<sub>18</sub>O<sub>2</sub></b> Er(C<sub>5</sub>O<sub>2</sub>HF<sub>6</sub>)<sub>3</sub></p>	<p><b>Tris(hexafluoroacetylacetonato)erbium</b> N.V. Tverdova, G. V. Girichev, V.V. Rybkin, S. A. Shlykov, N.P. Kuzmina, I.G. Zaitseva Structure by GED/MS and quantum chemical study Zh. Strukt. Khim. <b>49</b> (6) (2008), 1041-1051</p>
<p><b>C<sub>15</sub>H<sub>3</sub>F<sub>8</sub>O<sub>6</sub>Sm</b></p>	<p><b>Tris(hexafluoroacetylacetonato)samarium</b> G. V. Girichev, V. V. Rybkin, N. V. Tverdova, S. A. Shlykov, N. P. Kuzmina, I. G. Zaitseva Vapour composition by MS, r<sub>h1</sub> and r<sub>g</sub> structures by GED, <i>ab initio</i> calculations Zh. Strukt. Khim., submitted</p>
<p><b>C<sub>15</sub>H<sub>3</sub>F<sub>18</sub>HoO<sub>6</sub></b> HoC<sub>15</sub>F<sub>18</sub>O<sub>6</sub>H<sub>3</sub></p>	<p><b>Tris(hexafluoroacetylacetonato)holmium</b> G. V. Girichev, V. V. Rybkin, N. V. Tverdova, S. A. Shlykov, N. P. Kuzmina, I. G. Zaitseva Vapour composition by MS, r<sub>h1</sub> and r<sub>g</sub> structures by GED, <i>ab initio</i> calculations Zh. Strukt. Khim. <b>49</b> (6) (2008), 1041-1051</p>
<p><b>C<sub>15</sub>H<sub>3</sub>F<sub>18</sub>LaO<sub>6</sub></b> LaC<sub>15</sub>F<sub>18</sub>O<sub>6</sub>H<sub>3</sub></p>	<p><b>Tris(hexafluoroacetylacetonato)lanthanum</b> G. V. Girichev, V. V. Rybkin, N. V. Tverdova, S. A. Shlykov, N. P. Kuzmina, I. G. Zaitseva Vapour composition by MS, r<sub>h1</sub> and r<sub>g</sub> structures by GED, <i>ab initio</i> calculations Zh. Strukt. Khim., submitted</p>
<p><b>C<sub>15</sub>H<sub>3</sub>F<sub>18</sub>NdO<sub>6</sub></b> NdC<sub>15</sub>F<sub>18</sub>O<sub>6</sub>H<sub>3</sub></p>	<p><b>Tris(hexafluoroacetylacetonato)neodymium</b> G. V. Girichev, V. V. Rybkin, N. V. Tverdova, S. A. Shlykov, N. P. Kuzmina, I. G. Zaitseva Vapour composition by MS, r<sub>h1</sub> and r<sub>g</sub> structures by GED, DFT calculations Zh. Strukt. Khim., submitted</p>
<p><b>C<sub>15</sub>H<sub>3</sub>F<sub>18</sub>O<sub>6</sub>Sc</b> C<sub>15</sub>H<sub>3</sub>O<sub>6</sub>F<sub>18</sub>Sc</p>	<p><b>Scandium hexafluoroacetylacetonate</b> N. V. Belova, G. V. Girichev, H. Oberhammer Internal rotation of CH<sub>3</sub> groups by DFT calculations</p>

	Zh. Strukt. Khim., manuscript in preparation
<b>C<sub>15</sub>H<sub>3</sub>F<sub>18</sub>O<sub>6</sub>Yb</b> YbC <sub>15</sub> F <sub>18</sub> O <sub>6</sub> H <sub>3</sub>	<b>Tris(hexafluoroacetylacetonato)ytterbium</b> G. V. Girichev, V. V. Rybkin, N. V. Tverdova, S. A. Shlykov, N. P. Kuzmina, I. G. Zaitseva Vapour composition by MS, r <sub>h1</sub> and r <sub>g</sub> structures by GED, <i>ab initio</i> calculations Zh. Strukt. Khim. <b>49</b> (6) (2008), 1041-1051.
