Supporting Information

Molecular and Electronic Structures of Mononuclear Iron Complexes and their Oxidized Forms Using strongly Electron-donating Ligands

Julia B. H. Strautmann†, Serena DeBeer George‡, Eberhard Bothe§, Eckhard Bill§, Thomas Weyhermüller§, Anja Stammler†, Hartmut Bögge†, and Thorsten Glaser‡,*

Fakultät für Chemie, Universität Bielefeld, Universitätsstr. 25, D-33615 Bielefeld, Germany,

Stanford Synchrotron Radiation Laboratory, SLAC, Stanford University, Stanford, California 94309, USA,

Max-Planck-Institut für Bioanorganische Chemie, Stiftsstr. 34-36, D-45470 Mülheim, Germany

* To whom correspondence should be addressed.

† Fakultät für Chemie, Bielefeld

‡ Stanford Synchrotron Radiation Laboratory, Stanford

§ Max-Planck-Institut, Mülheim
Figure S1. a) Comparison of the normalized Fe K-edge data for [LFe(η²-NO₃)] as a solid in BN (black) and as a solution in dichloromethane (red). b) Comparison of the normalized Fe K-edge data for [LFeCl] as a solid in BN (black) and as a solution in dichloromethane (red).
**Figure S1.** Electronic absorption spectra of [LFe($\eta^2$-NO$_3$)] (black lines) and of [LFeCl] (red lines) measured in pentane (pentane), dichloromethane (CH$_2$Cl$_2$), acetonitrile (CH$_3$CN), and methanol (MeOH) at 25 °C.