Supplementary Material (ESI) for Green Chemistry

Supplementary Information for B411269E

Oxidation of 2,4,6-Trichlorophenol by Hydrogen Peroxide. Comparison of Different Iron-Based Catalysts

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Contents:

Fig. S1 Spectral observations in the 2,4,6-trichlorophenol - H_2O_2 system in the presence of methylrheniumtrioxide (CH_3ReO_3, MTO). [MTO] = 180 μM; [TCP] = 0.30 mM; [H_2O_2] = 60 mM; [H_2O] = 2.0 M in CH_3CN; reaction times: before the addition of MTO (a), 1 h (b), 5 h (c), 15 h (d); pathlength: 1 cm; T = 25.0 °C. The band forming and decomposing around 365 nm is characteristic of the bis-peroxo complex $CH_3ReO(O\text{-}O)_2$, whereas the band of TCP at 290 nm remains unchanged.

Fig. S2 Oxidation of chloride ion with peroxomonosulfate ion catalyzed by $Fe(TPPS)^+$. [HSO_5^-] = 50 mM; $[Cl^-]_0$ = 0.48 mM (a) 0.40 mM (b); [$Fe(TPPS)^+$] = 3.1 μM (a) 1.5 μM (b); μ = 0.14 M; T = 25.0 °C.

Fig. S3 Effect of citric acid on the spectrophotometric kinetic traces during the oxidation of 2,4,6-trichlorophenol with H_2O_2 catalyzed by $Fe(TPPS)^+$. [H_2O_2] = 320 mM; [$HClO_4$] = 64 mM; [citric] = 0 (a), 19 mM (b) 64 mM (c); [$Fe(TPPS)^+$] = 8.2 μM; [TCP] = 0.32 mM; T = 25.0 °C.

Fig. S4 Effect of citric acid on chloride ion buildup during the oxidation of 2,4,6-trichlorophenol with H_2O_2 catalyzed by $Fe(TPPS)^+$. [H_2O_2] = 46 mM; [$HClO_4$] = 91 mM; [citric acid] = 0 (a), 41 mM (b); [$Fe(TPPS)^+$] = 2.9 μM; [TCP] = 0.79 mM; T = 25.0 °C.

Fig. S5 Concentration of H_2O_2 as a function of time during the oxidation of 2,4,6-trichlorophenol with H_2O_2 catalyzed by *cis*- and *trans*-$[Fe(cyclam)]^{3+}$. [TCP] = 1.00 mM (a, b) 0 (c, d); [*cis*-$Fe(cyclam)^{3+}$] = 100 μM (a, c); [*trans*-$Fe(cyclam)^{3+}$] = 100 μM (b, d); T = 25.0 °C.

Fig. S6 Concentration of H_2O_2 as a function of time during the oxidation of 2,4,6-trichlorophenol with H_2O_2 catalyzed by $Fe(TPPS)^+$. [TCP] = 1.0 mM (a), 0 (b); [$Fe(TPPS)^+$] = 5.6 μM; T = 25.0 °C.

Fig. S7 Concentration of H_2O_2 as a function of time during the oxidation of 2,4,6-trichlorophenol with H_2O_2 catalyzed by $Fe(6\text{-}Me_2TPA)^{2+}$. [TCP] =1.0 mM (a), 0 (b); [$Fe(6\text{-}Me_2TPA)^{2+}$] = 28 μM; T = 25.0 °C.

Fig. S8 Concentration of H_2O_2 as a function of time during the oxidation of 2,4,6-trichlorophenol with H_2O_2 catalyzed by $Fe(TPA)^{2+}$. [TCP] =1.0 mM (a) 0 (b); [$Fe(TPA)^{2+}$] = 27 μM; T = 25.0 °C.

