

Dr. habil. 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>

C₄H₃FN₂O₂	5-Fluorouracil Molecular structure by ED and QC <i>D. N. Ksenafontov, N. Vogt, and A. N. Rykov</i> Work in progress
C₄H₄N₂O₂	Uracil Interpretation of vibrational spectra by quantum-chemical force field <i>L. S. Khaikin, O. E. Grikina, N. Vogt, and N. F. Stepanov</i> <i>Zh. Fiz. Khim., 86 (2012), 1993/ Russ. J. Phys. Chem. A, 86 (2012), 1855</i>
C₄H₄N₂O₂	Uracil r _a , r _e ^{se} , r _e (best ab initio) structure by ED and quantum chemical calculations <i>N. Vogt, L. S. Khaikin, O. E. Grikina, and A. N. Rykov</i> Manuscript in preparation
C₄H₄O₃	Dihydro-2,5-furandione (succinic anhydride) Molecular structure and conformations by ED and QC <i>N. Vogt, E. P. Altova, D. N. Ksenafontov, and A. N. Rykov</i> Work in progress
C₅H₇N₂O₂	1-Methyluracil r _a , r _e ^{se} , r _e (best ab initio) structure by ED and quantum chemical calculations <i>N. Vogt, I. I. Marochkin, O. V. Dorofeeva, and A. N. Rykov</i> Manuscript in preparation
C₆H₅NO₂ C₅H₄NCOOH	Pyridine-3-carboxylic acid (nicotinic acid) Molecular structure and conformations by ED and QC <i>I. I. Marochkin, N. Vogt, and A. N. Rykov</i> Work in progress
C₆H₅NO₂ C₅H₄NCOOH	Pyridine-2-carboxylic acid (picolinic acid) Molecular structure and conformations by ED and QC <i>I. N. Kolesnikova, N. Vogt, A. N. Rykov, and J. Vogt</i> Work in progress
C₆H₈N₂O₂	1-Methylthymine r _a , r _e ^{se} , r _e (best ab initio) structure by ED and quantum chemical calculations <i>N. Vogt, I. I. Marochkin, I. F. Shishkov, and A. N. Rykov</i> Manuscript in preparation
C₈H₁₀	o-Xylene r _e ^{se} and r _e (best ab initio) structure by MW and quantum chemical calculations <i>N. Vogt, J. Demaison, W. Geiger, and H. D. Rudolph</i> Manuscript in preparation

C₉H₁₃NO₃	(R)-4-(1-Hydroxy-2-(methylamino)ethyl)benzene-1,2-diol (adrenaline) Molecular structure and conformations by ED and QC <i>E. P. Altova, N. Vogt, A. N. Rykov, M. V. Popik, and I. F. Shishkov</i> Work in progress
	Structure of Free Polyatomic Molecules <i>E. Hirota, K. Kuchitsu, T. Steinle, M. Tanimoto, J. Vogt, and N. Vogt</i> Landolt-Börnstein New Series II/30A, (edited by K. Kuchitsu, N. Vogt, and M. Tanimoto), Springer, Berlin, in press
	Structure of Free Polyatomic Molecules <i>E. Hirota, K. Kuchitsu, T. Steinle, M. Tanimoto, J. Vogt, and N. Vogt</i> Landolt-Börnstein New Series II/30B, (edited by K. Kuchitsu, N. Vogt, and M. Tanimoto), Springer, Berlin, in press
	MOGADOC update 2011/2012 <i>J. Vogt, N. Vogt, R. Rudert, K. Deutzmann, and S. Schlagenhauf</i> update in preparation
	Equilibrium structure and its determination for some biomolecules <i>N. Vogt</i> Doctor of Science Thesis, Moscow State University 2012