Post-doctoral position available

Starting date : in early 2023

Project: The discovery and development of new versatile reactions is a challenging goal and a prerequisite toward the synthesis of complex molecular architectures. The aromatic Cope rearrangement (proceeding through a concerted mechanism) could be a useful and environmentally benign transformation to reach important challenges in modern synthetic chemistry like valuable aromatic CH functionalisation. Until now, the energetic impediments that must be overcome to use this reaction darkened its synthetic potential achievement. The organization of our project relies on three highly interconnected and interdependent works, involving two experimental teams and a theoretical investigation. Preliminary results arising from recent research efforts by the two partners (Reims, Strasbourg) of this collaborative project have established that a path to revive interest in this reaction may be found and, more importantly, the goal for implementing this reaction into the modern organic synthesis toolkit is achievable. The good accomplishment of our project requires a deep knowledge of the [3,3] sigmatropic step of the aromatic Cope rearrangement which is the rate determining step. Therefore, in a continuing interaction with organic chemists, theoretical calculations will be performed to save time and guide as quickly as possible the experimental preparation of a new generation library towards compounds both kinetically and thermodynamically more accessible. A big challenge of the project is to overcome the penalty for dearomatization occurring in the first [3,3] sigmatropic shift. To this end, we will make use of a Gold (I)/Gold(III) catalysis strategy to lower the barrier for this otherwise unfavorable dearomatization. The initial step of gold cation coordination to the substrate will be explored before simulating the [3,3] sigmatropic transformation in the presence of gold. Finally, the effort will be put on post-processing tools to allow a better control of the this transformation by understanding the subtle factors that may affect its specificity. So, quantum-mechanics tools based on the analysis of the electron density like AIM, ELF or IGM will be implemented to unravel specific events along the reaction path connecting reactants to products.

Location: The post-doctoral researcher will work at the University of Reims Champagne-Ardenne, in Reims (close to Paris, 45 minutes by train) in the Institute of Molecular Chemistry (ICMR, UMR CNRS 7312).

Candidates: Applicants should have a strong background in theoretical chemistry and experience in potential energy surface exploration for mechanistic studies (transition state search, energy profile determination). Skills in the electron density topology analysis will be appreciated.

Position details: the position is funded by the French ANR (Agence Nationale pour la Recherche) for 12 months starting in early 2023.

Selected references from the group on that topic:

C. Lefebvre et al. PCCP 19 (2017) 17928, H. Khartabil et al., Org. Biomol. Chem. 18 (2020) 1850
M. Bos and E. Riguet, Chem. Commun., 53 (2017) 4997
Pertschi, R et al. Helv. Chim. Acta. 104 (2021) e2100133, Pertschi, R. et al. Chem. Catal. 1 (2021) 129

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Please, provide a CV detailing your training, as well as previous research experience, a letter of motivation, and 2 letters of recommendation