

ION SPECTROSCOPY OF REACTION INTERMEDIATES

Jana Roithová

Department of Organic Chemistry, Faculty of Science, Charles University in Prague, Hlavova 2030/8, Prague 2, 128 43, Czech Republic
e-mail: roithova@natur.cuni.cz

The combination of electrospray ionization and mass spectrometry is often used for investigation of reaction mixtures. Many of the catalytic reactions lead via reactive complexes in which a catalyst facilitates coupling of the reactants and/or rearrangements within the complex. Isolation of such reactive intermediates in the gas phase and probing their uni- or bimolecular reactivities belong to one of the strongest contributions of mass spectrometry to the elucidations of reaction mechanisms. Interpretation of the reactivity must be based on knowing the structure of the isolated complexes. Infrared photodissociation spectroscopy allows obtaining infrared spectra for mass-selected ions and hence is one of the ideal tools for the molecular structure elucidation.^[1]

My presentation will be devoted to our approach to ion spectroscopy and its use in the investigation of transition-metal and organometallic complexes.^[2,3]

1) J. Roithová, *Chem. Soc. Rev.* **2012**, *41*, 547.

2) J. Roithová, A. Gray, E. Andris, J. Jašík, D. Gerlich, *Acc. Chem. Res.* **2016**, *10.1021/acs.accounts.5b00489*.

3) E. Andris, J. Jašík, L. Gómez, M. Costas, J. Roithová, *Angew. Chem. Int. Ed.* **2016**, DOI: 10.1002/anie.201511374.