

Tuning the Regioselectivity of Hydrocarbon Oxidation Catalyzed by Non-Heme Iron Complexes



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The selective oxidation of C-H bonds remains a challenge in organic synthesis. Recent work within the Goldsmith laboratory has focused on developing sterically encumbered ligands capable of modulating the regioselectivity of the oxygenation and halogenation catalyzed by non-heme iron complexes.

The **bbpc** compound was prepared as a bulkier analog of previous tetradentate N-donor ligands that supported iron-mediated oxidation chemistry. The $[\text{Fe}(\text{bbpc})(\text{MeCN})_2]^{2+}$ complex directs oxygenation towards the less sterically congested secondary carbons of alkane substrates rather than the thermodynamically weaker C-H bonds on tertiary carbons. The system is currently being adapted towards regioselective alkane chlorination and bromination.

Other accomplishments during the past year include the discovery of the first homogeneous Ga(III) catalyst for olefin epoxidation and the synthesis of a heptacoordinate Mn(II) complex that serves as an effective contrast agent for magnetic resonance imaging.

