

Supporting Information

Selective Formation of a Stable μ -Peroxo Ferric Heme-Cu^{II} Complex from the Corresponding μ -Oxo Fe^{III}-Cu^{II} Species with Hydrogen Peroxide

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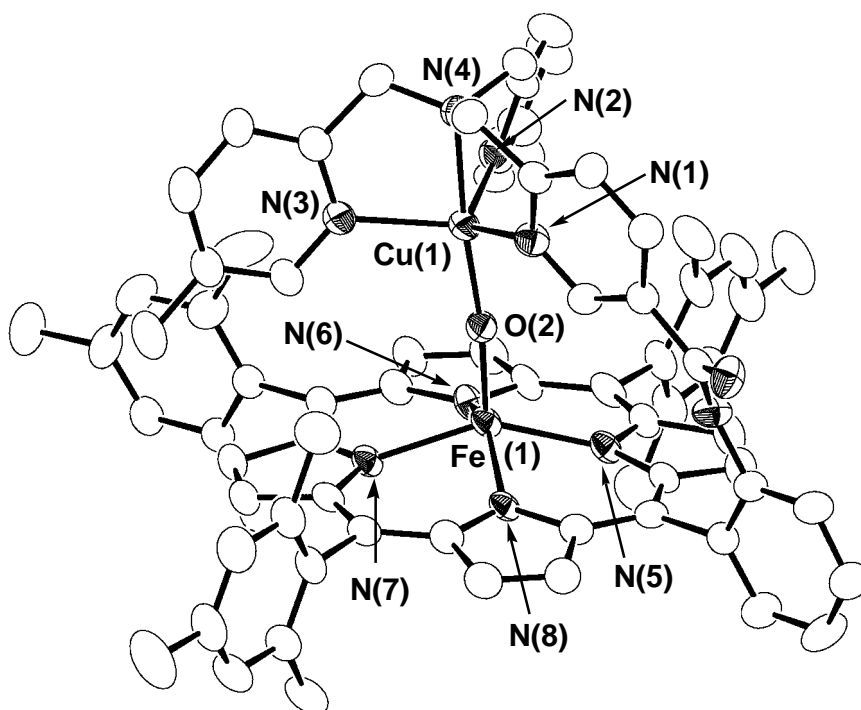


Fig. S1. ORTEP view of $[(\text{TMP})\text{Fe}^{\text{III}}-(\text{O})-(5\text{MeTPA})\text{Cu}^{\text{II}}]^+$ in crystals of **2** drawn with the thermal ellipsoids at the 50 % probability level. All hydrogen atoms were omitted for clarity. Selected bond length [\AA] and angles [deg]: Cu(1)-O(2) 1.856(3), Fe(1)-O(2) 1.758(3), Cu(1)-N(1) 2.069(4), Cu(1)-N(2) 2.079(4), Cu(1)-N(3) 2.144(4), Cu(1)-N(4) 2.095(4), Fe(1)-N(5) 2.121(4), Fe(1)-N(6) 2.113(4), Fe(1)-N(7) 2.106(4), Fe(1)-N(8) 2.119(4), Cu(1)-O(2)-Fe(1) 172.8(2).

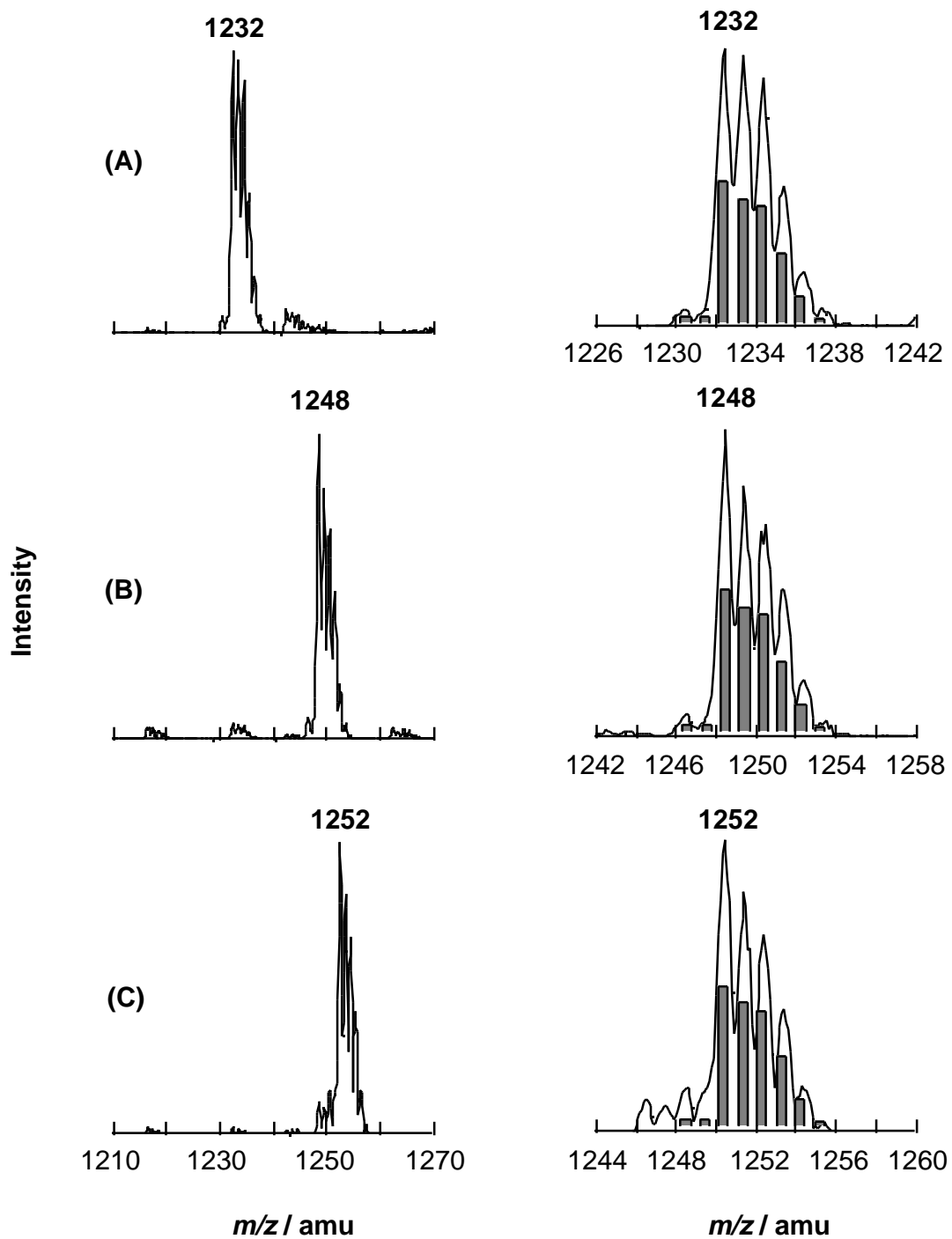


Fig. S2. ESI-mass spectra (CH_3CN , room temperature): (A) **2**, (B) **2** + $H_2^{16}O_2$ and (C) **2** + $H_2^{18}O_2$. The magnified ones are shown in the right side with their simulated isotope patterns in bars.