

Dr. Natalja Vogt
Dr. Jürgen Vogt
 Dr. Rainer Rudert
 Chemieinformationssysteme
 Universität Ulm
 D-89069 Ulm
 Germany

Telephone: (+49) 731 50-31050
 Telefax: (+49) 731 50-31059
 E-Mail: natalja.vogt@uni-ulm.de
juergen.vogt@uni-ulm.de
rainer.rudert@uni-ulm.de
 Homepage: <http://www.uni-ulm.de/nawi/cheminfo.html>

C₂H₅NO₂ C₃H₆O₃ $\text{HOH}_2\text{C-CHOH-CHO}$	<p>Nitroethane Equilibrium structure and internal rotation from GED and QC <i>I. F. Shishkov, V. A. Sipachev, P. I. Dem'yanov, O. V. Dorofeeva, N. Vogt, Yu. V. Vishnevskiy, and L. V. Vilkov</i> <i>J. Mol. Struct.</i>, in press</p> <p>Glyceraldehyde Equilibrium structure from GED and QC, relative stability of conformers from QC <i>N. Vogt, E. G. Atavin, A. N. Rykov, E. V. Popov, and L. V. Vilkov</i> <i>J. Mol. Struct.</i> 936 (2009) 125-131</p>
C₄H₂O₃ $\text{C}_2\text{H}_2(\text{CO})_2\text{O}$	<p>Maleic anhydride Equilibrium structure from GED+MW and QC (preliminary data) <i>E. P. Altova, N. Vogt, and N. Karasev</i> HRMS, 21st Colloquium, Castellamare di Stabia, Italy, 2009, P044.</p>
C₄H₂O₃ $\text{C}_2\text{H}_2(\text{CO})_2\text{O}$	<p>Maleic anhydride Equilibrium structure from GED+MW and QC <i>N. Vogt, E. P. Altova, and N. Karasev</i> <i>J. Mol. Struct.</i>, in press</p>
C₄H₄CIN	<p>N-Chlorosuccinimide The equilibrium structure from GED and QC <i>Yu. V. Vishnevskiy, N. Vogt, V. I. Korepanov, A. A. Ivanov, L. V. Vilkov, V. V. Kuznetsov, and N. N. Mahova</i> <i>Struct. Chem.</i> 20 (2009) 435-442</p>
C₄H₄O₄ HOOCCHCHCOOH	<p>Fumaric acid Equilibrium structure and conformational composition GED and QC <i>N. Vogt, M. Abaev, N.M. Karasev</i> manuscript in preparation</p>
C₄H₅NO₂	<p>2,5-Pyrrolidinedione (Succinimide) Equilibrium structure and flexibility of the saturated five-membered ring from GED and QC with use of spectroscopic data <i>N. Vogt, L. S. Khaikin, O. E. Grikina, N. M. Karasev, J. Vogt, and L. V. Vilkov</i> <i>J. Phys. Chem. A</i> 113 (2009) 931-937</p>
C₄H₆O₄ $\text{HOOCCH}_2\text{CH}_2\text{COOH}$	<p>Succinic acid Structure from QC and preliminary GED data <i>M. Abaev, N. Vogt, I.F. Shishkov, J. Vogt, A.N. Rykov, L.V. Vilkov, H. Oberhammer</i> 23rd Austin Symp.Mol.Struct.Dynamics, Austin, 2010, p.22</p>
	<p>Succinic acid</p>

C₄H₆O₄ HOOCCH ₂ CH ₂ COOH	Equilibrium structure and conformational composition from GED and QC <i>N. Vogt, M. Abaev, I. F. Shishkov, A.N. Rykov,</i> Manuscript in preparation
C₅H₅N₅	9H-Adenine Equilibrium structure from GED and QC <i>N. Vogt, O. Dorofeeva, V. A. Sipachev, and A. N. Rykov</i> <i>J. Phys. Chem. A</i> 113 (2009) 13816-13823
	Structure of free polyatomic molecules <i>E. Hirota, K. Kuchitsu, T. Steimle, M. Tanimoto, J. Vogt, and N. Vogt,</i> <i>Volume II/30, edited by K. Kuchitsu, N. Vogt, and M. Tanimoto</i> manuscript in preparation
	Molecular constants mostly from microwave spectroscopy, molecular beam and sub-Doppler laser spectroscopy Mostly from Microwave Spectroscopy, Molecular Beam and Sub-Doppler Laser Spectroscopy <i>J. Demaison, J. Vogt, and G. Wlodarczak</i> in press
	MOGADOC update 2010 <i>J. Vogt, N. Vogt, R. Rudert, K. Deutzmann</i> update in preparation
	3D visualization of molecular structures in the MOGADOC database <i>N. Vogt, E. Popov, R. Rudert, R. Kramer, and J. Vogt</i> <i>J. Mol. Struct., in press</i>
	Improved procedure of treatment of gas-phase electron diffraction (GED) images (IP) <i>N. Vogt, R. Rudert, J. Vogt, A. N. Rykov, N. M. Karasev, I. F. Shishkov, J. Crassous</i> HRMS, 21st Colloquium, Castellamare di Stabia, Italy, 2009
	DNA and RNA nucleobases Enthalpies of formation from G3X theory <i>O. Dorofeeva and N. Vogt</i> <i>J. Chem. Engin. Data</i> 20 (2009) 1348-1352