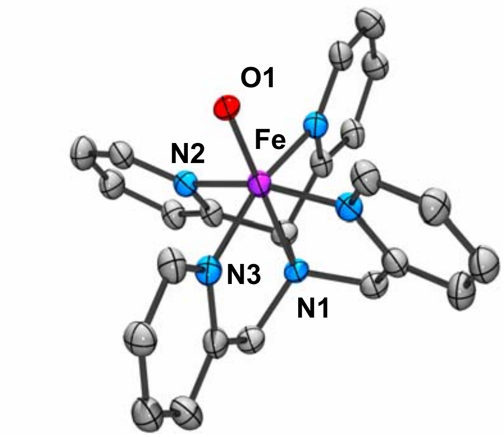
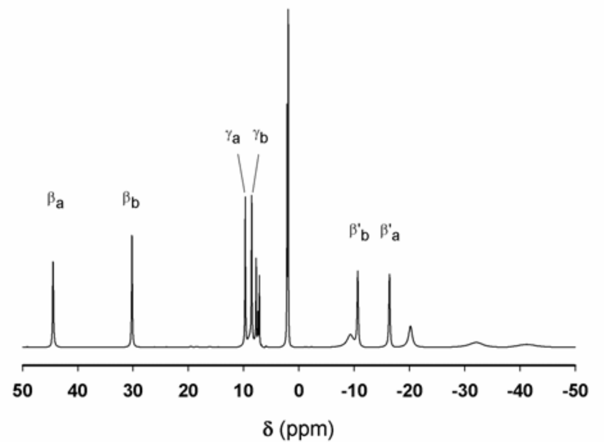
Structures and Reactivity of Non-heme Oxoiron(IV) Compounds

Eric J. Klinker, József Kaizer, William W. Brennessel, Lawrence Que, Jr.

Department of Chemistry and Center for Metals in Biocatalysis, University of Minnesota,
Minneapolis, MN 55455 (e-mail: klinker@chem.umn.edu)

High-valent oxoiron(IV) species are often invoked in the mechanisms of oxygen activating enzymes. Advances in modeling the chemistry of these enzymes have shown that such species can be isolated in non-heme nitrogen containing ligand environments. Recently, a new series of oxoiron(IV) species supported by pentadentate N5 ligands have been generated at room temperature. These systems provide remarkable solution state stability to the high-valent iron compounds that has allowed for their extensive characterization. A combination of X-ray crystallography and ^{1}H NMR has been used to develop a new method for determining ligand topology in oxoiron(IV) compounds by use of only ^{1}H NMR. Additionally, we have concluded that pyridine rings aligned parallel to the Fe=O bond greatly enhance the stability of these compounds. Despite their greater thermal stability, these oxoiron(IV) complexes react with a range of hydrocarbon substrates, an impressive reactivity that will be discussed in greater detail.





Supported by NIH GM-33162