Group	:	Homogeneous Catalysis & Biomimetic Synthesis
Project	:	**Study of Ru(0)-catalyzed cross-coupling reactions**
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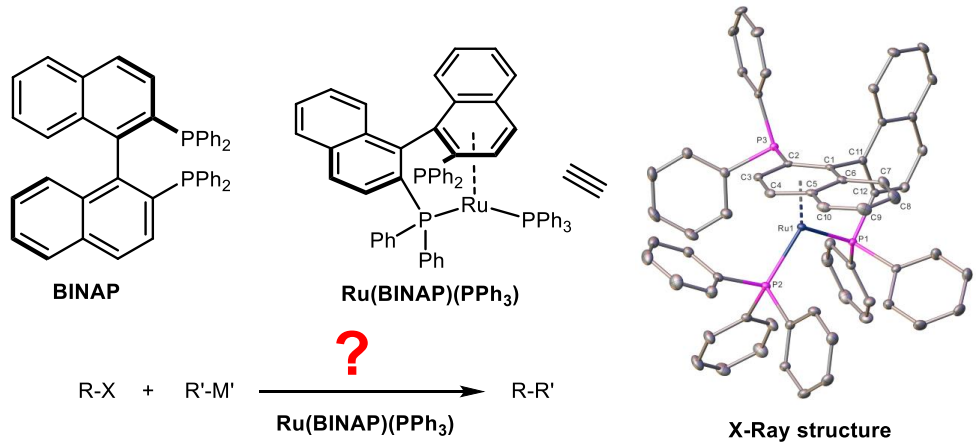
Keywords: Homogeneous Transition Metal Catalysis, Coordination Chemistry, Methodology Development

Introduction. Cross-coupling reactions are widely used for the construction of C-C bonds in the synthetic organic chemistry. These transformations are typically catalyzed by Pd complexes, which often demonstrate high levels of catalytic activity, stability and selectivity, making Pd-based catalysts unique for industrial applications.[1] However, the high price of Pd provides a high demand in cheaper catalytic systems based on other transition metals.

Ruthenium is approx. 10 times cheaper than Pd. The ability of Ru to activate inert C-H, C-F and C-C bonds, its well-defined coordination behavior and a clear tendency to undergo 2-electron rather than 1-electron redox processes (which are common for Fe, Co, Ni and Cu), make Ru highly attractive for cross-coupling reactions. However, the lack of only phosphine-based low-valent Ru-complexes precluded the research in this direction until now.[2-4]

Most recently we discovered a novel ruthenium(0) complex [Ru(BINAP)(PPh_3)], where the bidentate phosphine ligand BINAP[5] is coordinating with the ruthenium atom in a mixed π-arene/σ-P mode. With its unprecedented structure, this complex seems to be a promising molecule for efficient catalysis of homogeneous cross-coupling reactions.



Goal. In this project, we are going to investigate the potential of [Ru(BINAP)(PPh_3)] as a catalyst in cross-coupling reactions. The study will focus on the catalytic cross-coupling reactions between different types of substrates (combinations of aromatic halides with aryl boronic acids, silanes, alkenes and other C-based nucleophiles). For the successful transformation, the optimization of the reaction conditions will be performed and the synthetic scope of the transformation will be evaluated.

Topics to be studied. The project is focused on the development of a novel organic reaction methodology with elements of inorganic synthesis. The work will involve the set-up of catalytic reactions, analysis of reactions outcome, rational-based step by step development of novel catalytic methodology; reaction monitoring; analysis of reaction outcome by a combination of analytical methods with a significant use of NMR. Depending on the progress, research may involve elements of inorganic synthesis and study of stoichiometric reactions involving Ru-complexes.

Techniques to be used. The work will include the most up-to-date organic synthetic methods, including the work in inert atmosphere both on Schlenk-line and in glove box, reaction monitoring by TLC, GC-MS and NMR, column chromatography, crystallization, multinuclear NMR experiment, etc.

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