

Prof. Dr. Heinz Oberhammer
Institut für Physikalische Chemie
Universität Tübingen
Auf der Morgenstelle 8
D-72076 Tübingen, Germany

Telephone: (+49) 7071 29-76907

Telefax: (+49) 7071 29-5490

E-Mail: heinz.oberhammer@uni-tuebingen.de

Br₂Se SeBr ₂	Selenium dibromide S. A. Shlykov, A. V. Titov, H. Oberhammer, N. I. Giricheva, G. V. Girichev Structure by GED/MS and quantum chemical calculations Phys. Chem. Chem. Phys. 10 (2008), 6438 - 6445
Br₂Te TeBr ₂	Tellurium dibromide S. A. Shlykov, H. Oberhammer, A. V. Titov, N. I. Giricheva, G. V. Girichev Structure by GED/MS and quantum chemical calculations Eur. J. Inorg. Chem. (2008), 5220
CCl₃NOS ClC(O)N=SCl ₂	N-(Chloroformyl)iminosulfur dichloride N. L. Robles, E. H. Cutin, R. M. S. Alvarez, H. Oberhammer Vibrational spectroscopy and quantum chemical calculations J. Mol. Struct. 891 (2008), 40
C₃F₆OS CF ₃ C(O)SCF ₃	Trifluorothioacetic acid S-(trifluoromethyl) ester S. E. Ulic, C. O. Della Vedova, A. Hermann, H.-G. Mack, H. Oberhammer NMR, UV, vibrational spectra, GED, quantum chemical calculations J. Phys. Chem. A 112 (2008), 6211
C₄H₇NO₃ NH ₂ C(O)-CH ₂ - C(O)OCH ₃	Malonamic acid methyl ester N. Belova, H. Oberhammer, S. A. Shlykov Tautomeric properties, GED, quantum chemical calculations J. Phys. Chem. 112 (2008), 4355
C₅H₇ClO₂ CH ₃ C(O)-CHCl- C(O)CH ₃	3-Chloro-2,4-pentanedion N. V. Belova, H. Oberhammer, G. V. Girichev, S. A. Shlykov Tautomeric properties, GED, quantum chemical calculations J. Phys. Chem. A 112 (2008), 3209

<p>C₆H₃F₂NO₂ 2,6F₂-C₆H₃-NO₂</p>	<p>2,6-Difluoronitrobenzene O. V. Dorofeeva, A. V. Ferenets, N. M. Karasev, L. V. Vilkov, H. Oberhammer Structure and internal rotation by GED, quantum chemical calculations J. Phys. Chem. A 112 (2008), 5002</p>
<p>C₆H₃F₂NO₂ 3,5F₂-C₆H₃-NO₂</p>	<p>3,5-Difluoronitrobenzene O. V. Dorofeeva, A. V. Ferenets, N. M. Karasev, L. V. Vilkov, H. Oberhammer Structure and internal rotation by GED and quantum chemical calculations J. Phys. Chem. A 112 (2008), 5002</p>
<p>C₆H₄Cl₂O₂S 2-Cl-C₆H₄-SO₂Cl</p>	<p>2-Chlorobenzenesulfonyl chloride V. N Petrova, V. M. Petrov, G. M. Girichev, H. Oberhammer, S. N. Ivanov Structure and conformation by GED and quantum chemical calculations J. Struct. Chem. (Engl.) 49 (2008), 850</p>
<p>C₇H₅F₃S C₆H₅-SCF₃</p>	<p>(Trifluoromethyl)thiobenzene I. F. Shishkov, L. V. Khristenko, A. N. Rykov, L. V. Vilkov, N. I. Giricheva, S. A. Shlykov, G. V. Girichev, H. Oberhammer Structure and conformation by GED and quantum chemical calculations J. Mol. Struct. 876 (2008), 147</p>
<p>C₇H₇ClO₂S 2-CH₃-C₆H₄-SO₂Cl</p>	<p>2-Methylbenzene sulfonylchloride V. M. Petrov, V. N. Petrova, H. Oberhammer, A. V. Bardina, S. N. Ivanov, A. V. Krasnov Structure and conformation by GED and quantum chemical calculations J. Struct. Chem. (Engl.) 48 (2008), 1022</p>
<p>C₇H₈S C₆H₅SCH₃</p>	<p>Thioanisole I. F. Shishkov, L. V. Khristenko, N. M. Karasev, L. V. Vilkov, H. Oberhammer GED, Quantum chemical calculations J. Mol. Struct. 837 (2008), 137</p>
<p>C₇H₈S C₆H₅-SCH₃</p>	<p>Thioanisol I. F. Shiskov, L. V. Khristenko, N. M. Karasev, L. V. Vilkov, H. Oberhammer</p>

	<p>Structure and conformation by GED and quantum chemical calculations. J. Mol. Struct. 873 (2008), 137</p>
<p>C₇H₉NO₂S 4-CH₃-C₆H₄- SO₂NH₂</p>	<p>p-Methylbenzene sulfonamide V. M. Petrov, G. V. Girichev, H. Oberhammer, V. N. Petrova, N. I. Giricheva, A. V. Bardina, S. N. Ivanov Structure and Conformation by GED and quantum chemical calculations J. Phys. Chem. A 112 (2008), 2969</p>
<p>C₇H₉NO₂S 2-CH₃-C₆H₄- SO₂NH₂</p>	<p>o-Methylbenzene sulfonamide V. M. Petrov, G. V. Girichev, H. Oberhammer, V. N. Petrova, N. I. Giricheva, A. V. Bardina, S. N. Ivanov Structure and conformation by GED and quantum chemical calculations J. Phys. Chem. A 112 (2008), 2969</p>
<p>I₂Te TeI₂</p>	<p>Tellurium diiodide S. A. Shlykov, H. Oberhammer, A. V. Titov, N. I. Giricheva, G. V. Girichev Structure by GED/MS and quantum chemical calculations Eur. J. Inorg. Chem. (2008), 5220</p>