



Kolloquium des Wilhelm-Ostwald-Instituts

Prof. Dr. Héloïse Dossmann

Sorbonne Université, Paris

Montag, 21.11.2022, 16:15 Uhr

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Ligand effects on cyclopentadienyl Fe and Ru complexes probed by photoelectron spectroscopy

Abstract

In organometallic chemistry, the finest tuning of the catalytic reactions can be accessed through a detailed knowledge of the ligand electronic and steric effects surrounding the metallic center. To this end, various experimental approaches are available and aim to describe and quantify the donating and backdonating capability of a ligand towards a metal, such as the Tolman Electronic Parameter¹ or the Huynh Parameter.² Although widely used, these methods may reach some limitations and may not be able to deliver the desired information because for instance of a lack of sensitivity. Another reason may be the surrounding of the complex (solvent, counter ion,...) and gas-phase studies are therefore of particular interest. In this context, our group has developed different gas-phase experimental approaches based on mass spectrometry (MS)³ or photoelectron spectroscopy (PES) coupled with synchrotron radiation.⁴ One of our recent project concerns the study of iron and ruthenium tricarbonyl complexes used in various catalytic applications, especially hydrogenation reactions. The PES obtained for these complexes will be presented as well as their interpretation assisted by energy decomposition analysis (EDA).

References:

1. Tolman, C. A. *Chem. Rev.* 1977, 77, 313-348.
2. Huynh, H. V. *Chem. Lett.*, 2021, 50, 1831
3. Gatineau, D.; Lesage, D.; Clavier, H.; Dossmann, H.; Chan, C. H.; Milet, A.; Memboeuf, A.; Cole, R. B.; Gimbert, Y. *Dalton Trans.* 2018, 47, 15497-15505.
4. Dossmann, H.; Gatineau, D.; Clavier, H.; Memboeuf A.; Lesage, D. ; Gimbert, Y. *Phys. Chem. A* 2020, 124, 42, 8753–8765.

Ab 15:30 Uhr findet ein gemeinsames Kaffeetrinken in Raum 410 (TA) statt.