<b>C<sub>15</sub>H<sub>21</sub>O<sub>6</sub>Sc</b> C <sub>15</sub> H <sub>21</sub> O <sub>6</sub> Sc	<b>Scandium acetylacetonate</b> N. V. Belova, G. V. Girichev, H. Oberhammer Internal rotation of CH <sub>3</sub> groups by DFT calculations Zh. Strukt. Khim., manuscript in preparation
<b>C<sub>16</sub>H<sub>8</sub>N<sub>8</sub>OTi</b> C <sub>16</sub> H <sub>8</sub> N <sub>8</sub> OTi	<b>Oxotitaniumtetraazaporphyrin</b> A. V. Zakharov, G. V. Girichev Structure and vibrational frequencies by DFT calculations Journal of Molecular Structure: THEOCHEM, in press
<b>C<sub>16</sub>H<sub>14</sub>CuN<sub>2</sub>O<sub>2</sub></b> C <sub>14</sub> H <sub>16</sub> N <sub>2</sub> O <sub>2</sub> Cu	<b>N,N-bis(salicylidene)ethylenediaminocopper</b> N. V. Tverdova, G. V. Girichev, A. V. Zakharov, N. P. Kuzmina, O. V. Kotova Structure, IR spectra by QC Zh. Fiz. Khim., accepted
<b>C<sub>16</sub>H<sub>14</sub>CuN<sub>2</sub>O<sub>2</sub></b> CuC <sub>16</sub> H <sub>14</sub> N <sub>2</sub> O <sub>2</sub>	<b>N,N-Bis(salicylidene)ethylenediaminocopper(II)</b> N. I. Giricheva, G. V. Girichev, Yu. S. Medvedeva, N. P. Kuzmina, O. V. Kotova Structure by GED and QC calculations Zh. Strukt. Khim., submitted
<b>C<sub>16</sub>H<sub>14</sub>N<sub>2</sub>NiO<sub>2</sub></b> C <sub>14</sub> H <sub>16</sub> N <sub>2</sub> O <sub>2</sub> Ni	<b>N,N-Bis(salicylidene)ethylenediaminonickel</b> G. V. Girichev, N. V. Tverdova, A. V. Zakharov, N. P. Kuzmina, O. V. Kotova Structure, IR spectra by QC and experimental study Zh. Fiz. Khim., accepted
<b>C<sub>16</sub>H<sub>16</sub>N<sub>2</sub>O<sub>2</sub></b>	<b>N,N-Bis(salicylidene)ethylenediamine</b> V. V. Sliznev, G. V. Girichev Structure by QC calculation Manuscript in preparation
<b>C<sub>18</sub>H<sub>18</sub>N<sub>2</sub>O<sub>4</sub>Zn</b>	<b>N,N-Bis(3-methoxysalicylidene)ethylenediaminozinc</b>

$H_{18}C_{18}O_4N_2Zn$	N. V. Tverdova, G. V. Girichev, N. P. Kuzmina, O. V. Kotova Structure, IR spectra by QC Manuscript in preparation
$C_{20}H_{12}Br_2N_4Ti$ $C_{20}H_{12}N_4Br_2Ti$	<b>Dibromotitaniumporphyrin</b> A. V. Zakharov Vibrational spectra by DFT calculations Manuscript in preparation
$C_{20}H_{12}Cl_2N_4Ti$ $C_{20}H_{12}N_4Cl_2Ti$	<b>Dichlorotitaniumporphyrin</b> A. V. Zakharov Vibrational spectra by DFT calculations Manuscript in preparation
$C_{20}H_{12}F_2N_4Ti$ $C_{20}H_{12}N_4F_2Ti$	<b>Difluorotitaniumporphyrin</b> A. V. Zakharov Structure, conformations and vibrational spectra by DFT calculations Manuscript in preparation
$C_{20}H_{12}F_2N_4Ti$ $C_{20}H_{12}N_4I_2Ti$	<b>Diiodotitaniumporphyrin</b> A. V. Zakharov Structure, conformations and vibrational spectra by DFT calculations Manuscript in preparation
