Centrale Méditerranée

Proposition de sujet d'alternance 1A
2023-24

Laboratoire : iSm2

Titre du sujet : Neutral Frustrated Radical Pairs : Properties and Reactivity of Radical Carbene

Encadrant * (s) :
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* *un co-encadrement est possible.*
** *l'encadrement devra être assuré de préférence par un permanent du laboratoire, au minimum titulaire d'un Doctorat.*

Descriptif du sujet et de la mission (au moins sur la 1er année) :

Since the seminal work from Scott et al. in 2006, the chemistry of Frustrated Lewis Pairs has received a lot of attention, because of the capability of these systems to cleave small molecules. In this context, we aim at exploring new systems that could be defined as neutral Frustrated Radical Pairs (FRP). They are constructed by a hindered Lewis base LB, together with a hindered radical Lewis acid. We are interested to computationally evaluate the electronic and structural properties of these chemical objects. After having assessed the FRP capability of splitting H_2, we shall explore the behavior of the obtained radical fragment of type LB-H$^{\cdot}$. These are transient species that are difficult to characterize from experiments. The computational study allows for predicting their fate, by evaluating their capability to either transfer a hydrogen atom, or to promote other kinds of reactions, such as addition reactions. Predictions are important to drive the synthetic chemists in their work.The study will focus mainly on N-heterocyclic carbenes (NHC) as Lewis bases. Their properties can be moduled by a fine design of substituents groups that decorate the NHC backbone.

Validation pour mise en ligne ECM :