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H-Bonds in Photo- and Ion Pair Catalysis: NMR Spectroscopy as Mechanistic Tool

Tuesday 16 September 2025 14:30 (30 minutes)

H-bonds play a crucial role in many mechanistic aspects of catalytic reactions. However, in many rapidly expanding fields of catalysis and asymmetric catalysis, mechanistic studies as well as structural investigations on intermediates, intermolecular interactions or aggregate formation are scarce. In addition, to dissect the contribution of H-bonds in these mechanistic cycles is extremely challenging. In this talk I will present techniques and methods to get insights via NMR spectroscopy into various H-bond contributions in photocatalysis and ion pair catalysis and explain their impact on examples.

Hydrogen bond assisted ion pair catalysis will be a main topic in this talk. In depths studies of the H-bonds between the catalyst and the substrate and their characterization will be addressed. Kinetic studies show that the intrinsic H-bond strengths is responsible for activation of the substrates, which is deviating from external measurements. Furthermore, the structure stabilization via a strong H-bond explains the broad substrate scope of the reaction. Beyond the binary catalyst substrate complexes also ternary intermediates are discussed including special relaxation optimized NMR pulse sequences enabling structure determination using the special properties of H-bonds. In addition, the SOFAST method can be used to detect megnetisation transfers via H-bonds even without 15N labelling.

In photocatalysis it will be shown that H-bond analysis can be used to reveal so far hidden properties of well known H atom transfer reagents. There NMR spectroscopy can be even used to reveal indirect insights about the light part of a photocatalytic reaction. Last but not least first attempts to detect H-bond activation at oil water interfaces in photochemical reactions will be presented.

Keywords

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