$C_{20}H_{12}N_4OTi$ $C_{20}H_{12}N_4OTi$	<b>Oxotitaniumporphyrin</b> A. V. Zakharov, G. V. Girichev Structure and vibrational frequencies by DFT calculations Journal of Molecular Structure: THEOCHEM, in press
$C_{20}H_{14}N_2O_2Zn$ $H_{14}C_{20}O_2N_2Zn$	<b>N,N-(o-Phenylen)-bis(salicylidenediamino)zinc</b> N. V. Tverdova, G. V. Girichev, N. P. Kuzmina, O. V. Kotova Structure, IR spectra by QC Manuscript in preparation
$C_{22}H_{18}N_2O_4Zn$ $H_{18}C_{22}O_4N_2Zn$	<b>N,N-(o-Phenylen)-bis(3-methoxysalicylidenediamino)zinc</b> N. V. Tverdova, G. V. Girichev, N. P. Kuzmina, O. V. Kotova Structure, IR spectra by QC Manuscript in preparation
$C_{22}H_{38}CaO_4$ $C_{22}H_{38}O_4Ca$	<b>Calcium dipivaloylmethanate</b> N. V. Belova, G. V. Girichev, H. Oberhammer Internal rotation of $CH_3$ groups by DFT calculations Zh. Strukt. Khim., manuscript in preparation



<p><b>C<sub>22</sub>H<sub>38</sub>CoO<sub>4</sub></b> C<sub>22</sub>H<sub>38</sub>O<sub>4</sub>Co</p>	<p><b>Cobalt dipivaloylmethanate</b> N. V. Belova, V. V. Sliznev, G. V. Girichev Molecular structure and electronic states by QC Manuscript in preparation</p>
<p><b>C<sub>22</sub>H<sub>38</sub>FeO<sub>4</sub></b> C<sub>22</sub>H<sub>38</sub>O<sub>4</sub>Fe</p>	<p><b>Iron dipivaloylmethanate</b> N. V. Belova, V. V. Sliznev, G. V. Girichev Molecular structure and electronic states by QC Manuscript in preparation</p>
<p><b>C<sub>22</sub>H<sub>38</sub>MnO<sub>4</sub></b> C<sub>22</sub>H<sub>38</sub>O<sub>4</sub>Mn</p>	<p><b>Manganese dipivaloylmethanate</b> N. V. Belova, V. V. Sliznev, G. V. Girichev Molecular structure and electronic states by QC Manuscript in preparation</p>
<p><b>C<sub>28</sub>H<sub>28</sub>CuN<sub>4</sub></b> C<sub>28</sub>H<sub>28</sub>N<sub>4</sub>Cu</p>	<p><b>Copperoctamethylporphyrine</b> G. V. Girichev, N. I. Giricheva, O. A. Golubchikov, Yu. V. Minenkov, A. S. Semeikin, S. A. Shlykov. r<sub>h1</sub> structure, vapor composition by means of GED and MS, structure and frequencies by ROB3LYP calculations (6-31G*, TZV) Manuscript in preparation</p>
<p><b>C<sub>28</sub>H<sub>28</sub>N<sub>4</sub>Ni</b> C<sub>28</sub>H<sub>28</sub>N<sub>4</sub>Ni</p>	<p><b>Nickeloctamethylporphyrine</b> G. V. Girichev, O. A. Golubchikov, Yu. V. Minenkov, A. S. Semeikin, S. A. Shlykov. r<sub>h1</sub> structure, vapor composition by means of GED and MS, structure and vibrational frequencies by B3LYP calculations (6-31G*, TZV, TZV2, DGDZVP2), energy difference between ruffling and planar structures Manuscript in preparation</p>
<p><b>C<sub>28</sub>H<sub>28</sub>N<sub>4</sub>OTi</b> C<sub>28</sub>H<sub>28</sub>N<sub>4</sub>OTi</p>	<p><b>Oxotitaniumoctamethylporphyrin</b> A. V. Zakharov, G. V. Girichev Structure and vibrational frequencies by DFT calculations Journal of Molecular Structure: THEOCHEM, in press</p>
