SAPIENZA
UNIVERSITÀ DI ROMA

Avviso di seminario

Aula B alle 14:30, Venerdì 27 Settembre.

Understanding organometallic reactivities inside cyclodextrins

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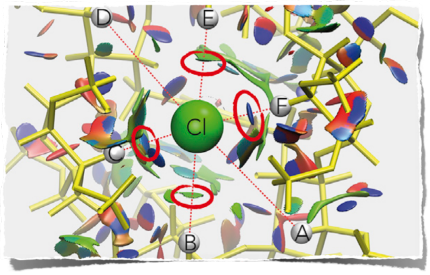
Encapsulating a metallic center in a cavity with a defined and specific shape is an efficient way to promote selectivity in catalytic processes. This is the strategy that nature uses in metalloenzymes, and it has naturally become a source of inspiration to the chemist. Cyclodextrins (CDs) have become popular in this area because they provide a system with a well-defined naturally occurring chiral cavity. Capping of cyclodextrins with a carbene ligand positions the metal inside this natural cavity, inducing a large organisation in the cavity shape (see picture), which in turn is responsible for the selectivity of these catalytic systems.



It will be demonstrated by various modeling methods how these CDs ligands can modified the classical gold catalysis of enynes,[1] and also how this unusual ligand can induce a mechanistic switch in copper-catalyzed hydroboration.[2]

References

1. Zhang, P.; Tugny, C.; Meijide Suarez, J.; Guitet, M.; Derat, E.; Vanthuyne, N.; Zhang, Y.; Bistri, O.; Mouriès-Mansuy, V.; Ménand, M.; et al. *Chem* **2017**, *3*, 174–191.
2. Zhang, P.; Meijide Suarez, J.; Driant, T.; Derat, E.; Zhang, Y.; Ménand, M.; Roland, S.; Sollogoub, M. *Angew. Chem. Int. Ed.* **2017**, *56*, 10821–10825.

Short Bio

I am associate professor of computational chemistry at the Institut Parisien de Chimie Moléculaire, a joint lab between Sorbonne Université and CNRS (UMR 8232). My research is focusing on understanding mechanistic details of various chemical transformations, with a focus on reactions involving metals and radicals, using either pure quantum mechanics calculations or hybrid quantum mechanics/molecular mechanics. I have been a member of the section dedicated to molecular chemistry at the french national committee for scientific research and I have been invited professor at Tokyo University and at the Indian Institute of Chemical Technology.

Enrico Bodo