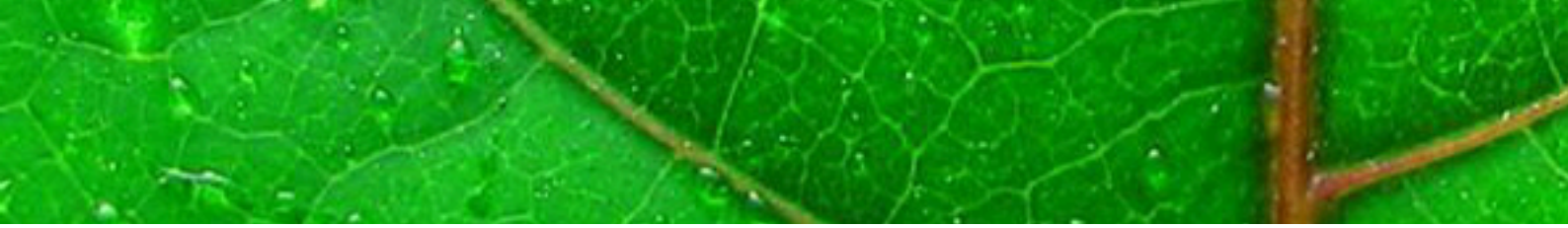

Séminaire - Christophe Raynaud

Lundi 17 juin 2019, 14h - Salle S112

Le 16 juin 2019

Christophe Raynaud
(Institut C. Gerhardt, Université de Montpellier)

Titre: "Information about reactivity from 13C NMR?"

Abstract:

While isotropic chemical shift is universally used to characterize a chemical compound in so- lution, the chemical shift tensor which is accessible not only by solid-state NMR spectroscopy but also by quantum chemistry calculations, can provide detailed information about the elec- tronic structure of the observed nuclei. We have recently established that the NMR chemical shift tensor is a powerful reporter for the electronic structure, i.e. of frontier molecular orbitals that encode the reactivity patterns of organometallic compounds. We will show how the 13C NMR chemical shift is linked to the electronic structure of some major classes of organome- tallic compounds (metal alkyls, metal alkylidenes and metal alkylidynes) and deal with their most prominent reactivity patterns, e.g., C–H bond activation, olefin polymerization, olefin metathesis and alkyne metathesis. We will highlight that chemical shifts, accessible to calcu- lations for molecules of chemical interest, are not only easy to understand with the help of molecular orbitals but can inform on reactivity pattern.