



The Department of Chemistry Presents:

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Title: High-valent Cu(III) species in bioinorganic chemistry and C-H functionalization

High-valent Cu(III) complexes have long been proposed as important intermediates in biological redox processes and organic transformations involving the activation of C-H bonds. However, the proposed high-valent Cu(III) intermediates often elude detection due to their fleeting lifetimes.

In the first part of my talk, we employ a general CuII/CuIII platform to activate simple nucleophiles (Nu) toward C-H functionalization. Oxidation of CuII-Nu to formal CuIII-Nu endows the Nu moiety with hydrogen atom transfer and radical capture reactivity. Building on this platform, we have established several (electro)catalytic C-H functionalization methods that selectively produce functionalized hydrocarbon products at mild conditions.

In the second part of my talk, I will present a newly discovered reactivity of Cu(III) complexes toward deoxyhalogenation. While C-H halogenation is typically proposed to proceed via a halogen rebound mechanism, our results support an alternative stepwise pathway in which copper first mediates C-H hydroxylation—reactivity well established for copper enzymes and coordination complexes—followed by deoxyhalogenation. This mechanistic framework offers a plausible means by which nature repurposes copper cofactors for C-H hydroxylation to achieve C-H halogenation.

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