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## MS32-P15

## Supramolecular analysis of intramolecular H-bonds in (P,N) chelates and (P,C) palladacycles: towards understanding the mechanism of asymmetric induction *via* crystal engineering

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(P,N) chelates and (P,C) palladacycles [1] are very important complexes, especially in catalytic research. A set of pentane-2,4-diyl based chiral aminoalkylphosphine ligands Ph PCH(CH<sub>3</sub>)CH<sub>2</sub>CH(CH<sub>3</sub>)NHR and their palladium complexes were prepared (as an example, see Figure). Single crystal X-ray diffraction; solution phase 1D and 2D NMR studies and theoretical calculations [2] were applied to verify the results and outcome of crystal engineering and to support catalytic studies. According to our latest results, mild oxidation of the complexes bearing suitable R substituents resulted in intramolecular C-H activation and concomitant formation of (P,C) coordinated palladacycles. Intramolecular H-bond between the coordinated chloride as acceptor and methylene/NH proton seems to play crucial role in stabilizing the conformation of the ring and fixing the stereogenic nitrogen atom, hence in transmission of chiral information in enantioselective catalysis. This opens the possibility to engineer suitable structures for enantioselective catalytic reactions of various substrates. Palladium was replaced with other metals having square planar coordination geometry and their structures were also studied.

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