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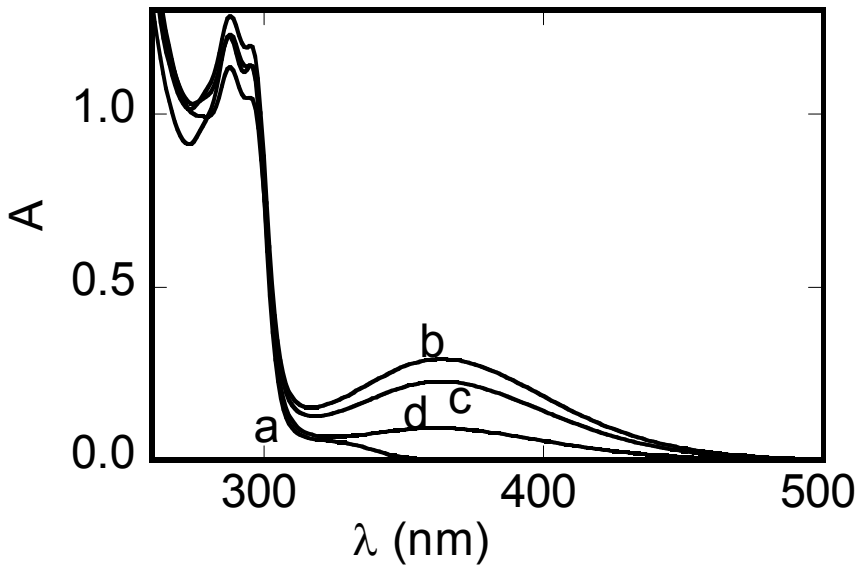

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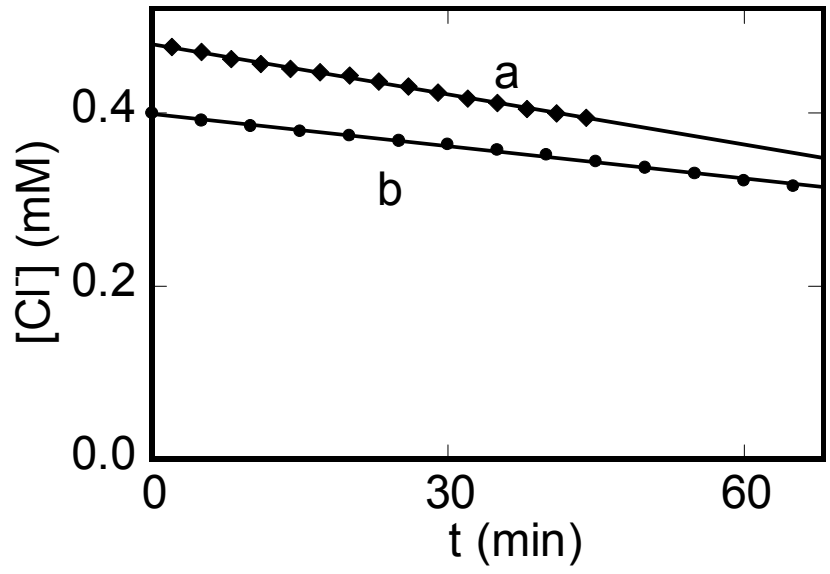

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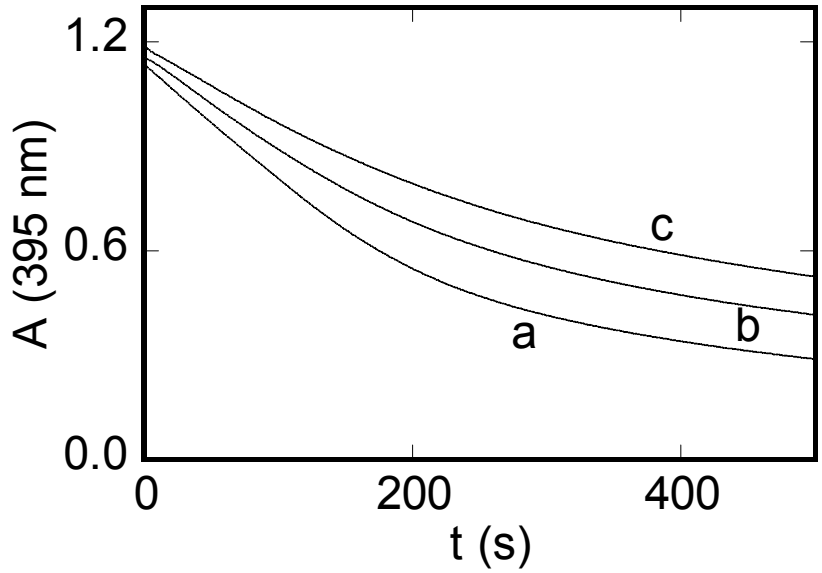

