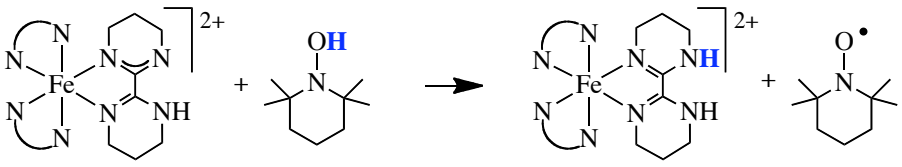
Abstract for Jim Mayer talk
UCSB, PIRE-ECCI seminar,
February, 2011

Proton-Coupled Electron Transfer: Metal Complexes, Organic Reactions, Metal Oxides, and Marcus Theory

The coupled transfer of electrons and protons is fundamental to a wide variety of chemical and biochemical processes. These range from classical organic hydrogen atom transfer reactions to the multielectron/multiproton transformations central to chemical and biological energy transduction. The first part of this presentation will discuss a number of reactions involving transition metal and/or organic compounds that involve concerted transfer of one electron and one proton. Some of these reactions 'look like' hydrogen atom transfers, such as oxyl radicals abstracting H• from vitamin C and the oxidation of a hydroxylamine by an iron(III) complex (eq 1). Other reactions cannot be described a transfer of an H-atom because the electron and proton are quite separated in the reactants or products. Both types of reactions can be analyzed using versions of Marcus Theory, in many cases with good accuracy. The Marcus approach shows the commonality of organic and transition metal H-atom transfer reactions, and raises fundamental issues of intrinsic barriers, driving force dependence, and hydrogen bonding. The second portion of the presentation will present initial results on projects extending these ideas to new water-oxidation catalysts and to the reactivity of zinc oxide nanoparticles.



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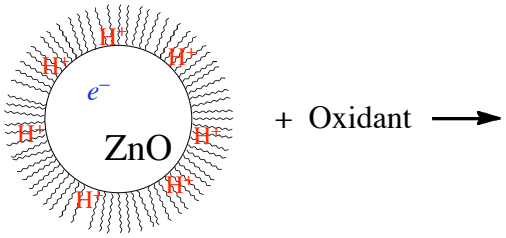

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