

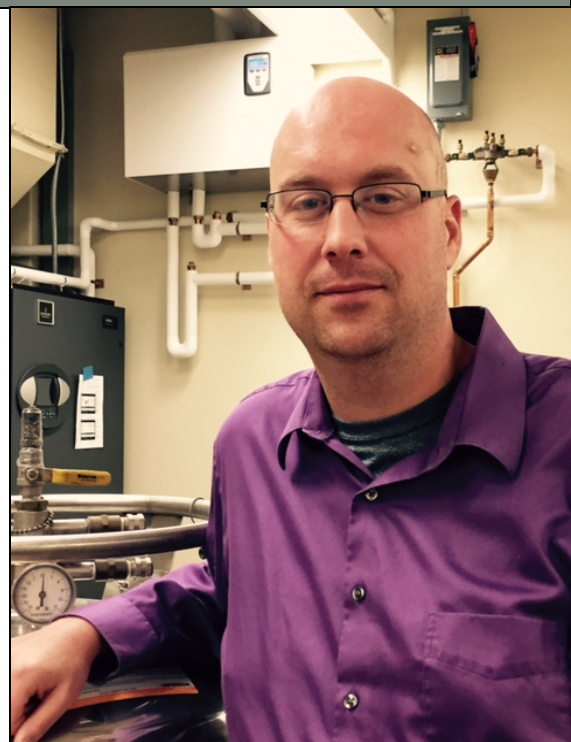
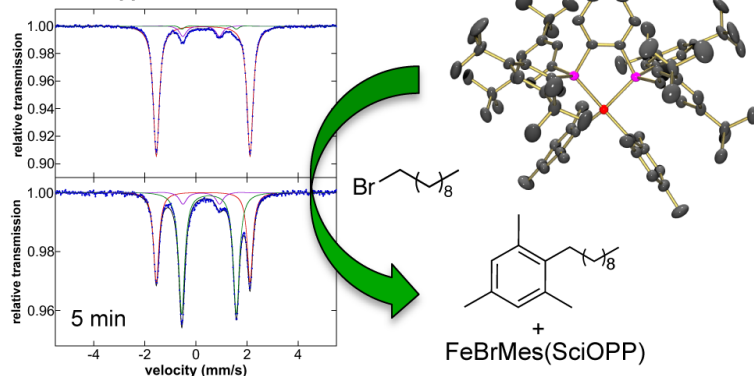
CHEMISTRY COLLOQUIUM

Structure, Bonding and Mechanism in Iron-Catalyzed Cross-Coupling

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Freeze-Trapped Solution Mössbauer



Abstract:

Iron-catalyzed C-C cross-coupling reactions have attracted significant interest as versatile and cost effective alternatives to traditional precious metal catalysts, including reactions that have proven difficult for precious metals such as cross-couplings of non-activated alkyl halides. Despite the success of these reactions, the design and development of improved catalysts requires a detailed understanding of the in situ formed iron species and mechanism of catalysis in these systems. However, such investigations are challenging due to the prevalence of paramagnetism in iron species involved in cross-coupling as well as the need to elucidate the individual iron components present in potentially complex mixtures in solution. Our group has pioneered an approach combining inorganic spectroscopic methods (e.g. Mössbauer, MCD, EPR), DFT investigations and synthetic/reaction studies that provides a powerful method to address these challenges and define the active iron species and mechanisms involved in iron-catalyzed cross-coupling. The utilization of this research methodology in several iron-based systems will be presented, including iron-bisphosphine and simple ferric salt systems.

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