

Bioinspired catalysis investigated by mass spectrometry

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Analysis of reactivity of reactive intermediates is difficult because of their low concentrations and short life times. This is particularly evident for intermediates in bioinspired catalysis, where we aim to design and prepare complexes capable of challenging transformations such as C-H activation of alkanes. During the lecture I will show how mass spectrometry can contribute to detecting and characterizing transient reactive complexes and how it can help in understanding the reaction processes happening in solutions.¹

Mass spectrometry methods require to transfer the reactive complexes to the gas phase which is usually achieved via electrospray or cryospray interfaces. Once the reactive species are isolated in the gas phase, their life time is sufficient for their characterization by IR and UV/vis photodissociation spectroscopy.² I will show how this approach led to characterization of highly reactive metal-oxo complexes. In order to trap the reactive complexes, the reaction time has to be short. I will show the techniques that allow us to study short lived complexes and connect their mass-spectrometric signature with reaction kinetics in solution.³ Finally, I will present a coupling of mass spectrometry with an electrochemical cell that allows us to detect and study complexes in reactive oxidation states. I will demonstrate this for a study of the mechanism of CO₂ reduction in an iron porphyrine cage⁴

¹ J. Mehara, J. Roithova, *Chem. Sci.* **2020**, *11*, 11960 – 11972.

² J. Roithová, A. Gray, E. Andris, J. Jašík, D. Gerlich, *Acc. Chem. Res.* **2016**, *49*, 223–230.

³ G. L. Tripodi, M. T. G. M. Derks, F. P. J. T. Rutjes, J. Roithová, *Chem. Methods* **2021**, *1*, 430 – 437.

⁴ A. Koovakattil Surendran, G. L Tripodi, E. Pluharova, A. Y. Pereverzev, J. P. J. Bruekers, J. A. A. W. Elemans, E. J. Meijer, J. Roithova, <https://doi.org/10.26434/chemrxiv-2022-0dkm2>.