

Vogt

Dr. habil. Natalja Vogt

Dr. Jürgen Vogt

Dr. Rainer Rudert

Chemieinformationssysteme

Universität Ulm

Albert-Einstein-Allee 47

D-89081 Ulm

Germany

Telephone: (+49) 731 50-31054

Telefax: (+49) 731 50-31059

E-Mail: Natalja.Vogt@uni-ulm.de

Homepage: <https://www.uni-ulm.de/cheminfo>

	Sulfine
CH₂OS	Equilibrium structure by MW and coupled-cluster calculations
H₂C=S=O	<i>J. Demaison, N. Vogt, and D. N. Ksenafontov</i> <i>J. Mol. Struct. 1206 (2020) 127676</i>
	Methylarsine
CH₅As	Equilibrium structure by MW and coupled-cluster calculations
CH₃AsH₂	<i>R. A. Motiyenko, V. V. Ilyushin, J. Demaison, N. Vogt, L. Margulès, H. Mollendal, and J.-C. Guillemin</i> <i>J. Mol. Struct. 1213 (2020) 128037</i>
	5-Fluorouracil
C₄H₃FN₂O₂	Equilibrium structure by ED and coupled cluster calculations
	<i>N. Vogt, D. N. Ksenafontov, D. Savelev, and A. N. Rykov</i> <i>Mendeleev Commun. 30 (2020) 660-662</i>
	Succinic anhydride
C₄H₄O₃	Equilibrium structure by MW and coupled-cluster calculations
	<i>M. K. Jahn, D. A. Obenchain, K. P. R. Nair, J.-U. Grabow, N. Vogt, J. Demaison, P. D. Godfrey, and D. McNaughton</i> <i>Phys. Chem. Chem. Phys. 22 (2020) 5170-5177</i>
	Pyridine-3-carboxylic acid (nicotinic acid)
C₆H₅NO₂	Structure and conformations by ED and coupled cluster calculations
	<i>N. Vogt, I. I. Marochkin, and R. A. Rykov</i> <i>Work in progress</i>
	Phthalic anhydride
C₈H₄O₃	Equilibrium structure by MW and coupled-cluster calculations
	<i>A. V. Belyakov, R. Yu. Kulishenko, N. Vogt, and J. Demaison</i> <i>Manuscript in preparation</i>
	3-Aminophthalimide
C₈H₆N₂O₂	Equilibrium structure by ED and coupled-cluster calculations
	<i>N. Vogt, D. Savelev, N. I. Giricheva, and G. V. Girichev</i> <i>Phys. Chem. Chem. Phys. 22 (2020) 27539-27546</i>
	3-Aminophthalimide
C₈H₆N₂O₂	Back cover
	<i>N. Vogt, D. Savelev, N. I. Giricheva, and G. V. Girichev</i> <i>Phys. Chem. Chem. Phys. 22 (2020) back cover of issue 47</i>
	Erythrulose
C₄H₈O₄	Equilibrium structure by MW and coupled-cluster calculations
	<i>A. Insausti, E. R. Alonso, B. Tercero, J. I. Santos, C. Calabrese, N. Vogt, F. Corzana, J. Demaison, J. Cernicharo, and E. J. Cocinero</i> <i>J. Phys. Chem. Lett. 12 (2021) 1352-1359</i>
	Erythrulose
C₄H₈O₄	Cover

Vogt

	<p><i>A Insausti, E. R. Alonso, B. Tercero, J. I. Santos, C. Calabrese, N. Vogt, F. Corzana, J. Demaison, J. Cernicharo, and E. J. Cocinero</i> <i>J. Phys. Chem. Lett. 12 (2021) cover of issue 4</i></p>
$C_5H_4N_2O_4$	<p>Orotic acid (6-uracilcarboxylic acid) Equilibrium structure by ED and coupled-cluster calculations <i>E. P. Altova, A. N. Rykov, N. Vogt, and I. F. Shishkov</i> <i>Mendeleev Commun. 31 (2021) 81–83</i></p>
$C_6H_6O_2$	<p>2-Acetylfuran Equilibrium structure by MW and coupled-cluster calculations <i>C. Dindic, A. Lüchov, N. Vogt, J. Demaison, H. V. L. Nguyen</i> <i>Manuscript in preparation</i></p>
CN_2O_2 CO...NNO	<p>Carbon monoxide - dinitrogen monoxide (1/1) Equilibrium structure of van der Waals complex by MW and coupled-cluster calculations <i>N. Vogt, J. Demaison, A. Lesarri et al.</i> <i>Manuscript in preparation</i></p>
	<p>MOGADOC Update <i>J. Vogt, N. Vogt, and R. Rudert</i> <i>Update ready</i></p>
	<p>Databases with structural information Chapter in textbook <i>A. A. Ischenko, N. Vogt, et al.</i> "Analytical Chemistry, V. 2, Instrumental methods of analysis." Part 2, Textbook. (ed. A. A. Ishchenko), Ch. 3 (2020), Fizmatlit, Moscow (in Russian)</p>
	<p>Multidimensional hypersurfaces Visualization and minima finding <i>E. V. Popov, A. A. Batiukov, N. Vogt, T. P. Popova, and J. Vogt</i> <i>IGI Golbal Disseminator of Knowledge, Chapter 15 (2020) 282-309</i></p>
	<p>Potential energy surfaces Visualization and analysis of molecular potential energy surface (PES) and its minima <i>E. V. Popov, A. A. Batiukov, N. Vogt, T. P. Popova, and J. Vogt</i> <i>IADIS International Conference Interfaces and Human Computer Interaction 2019 (part of MCCSIS 2019) p 411-415 (ISBN: 978-989-8533-91-3)</i></p>
	<p>Structure data of free polyatomic molecules Monograph <i>N. Vogt and J. Vogt</i> <i>Springer Nature Switzerland (2019) 926 pp.</i></p>
	<p>Accurate structure determinations Accurate structure determinations of free molecules <i>J. Demaison and N. Vogt</i> <i>Springer Nature Switzerland (2020) 277 pp.</i></p>