

A Tale of Two States: From Iron Oxo Diatomic to Cytochrome P450 and Other Oxidation Catalysts

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The talk will describe the phenomenon of two-state or multi-state reactivity (TSR/MSR) in high-valent metal-oxo reagents, projecting its wide-ranging applicability starting from the bare diatomic species, through the reagents made by Que and collaborators, to the Mn(V)-oxo substituted polyoxometalate, all the way to Compound I species of cytochrome P450 and other heme enzymes. *The paper shows how the TSR/MSR behaviors of all these variegated species derive from a simple set of electronic structure principles.* Controversial experimental trends concerning radical lifetimes and product isotope effect will be reconciled with the TSR/MSR picture. Diagnostic mechanistic probes will be proposed for the TSR/MSR scenario, based on kinetic isotope effect, stereochemical studies, and magnetic- and electric-field effects.