<p><b>C<sub>32</sub>H<sub>16</sub>Br<sub>2</sub>N<sub>8</sub>Ti</b> C<sub>32</sub>H<sub>16</sub>N<sub>8</sub>Br<sub>2</sub>Ti</p>	<p><b>Dibromotitaniumphthalocyanin</b> A. V. Zakharov Structure, conformations and vibrational spectra by DFT calculations Manuscript in preparation</p>
<p><b>C<sub>32</sub>H<sub>16</sub>Cl<sub>2</sub>N<sub>8</sub>Ti</b> C<sub>32</sub>H<sub>16</sub>N<sub>8</sub>Cl<sub>2</sub>Ti</p>	<p><b>Dichlorotitaniumphthalocyanin</b> A. V. Zakharov</p>

	Vibrational spectra by DFT calculations Manuscript in preparation
$C_{32}H_{16}CuN_8$ $CuN_8C_{32}H_{16}$	<b>Copperphthalocyanine</b> G. V. Girichev, N. V. Tverdova, N. I. Giricheva $r_{h1}$ and $r_g$ structures by GED, <i>ab initio</i> and DFT calculations Manuscript in preparation
$C_{32}H_{16}F_2N_8Ti$ $C_{32}H_{16}N_8F_2Ti$	<b>Difluorotitaniumphthalocyanin</b> A. V. Zakharov Structure, conformations and vibrational spectra by DFT calculations Manuscript in preparation
$C_{32}H_{16}I_2N_8Ti$ $C_{32}H_{16}N_8I_2Ti$	<b>Diiodotitaniumphthalocyanin</b> A. V. Zakharov Vibrational spectra by DFT calculations Manuscript in preparation
$C_{32}H_{16}N_8OTi$ $C_{32}H_{16}N_8OTi$	<b>Oxotitaniumphthalocyanin</b> A. V. Zakharov, G. V. Girichev Structure and vibrational frequencies by DFT calculations Journal of Molecular Structure: THEOCHEM, in press
$C_{32}H_{16}N_8OTi$	<b>Oxotitaniumphthalocyanine</b> A. V. Zakharov, S. A. Shlykov, G. V. Girichev Structure by GED experiment and DFT calculations Manuscript in preparation
$C_{33}H_{57}O_6Sc$ $C_{33}H_{57}O_6Sc$	<b>Scandium dipivaloylmethanate</b> N. V. Belova, G. V. Girichev, H. Oberhammer Internal rotation of $CH_3$ groups by DFT calculations Zh. Strukt. Khim., manuscript in preparation
$C_{42}H_{39}N_{15}S_3$ $C_{42}H_{39}N_{15}S_3$	<b>Trithiadiazoletri(5-tert-butylisindole)macrocycle</b> A. V. Zakharov, S. A. Shlykov, N. V. Bumbina, E. A. Danilova, A. V. Krasnov, M. K. Islyaikin, G. V. Girichev Molecular structure by GED and QG, enthalpy of sublimation by MS Angew. Chemie Int. Ed., submitted
$Cl_3Er$ $ErCl_3$	<b>Erbium trichloride</b> N. I. Giricheva, S. A. Shlykov, G. V. Girichev, E. V. Chernova and E. Lapykina Structure by GED/MS and QC

	Zh. Strukt. Khim., submitted
<b>Cl<sub>3</sub>Yb</b> YbCl <sub>3</sub>	<b>Ytterbium trichloride</b> N. I. Giricheva, S. A. Shlykov, G. V. Girichev, E. V. Chernova and E. Lapykina Structure by GED/MS and QC Zh. Strukt. Khim., submitted
<b>Cl<sub>4</sub>Te</b> TeCl <sub>4</sub>	<b>Tellurium tetrachloride</b> G. V. Girichev, N. I. Giricheva, D. Lentz, S. A. Shlykov, A. V. Titov GED, MS and QC, structure Manuscript in preparation.
