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From Organometallics to Artificial Metalloenzymes: Cu-Catalyzed Enantioselective Hydration of Alkenes

Agustín Lledós

Universidad Autónoma de Barcelona

16/05/19

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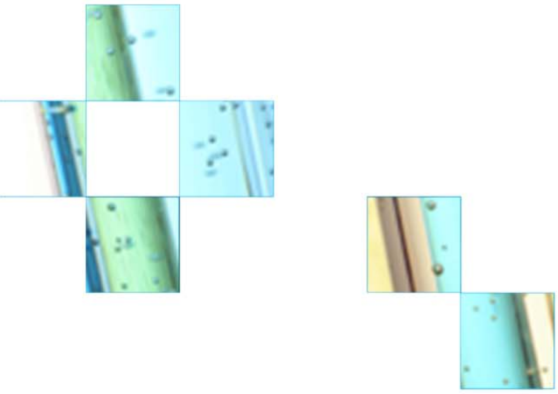

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From Organometallics to Artificial Metalloenzymes: Cu-Catalyzed Enantioselective Hydration of Alkenes

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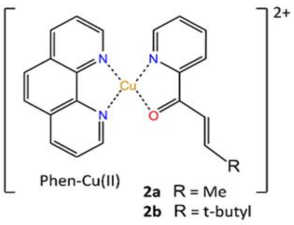
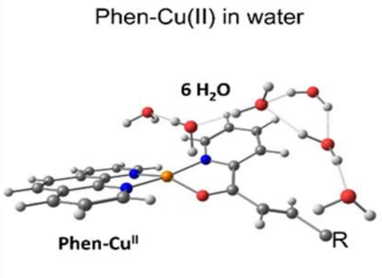
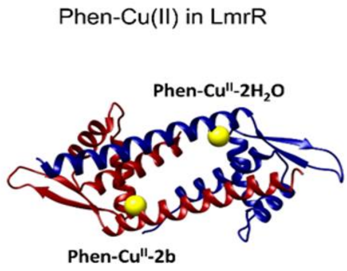
Chirally pure alcohols are transversal intermediates in chemical industries. One of the most interesting routes to synthesize these compounds is the enantioselective direct addition of a water molecule to alkenes. However, achieving this transformation with high enantiomeric excesses represents a major challenge in synthetic chemistry. The reaction faces two major challenges: i) water is a poor nucleophile that needs to be activated and ii) an asymmetric environment is required to enantioselectively add the water substrate. The use of Artificial metalloenzymes (ArMs) appears as a promising solution to these issues. In the last years Roelfes and coworkers have designed a variety of biohybrids embedding a Cu(II) catalyst, with phenanthroline (phen) or bipyridine (bipy) as a ligand, in a protein (LmrR), able to perform the addition of water to conjugated alkenes with promising enantioselectivities.[1] Our group has been collaborating with the experimental team to understand the catalytic mechanism and, from this knowledge, to improve the enantioselectivity.[2] Both the isolated catalyst in aqueous medium and embedded in the LmrR protein have been simulated using an integrated computational protocol which includes DFT calculations, ab initio molecular dynamics, protein-ligand docking, classical molecular dynamics and full-QM cluster models. [3] These studies will be the subject of the lecture.







References

1. Bos, J.; García-Herraiz, A.; Roelfes, G. *Chem. Sci.* **2013**, *4*, 3578.
2. Drienovska, I.; Alonso-Cotchico, L.; Vidossich, P.; Lledós, A.; Maréchal, J.-D.; Roelfes, G. *Chem. Sci.* **2017**, *8*, 7228.
3. Alonso-Cotchico, L.; Sciortino, G.; Vidossich, P.; Lledós, A.; Roelfes, G.; Maréchal, J.-D. *ACS Catal.* **2019**, *9*, 4616.

Agustí Lledós

Prof. Agustí Lledós was born in Barcelona (Spain) in 1955. He obtained a Ph. D. in Chemistry from the Universitat Autònoma de Barcelona (UAB) in 1984. He entered into the field or organometallic chemistry during a postdoctoral stay at the "Laboratoire de Chimie Thèorique" of the "Université de Paris-Sud" (1985-86). Then, he returned to UAB (1987), where he started a research group devoted to the computational study of organometallic reactivity and reaction mechanisms of homogeneous catalysis. He was appointed Full Professor of Physical Chemistry at UAB in 1994. Guided by a strong motivation to use computational techniques to do "real" chemistry, the UAB group has pioneered the collaborative experimental-theoretical research in organometallic chemistry. A significant part of the Dr. Lledós' scientific production (more than 300 papers) has been published in collaboration with experimental groups. He has also contributed to the formation of researchers in theoretical organometallic chemistry (25 Ph. D. Thesis supervised and training in computational techniques of more than 30 experimental researchers). Some of the main scientific achievements of Dr. Lledós are his contributions to the transition metal hydride and dihydrogen chemistry, cross-coupling processes, gold-catalyzed homogeneous catalysis, asymmetric catalysis and organometallic reactivity in water. Recently he has started collaborating with Dr. Maréchal in the computational design of artificial metalloenzymes applied to organic synthesis. He has served (2012-2017) as vice-president of the Spanish Chemical Society (RSEQ). He has been awarded with the RSEQ-Bruker Award for Physical Chemistry (2008), the RSEQ-GEQO Gold Medal (2018) and the Narcis Monturiol Scientific Merit Medal (2018).