

Curriculum vitae

Name: Jana Roithová

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Titles: Mgr. (*MSc. equivalent*), *PhD.*

Position: Professor of Organic Chemistry, Faculty of Science, Charles University in Prague



Education: MSc. in Organic Chemistry at the Charles University in Prague (Czech Republic), Faculty of Science, Department of Organic Chemistry (Diploma Thesis: '*Derivatives of betulinic acid*', supervisor: Prof. J. Klinot, defended 1998)

Ph.D. in Physical Chemistry at the Institute of Chemical Technology in Prague (Czech Republic), Faculty of Chemical Engineering, Physical Chemistry Department (Ph.D. Thesis: '*Structure, stability and reactivity of molecular dications: System $CHCl^{2+} + D_2, Ar, Kr, Xe$* ', supervisor: Prof. Z. Herman, defended 2003)

• CHRONOLOGY OF EMPLOYMENT

- since 2014 **Professor** of organic chemistry, Charles University in Prague
- since 2011 **Head of the Department of Organic Chemistry**, Charles University in Prague
- 2011 – 2014 **Associate professor** for organic chemistry, Charles University in Prague
- 2007 - 2010 **Assistant professor** for physical organic chemistry, Charles University in Prague, Faculty of Science, Department of Organic and Nuclear Chemistry
- 2006 - 2010 **Senior researcher** in ion chemistry (group of Dr. D. Schröder), Institute of Organic Chemistry and Biochemistry, Academy of Sciences of the Czech Republic (ASCR)
- 2005 - 2006 **Research scientist**, Ion chemistry (group of Prof. Z. Herman), J. Heyrovsky Institute of Physical Chemistry, ASCR
- 2003 - 2005 **Postdoctoral fellow**, Ion chemistry (group of Prof. H. Schwarz), Technische Univ. Berlin
- 2000 - 2003 **Ph. D. student**, Dynamics of chemical reactions in the gas phase (group of Prof. Z. Herman), J. Heyrovsky Institute of Physical Chemistry, ASCR
- 1998 – 2000 **Ph. D. student**, quantum chemical calculations (group of Doc. R. Ponec), Institute of Chemical Process Fundamentals, ASCR

• MAJOR RESEARCH INTERESTS

- Reaction mechanisms: investigation of mechanisms of organic and organometallic reactions by means of mass spectrometry, ions spectroscopy and theoretical computations. The research spans from kinetic studies to the construction of potential energy-surfaces for a given reaction system.
- Fundamental properties of molecules: Experimental and theoretical investigation of basic thermodynamic properties of molecules such as ionization energies, proton affinities, or bonding energies. Studies of complexation abilities of molecules and their redox properties.
- Ion spectroscopy: Infrared dissociation spectroscopy of mass-selected ions. Research is focused on spectroscopy of ionic intermediates isolated from reaction mixtures by ESI-MS approach using a standard set-up (infrared multiphoton dissociation spectroscopy using free-electron laser) and laboratory system based on preparation of helium-tagged ionic complexes (infrared predissociation spectroscopy).

• QUALIFICATIONS AND PROFESSIONAL EXPERIENCE

- Profound expertise in mass spectrometry (MS): different types of multipole systems, ion traps, ion cyclotron resonance MS, sector MS, selected ion flow tubes, crossed-beam experiments.
- Leadership of measurements with free-electron laser systems and synchrotron beamlines.
- Advanced expertise in quantum chemistry (ab-initio calculations, density functional theory calculations).

• PRIZES/AWARDS/GRANTS

- **2003:** Prize „Chemistry 2003 Rhodia CZ/ French Embassy”, **2005:** Hlavka Prize (The Hlavka Foundation), **2008:** L’Oreal “For women in science” stipend, **2009:** Prize of the Dean of the Faculty of

Science of the Charles University in Prague, **2014**: Neuron Prize; **2014**: Prize of the Czech Learned Society for young scientists

- **2010**: Starting Grant ISORI from European Research Council, PI of 5 national grants
- **SCIENTIFIC COMMUNITY ACTIVITIES**
 - *Chairperson* of the Czech Society for Mass Spectrometry (since 2011)
 - *Reviewer*: Peer-reviewing for major international journals (e.g. *J. Am. Chem. Soc.*, *J. Org. Chem.*, *Phys. Chem. Chem. Phys.*, *Angew. Chem. Int. Ed.*, *Chem. Eur. J.*, *J. Am. Soc. Mass Spectrom.*, *J. Mass Spectrom.*, etc.), currently with a frequency of ~30 ms/year
 - *Grant reviewing* for NSF (National Science Foundation), FRC (Frontier Research in Chemistry), and other grant agencies
- **ORGANISATION OF CONFERENCES**
 - Main organiser (together with J. Michl) of the *European Symposium on Organic Reactivity* (Prague 2013)
 - Main organiser of the *Annual Conference of the Czech Society for Mass Spectrometry* (Hradec Králové, 2011, 2012, and 2013)
- **TEACHING AND MENTORING**
 - MSc. Courses ‘*Computational Chemistry for Experimental Chemists, Organic Chemistry, Stereochemistry, Mass Spectrometry, Physical Organic Chemistry*, (all at the Charles Univ. in Prague)
 - Supervisor of Ph.D. students (Petr Milko - defended in 2009; Lucie Jašíková, Anton Škríba, Alexandra Tsybizova, Erik Andris), postdoctoral fellows (Andrew Gray, Jiří Schulz, Jiří Váňa, Pramod Kumar, Susanta Hazra, Štěpánka Janková), and undergraduate students
- **KEY SCIENTIFIC COLLABORATIONS**
 - *Domestic*: Martin Katora, Jan Veselý, P. Kočovský (all: *Charles Univ. in Prague*), Ivo Starý, Lubomír Rulišek (both: *Inst. of Organic Chemistry and Biochemistry, Prague*), Petr Klán (*Masaryk Univ. in Brno*), Karel Lemr (*Palacký Univ. in Olomouc*)
 - *International*: Dieter Gerlich (*Technical Univ. Chemnitz, Germany*), Daniela Ascenzi (*Univ. Trento, Italy*), Philippe Maitre (*Univ. Paris Sud, France*), Stephen D. Price (*Univ. Coll. London, UK*), Helmut Schwarz (*Technical Univ. Berlin, Germany*), Mirjana Eckert-Maksic (*Ruder Boskovic Inst., Croatia*)
- **BIBLIOGRAPHIC OVERVIEW**

At present, JR has published more than **130 research articles**, mostly in leading journals. **29 papers** have been published in top-ranked journals, e.g. *J. Am. Chem. Soc.* (8), *Angew. Chem. Int. Ed.* (6), *Chem. Eur. J.* (12), and *Chem. Commun.* (2), recent contributions include *inter alia* two invited reviews (*Chem. Rev.* **2010** and *Chem. Soc. Rev.* **2012**). The work has been **cited ~2,200 times** (~1500 citations without self-citations; source: ISI WoS Core Collection, February 20, 2014). **H-index** is **27**.