Electronic Supporting Information for:

Structural, Spectroscopic, and Electrochemical Properties of Nonheme Fe(II)-Hydroquinonate Complexes: Synthetic Models of Hydroquinone Dioxygenases

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Contents

Figures S1-S3 S2-S4
Computational Details S5
Figure S1. Electronic absorption spectra of $2E$ and $2F$(MeCN) in CH$_2$Cl$_2$ at room temperature.
Figure S2. $^1$H NMR spectra of 1A-1D, and 1F in CD$_2$Cl$_2$ at ambient temperature. Peaks marked with an asterisk (*) disappeared upon addition of a small amount of MeOH-$d_4$ and are therefore assigned to the exchangeable proton of the distal –OH moiety. Resonances arising from protons at the 4-positions of the Ph$_2$Tp pyrazole rings (4-pz) were identified on the basis of peak integrations.
Figure S3. X-band EPR spectra of $1A_{ox}-1C_{ox}$ in frozen CH$_2$Cl$_2$ solutions. The $1X_{ox}$ species were obtained by treating the Fe(II) precursors with one equivalent of acetylferrocenium ($1A_{ox}$) or [N(C$_6$H$_4$Br-4)]$^+$ ($1B_{ox}$ and $1C_{ox}$). The spectra were collected under the following conditions: frequency = 9.63 GHz; power = 2.0 mW; modulation = 12 G; temperature = 10 K.
Computational Details.

Density functional theory (DFT) calculations of complex 1B were performed using the ORCA 2.0 software package developed by Dr. F. Neese. Atomic coordinates were obtained from the corresponding X-ray structure, although the 5-Ph groups of the Ph2Tp ligand were replaced by -CH3 groups in the computational model. The DFT calculations employed the Becke-Perdew (BP86) functional and Ahlrichs’ valence triple-ζ basis set (TZV) for all atoms, in conjunction with the TZV/J auxiliary basis set. Extra polarization functions were used on non-hydrogen atoms. Time-dependent DFT (TD-DFT) calculations provided absorption energies and intensities within the Tamm-Dancoff approximation. Forty excited states were calculated.

(1) Neese, F.; ORCA - An ab initio, Density Functional and Semi-empirical Program Package, version 2.8; University of Bonn: Bonn, Germany, 2010.