Richard M W Wong, J Chemical Sci 2018, Volume: 9
DOI: 10.4172/2150-3494-C4-025

5th International Conference on

Organic and Inorganic Chemistry

July 12-13, 2018 | Paris, France

Richard M W Wong

National University of Singapore, Singapore

Application of halogen bonding to organocatalysis

Halogen bond, a noncovalent interaction involving a halogen atom as an acceptor of electron density, has emerged in recent years as an important element of molecular recognition and has numerous applications such as molecular self-assembly of functional materials and protein-drug interaction. Due to its bond strength and directionality, halogen bonding has great potential to become a complementary molecular tool to hydrogen bonding in rational catalyst design. Using density functional calculations, we have shown the use of halogen-bond donors as noncovalent activators in Lewis acid catalysis. In particular, we have proposed a new type of triaryl benzene organocatalysts via multiple halogen bond donors (e.g. perfluoro-iodophenyl group). This *in silico* designed halogen bonding (XB) based catalyst was applied to several important types of organic reactions, namely Diels-Alder reaction, Claisen rearrangement and cope-type hydroamination. The calculated catalytic mechanisms and activation barriers of these reactions readily demonstrate that the designed system is a promising Lewis acid catalyst via halogen bond mode of activation. On the basis of our DFT calculations and calculated turnover frequencies, the XB-catalyzed reactions are found to be competitive with the corresponding hydrogen bonding catalysis reported in literature. The calculated transition states unravel multiple halogen bonds between the iodine atoms and various types of halogen bond acceptors (lone pair, π and σ bonds). These cooperative non-covalent interactions provide efficient binding between the catalyst and substrate (~15 kcal/mol binding energy) and are the key factors for transition-state stabilization and molecular recognition.

Biography

Richard M W Wong received his PhD degree from Australian National University in 1989. Subsequently, he held Post-doctoral position at IBM Kingston and Yale University. Currently, he is a full-time Professor and Head of Department at the National University of Singapore. Recently, he was the Recipient of Fukui Award for his outstanding work in Theoretical and Computational Chemistry. He has published about 200 scientific publications, which received over 9300 citations and H-index of 43. His research interests include application of computational quantum chemistry to a range of chemical problems, including reactive intermediates, catalysis, materials design, chemical sensors and weak intermolecular interactions. He is an International Advisory Board Member of Asian Journal of Chemistry, Journal of Analytical and Applied Pyrolysis and Advanced Theory and Simulations.

chmwmw@nus.edu.sg

Notes: