Understanding organometallic reactivities inside cyclodextrins

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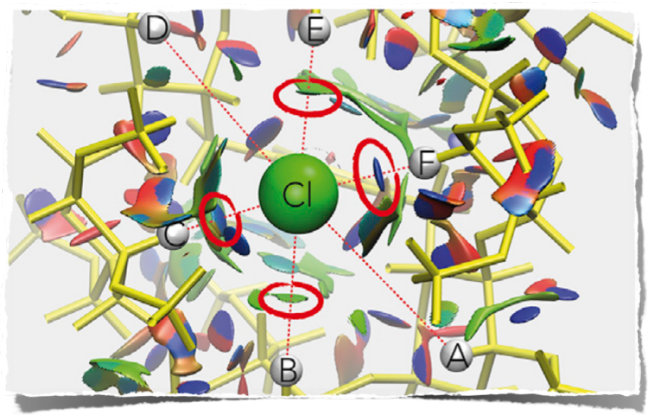
Encapsulating a metallic center in a cavity with a defined and specific shape is an efficient way to promote selectivity in catalytic processes. This is the strategy that nature uses in metalloenzymes, and it has naturally become a source of inspiration to the chemist. Cyclodextrins (CDs) have become 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 modify the classical gold catalysis of enynes,[1,2] how this unusual ligand can induce a mechanistic switch in copper-catalyzed hydroboration,[3] or why the cylodextrin is modifying the chemoselectivity in copper-catalyzed hydrosilylation of unsaturated ketones.[4]

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