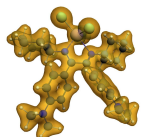


Monday 12/01/2015 - Amphithéâtre EGIM SUD, Faculté des Sciences de Saint Jérôme

8:35-8:55	Registration
8:55-9:00	Introducing remarks
9:00-9:40	Making and breaking bonds: X-ray spectroscopic insights into small molecule activation. <b>S. DeBeer</b>
9:40-10:00	Nickel(II) complex towards mCPBA: formation of a highly reactive intermediate. <b>T. Corona</b> , F. Pfaff, K. Ray, A. Company
10:00-10:20	Cu(II) in Alzheimer's Disease, view at the molecular level. P. Faller, F. Collin, <b>C. Hureau</b>
10:20-10:40	Bispidine-metal-oxo complexes - transition state spin, geometry and reactivity. <b>P. Comba</b>
10:40- 11:10: Coffee	
11:10-11:30	Exploring electronic structure and photodynamics of ruthenium complexes. A challenge for theory. <b>L. Freitag</b> , S. Knecht, M. Reiher, L. González
11:30-11:50	Electrochemical study of a non heme Fe(II) complex in the presence of dioxygen. Insights into the reductive activation of O <sub>2</sub> at Fe(II) centers. N. Ségaud, E. Anxolabéhère-Mallart, K. Sénéchal-David, L. Acosta-Rueda, M. Robert, <b>F. Banse</b>
11:50-12:10	Magnetic anisotropy and spin transition: Weighing the fine balance of ligand field, spin orbit and lattice effects. <b>M. Cimpoesu</b>
12:10-12:30	Monitoring the copper binding to dendrimers with electron spin resonance and molecular modeling. S. Furlan, <b>G. La Penna</b> , M. F. Ottaviani, A. Danani
Lunch (buffet, salle des actes)	
14:00-15:00	Biomimetic metal-oxygen intermediates in dioxygen activation reactions. <b>W. Nam</b>
15:00-15:20	Metal glyoximes complexes for H <sub>2</sub> production, not that «molecular» after all? A. Aukauloo, S. Cherdo, S. El Ghachtouli, M. Orio, <b>M. Sircoglou</b>
15:20-15:40	Spin state energetics in first-row transition metal complexes: role of (3s3p) correlation. <b>K. Pierloot</b>
15:40-16:00	Magnetic anisotropy of spin systems studied by EPR spectroscopy. <b>B. Rakvin</b>
16:00-17:00: WGs discussions	
17:00-19:00	Poster session / "Pica Pica" / Salle des Actes



Tuesday 13/01/2015 - Amphithéâtre Gastaut, Jardin du Pharo

- 9:00-9:40 In Silico Discovery of New Spin Crossover Complexes  
**Rob Deeth**
- 9:40-10:00 Understanding the outer-valence electronic structure of metal-organic compounds with density functional theory and many-body perturbation theory.  
**L. Kronik**
- 10:00-10:20 Binuclear copper active site: tyrosinase vs. pMMO.  
C. Belle, H. Jamet, M. Orio, R. Hardré, B. Faure, J. Simaan, **M. Réglie**
- 10:20-10:40 Magnetostructural correlations in tetrahedral  $[M(II)\{(E)P(Pr)_2\}_2N\}_2]$ ,  $M = Fe, Co, Ni$ ;  $E = S, Se$ , and octahedral  $[Mn(III)\{(OPPh_2)(OPPh_2)N\}_3]$  or trans- $[Ni(II)\{(OPPh_2)(E)P(Ph)_2\}_2(sol)_2]$ ,  $E = S, Se$ ; sol = dmf, thf, dmsO, complexes.  
**P. Kyriltis**

10:40- 11:10: Coffee and group picture

- 11:10-11:30 Nitrene radicals' in the coordination sphere of cobalt complexes - characterization and reactivity.  
**M. Goswami**, B. de Bruin, S. DeBeer, K. Ray
- 11:30-11:50 Fe(II) spin crossover complexes: Using 1-substituted tetrazole ligands to tune the spin transition properties.  
D. Müller, C. Knoll, M. Reissner, G. Giester, **P. Weinberger**.
- 11:50-12:10 Spectroscopy-constrained modelling of metalloenzymes.  
**D. A. Pantazis**
- 12:10-12:30 On line monitoring of reaction intermediates and their kinetics using MS.  
**J. Roithová**

Lunch (New Hotel of Marseille)

- 14:00-14:40 Spin states of myoglobin. Insights from QM/MM and MD.  
**J. Harvey**
- 14:40-15:00 Non-empirical prediction of the photophysical and magnetic properties of systems with open d- and f-shells.  
**C. A. Daul**
- 15:00-15:20 O<sub>2</sub> activation by Mn thiolate complexes.  
**M. Gennari**, D. Brazzolotto, C. Duboc
- 15:20-15:40 Spin-crossover in cobalt(II) complexes as a means of switching organic ligands from a closed-shell to an open-shell state.  
R. Dolai, M. Graf, H.-**J. Krüger**
- 15:40-16:00 An ionizable active-site tryptophan imparts catalase activity to a peroxidase core.  
P. Vidossich, X. Carpena, P. Loewen, I. Fita, **C. Rovira**

16:00-18:00: MC meeting