

On the Mechanism of Stereoselection in the Important Enantioselective Reactions: Combined NMR and DFT Studies

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The talk will describe combined experimental (NMR) and computational studies on the elucidation of the mechanism of induction of chirality in the reactions catalyzed by transition metal complexes with chiral ligands. Short review of the trial-and-error mechanism in asymmetric hydrogenation [1] will be followed by the most recent results [2,3]. Other topics are Ru catalyzed asymmetric Michael addition [4] and two conjugated addition reactions of alpha-cyanoesters that give opposite sign of chirality with the same combination of the catalyst and cyanoester [5,6].

[1] Chem.Comm. 2009, 7447-7465

[2] JACS 2012 1754-1769

[3] Chem.Comm. 2012 2186-2188

[4] JACS 2010 16637-16650

[5] JACS 2007 2158-2159

[6] ACIE 2010 8157-8160