

Supporting Information for

**A New Example of NonHeme Mononuclear
Fe(IV)-Oxo complex. Spectroscopic data and
Oxidation Activity.**

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Figure S1. Oxygen-atom exchange between $[(\text{TPEN})\text{FeO}]^{2+}$ (m/z 248.2) and H_2^{18}O monitored by EI-MS. The peak that progressively increases in intensity at m/z 249.2 corresponds to $[(\text{TPEN})\text{Fe}^{18}\text{O}]^{2+}$ (time is increasing from upper to lower spectrum).

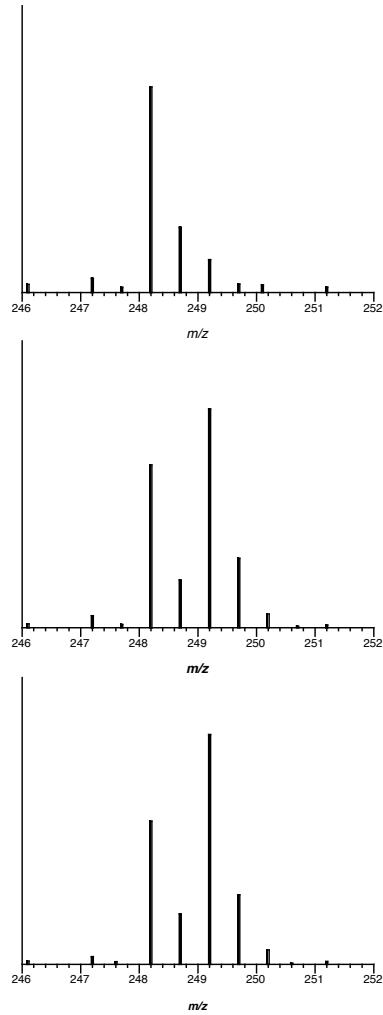


Figure S2. Zero-field Mössbauer spectrum of solid $[(\text{TPEN})\text{Fe}^{\text{IV}}(\text{O})](\text{PF}_6)_2$ at 4.2 K. Full width at half-maximum of the Lorentzian lines : 0.15 mm/s (lower energy line) and 0.18 mm/s (higher energy line). The spectrum was fitted (solid line) with the parameters: $\Delta E_Q = 0.87$ (1) mm/s; $\delta = 0.01$ (1) mm/s (relative to Fe metal). Standard deviations are given in parentheses. An impurity is also present, but has not been considered in the fitting procedure.

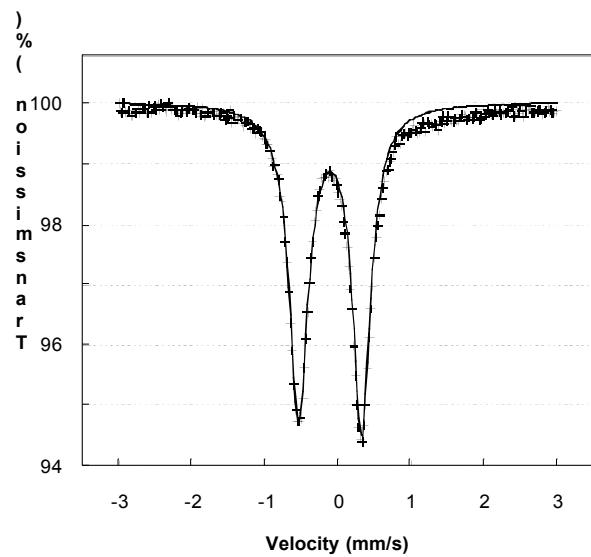


Figure S3. evolution of $[(\text{TPEN})\text{FeO}]^{2+}$ (m/z 248.2) monitored by ESI-MS. The peak at m/z 240.2 corresponds to $[(\text{TPEN})\text{Fe}]^{2+}$, m/z 193.7, m/z 108.1 and m/z 201.7 correspond to $[(\text{SBPy})_3\text{Fe}]^{2+}$, protonated pyridine carboxaldehyde, and $[(\text{SBPy})_3\text{FeO}]^{2+}$ respectively.

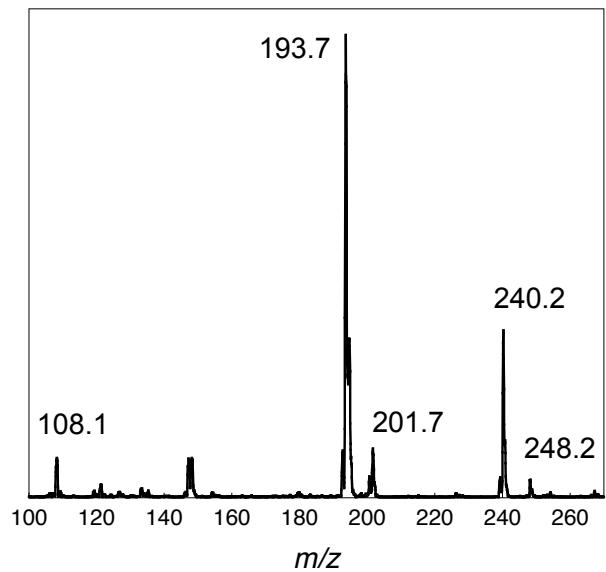


Figure S4. plots of the absorbance at 730 nm (λ_{\max} for $[(\text{TPEN})\text{FeO}]^{2+}$) and 556 nm (λ_{\max} for $[(\text{SBPy}_3)\text{Fe}(\text{CH}_3\text{CN})]^{2+}$) resolved in time. Data extracted from the decay of a 4 mM solution of $[(\text{TPEN})\text{Fe}]^{2+} + 1 \text{ }m\text{CPBA}$ in $\text{CH}_2\text{Cl}_2 / \text{CH}_3\text{CN}$ at room temperature.