<b>Cl<sub>4</sub>Ti</b> TiCl <sub>4</sub>	<b>Titanium tetrachloride</b> N. I. Giricheva, S. A. Shlykov, G. V. Girichev, S. V. Smorodin and A. V. Titov Structure changes by GED (T=273-873K), applicability of models of nuclear dynamics Izv. Vuzov. Khim. Khim. Tekhnol. <b>51</b> (9) (2008), 68-72.
<b>F<sub>4</sub>Te</b> TeF <sub>4</sub>	<b>Tellurium tetrafluoride</b> N. I. Giricheva, S. A. Shlykov, G. V. Girichev, D. Lentz and A. V. Titov Structure by GED/MS and QC Manuscript in preparation
<b>I<sub>2</sub>Be</b> BeI <sub>2</sub>	<b>Beryllium diiodide</b> S. A. Shlykov, Yu. A. Zhabanov, A. V. Zakharov, G. V. Girichev, N. I. Giricheva Structure by GED/MS and QC (CCSD(T)) Manuscript in preparation
<b>I<sub>2</sub>Te</b> TeI <sub>2</sub>	<b>Tellurium diiodide</b> S. A. Shlykov, N. I. Giricheva, G. V. Girichev, H. Oberhammer and A. V. Titov Structure by GED/MS and QC Manuscript in preparation
<b>I<sub>3</sub>Dy</b> DyI <sub>3</sub>	<b>Dysprosium triiodide</b> S. A. Shlykov, N. I. Giricheva, H. Oberhammer and G. V. Girichev Structure by GED/MS Manuscript in preparation
<b>I<sub>3</sub>Er</b>	<b>Erbium triiodide</b>

ErI <sub>3</sub>	S. A. Shlykov, N. I. Giricheva, H. Oberhammer and G. V. Girichev Structure by GED/MS Manuscript in preparation
I <sub>3</sub> Gd GdI <sub>3</sub>	<b>Gadolinium triiodide</b> S. A. Shlykov, N. I. Giricheva, H. Oberhammer, G. V. Girichev Structure by GED/MS Manuscript in preparation
I <sub>3</sub> Ho HoI <sub>3</sub>	<b>Holmium triiodide</b> S. A. Shlykov, N. I. Giricheva, H. Oberhammer and G. V. Girichev Structure by GED/MS Manuscript in preparation
I <sub>3</sub> Pr PrI <sub>3</sub>	<b>Praseodymium triiodide</b> S. A. Shlykov, N. I. Giricheva, G. V. Girichev, I. E. Galanin Molecular structure, GED/MS Manuscript in preparation
I <sub>3</sub> Tb TbI <sub>3</sub>	<b>Terbium triiodide</b> S. A. Shlykov, N. I. Giricheva, H. Oberhammer and G. V. Girichev Structure by GED/MS Manuscript in preparation
	<b>Scanner application</b> A. V. Zakharov, Yu. A. Zhabanov Software for a scanner application for GED Manuscript in preparation
	Yu. S. Medvedeva Molecular structure of 4-fluoro- and 3,4-difluorodanisole, N,N-bis(salicylidene)ethylenediamino- and N,N'-ethylene-bis(acetylacetoniminato)nickel(II) and copper(II) by GED and quantum chemical calculations, Ph.D. thesis Sept. 2008