Supporting Information

Characterization of the Arene-Oxidizing Intermediate in ToMOH as a Diiron(III) Species

Leslie J. Murray,[1] Sunil G. Naik,[2] Danilo O. Ortillo,[2] Ricardo García-Serres,[2] Jessica K. Lee,[1] Boi Hanh Huynh,[2] and Stephen J. Lippard[1]

[1]Department of Chemistry, Massachusetts Institute of Technology, Cambridge, MA 02139 and

[2]Department of Physics, Emory University, Atlanta, GA 30322

lippard@mit.edu; vhuynh@emory.edu

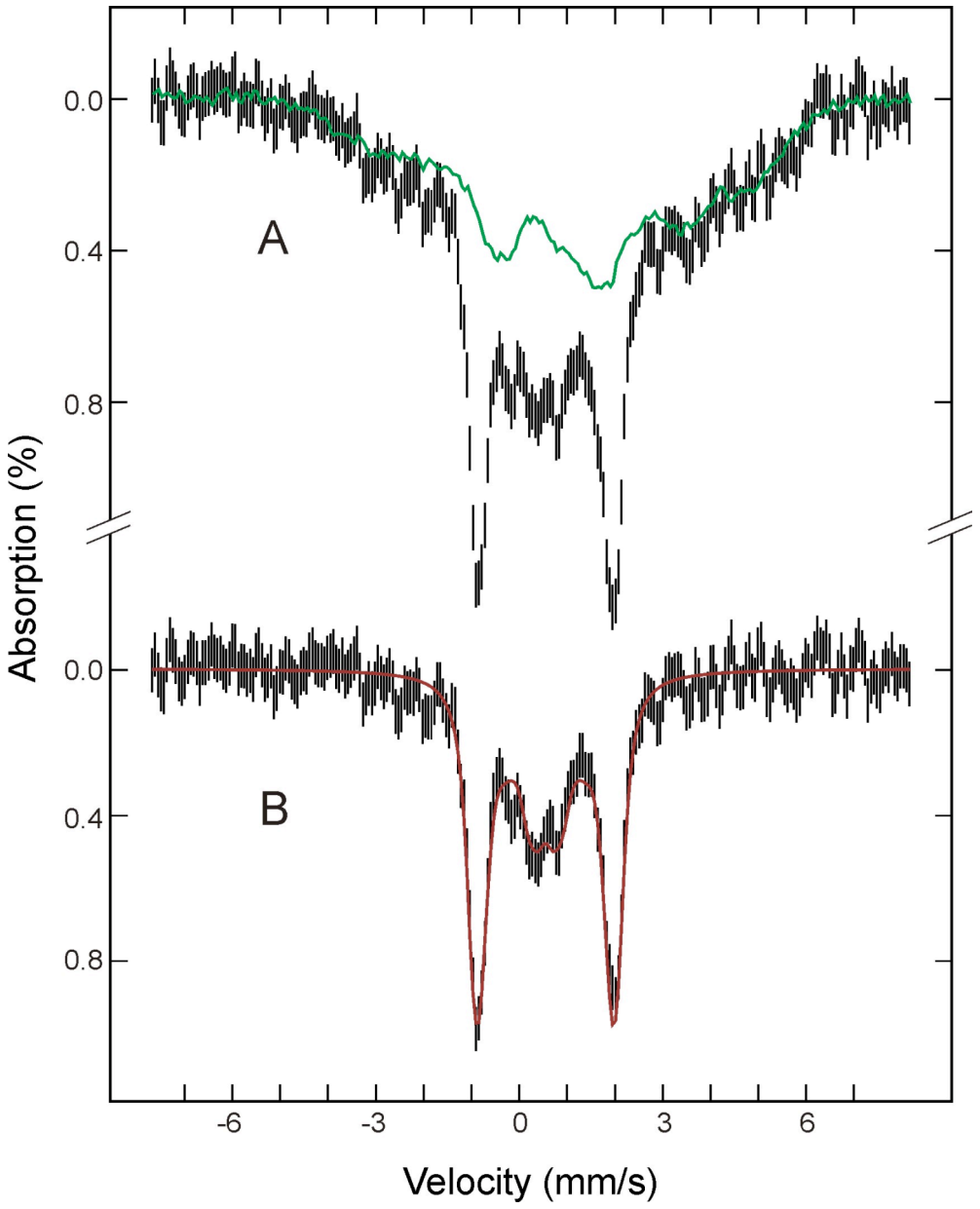

Figure S1. High-field Mössbauer spectrum (vertical bars in A) of a freeze-quench sample from the reaction of reduced ToMOH:2ToMOD with O_2 frozen at 0.14 s after mixing the reduced protein with O_2. The spectrum was collected at 4.2 K in an applied field of 8 T parallel to the γ-beam. The green line in A is the spectrum of the diiron(II) protein before mixing recorded under the same experimental conditions, and is plotted at 56% of the total Fe absorption of the freeze-quenched sample. Removal of the diiron(II) contribution from spectrum A yields spectrum B (vertical bars). The red line in B is a theoretical spectrum of the diiron(III) intermediate simulated with parameters determined at low field (see caption of Figure 1) and assuming diamagnetism. The excellent agreement between theory and experiment indicate the ground state of the diiron(III) intermediate is diamagnetic, revealing antiferromagnetic coupling between the two ferric ions.