

# Dynamic Catalytic Systems in the Heck Reaction and C-S Cross-Coupling Revealed by Mass Spectrometry

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Catalytic systems based on Pd complexes are well established for a variety of C-C, and C-Heteroatom bond formation processes including the Mizoroki-Heck reaction and C-S cross-coupling. Most commonly, well-defined catalyst precursors containing strong metal-ligand bonds are developed to ensure molecular homogeneous catalysis. However, recent studies indicate diversity of dynamic processes, which occur in the reaction mixture and affect the catalytically active species.<sup>1,2</sup>

The impact of the nanoscale organization of reactive species on their reactivity creates various opportunities for fine-tuning of reaction parameters.<sup>3</sup> In order to reveal intermediates and study the mechanisms of these highly valuable reactions, electrospray ionization mass spectrometry was applied (Figure 1).

Catalytic systems based on Pd-NHC and Pd/Ni(SAr)<sub>2</sub> complexes were studied and indicated involvement of cocktail-type reactions.<sup>1-3</sup> The resulting mechanistic insights and their synthetic implementations will be presented and discussed.

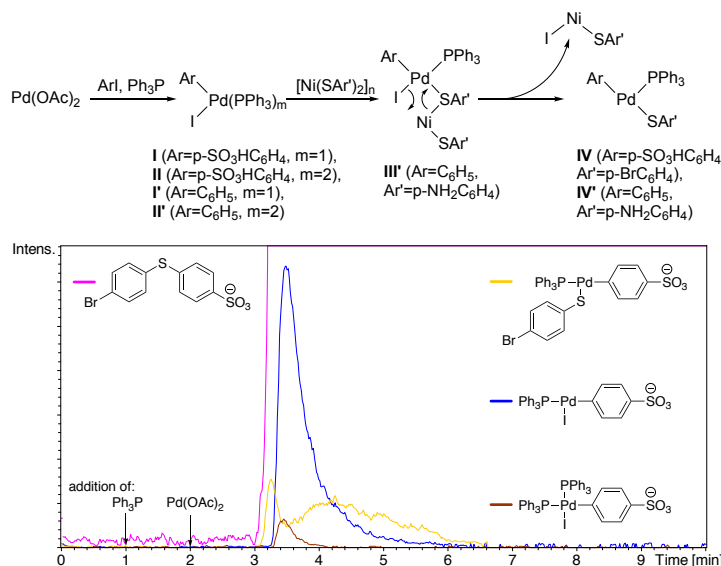


Figure 1. An example of the ESI-MS study of reaction mechanism in solution, with the intermediates detected and ESI-MS traces in the negative ion mode.

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