

COMPUTATIONAL HINTS IN OLEFIN METATHESIS

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In recent years olefin metathesis catalyzed by N-heterocyclic carbene ruthenium complexes has attracted remarkable attention as a versatile tool to form new C=C bonds.[1] The last developed (pre)catalysts show excellent performances, and this achievement has been possible because of continuous experimental and computational efforts to understand the laws controlling the behavior of these systems. This perspective talk rapidly traces the ideas and discoveries that computational chemistry contributed to the development of these catalysts, with particular emphasis on catalysts presenting a N-heterocyclic carbene ligand. Specifically, one of the most important challenges in ruthenium-catalyzed olefin metathesis is to increase the stability of the catalysts under reaction conditions and this hopefully without loss of activity. Although, in the solid state, most ruthenium-based olefin metathesis catalysts are stable to oxygen and moisture, in solution decomposition usually occurs readily. Understanding the decomposition routes of catalysts is extremely important as any insight gained in this area can guide catalyst design efforts, to participate then in the synthesis of drugs.[2] Furthermore, new challenging projects plan to modify the structure of the NHC ligands, or replace this ligand by alkylidene ligands, and even the substitution of the metal is a goal, moving to more environmentally friendly metals.

[1] G. C. Vougioukalakis, R. H. Grubbs, *Chem. Rev.* 110, 1746 (2010).

[2] S. Manzini, C. A. Urbina-Blanco, A. Poater, A. M. Z. Slawin, L. Cavallo, S. P. Nolan, *Angew. Chem. Int. Ed.* 51, 1042 (2012).