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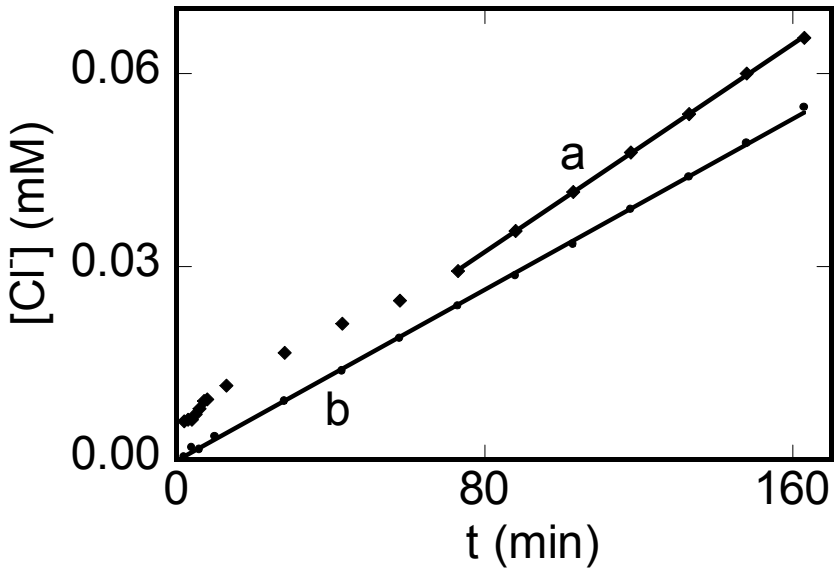

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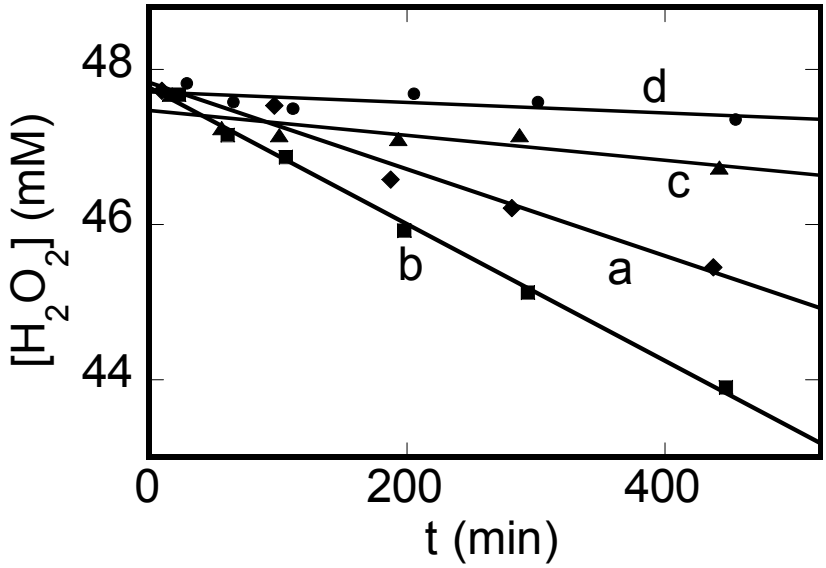

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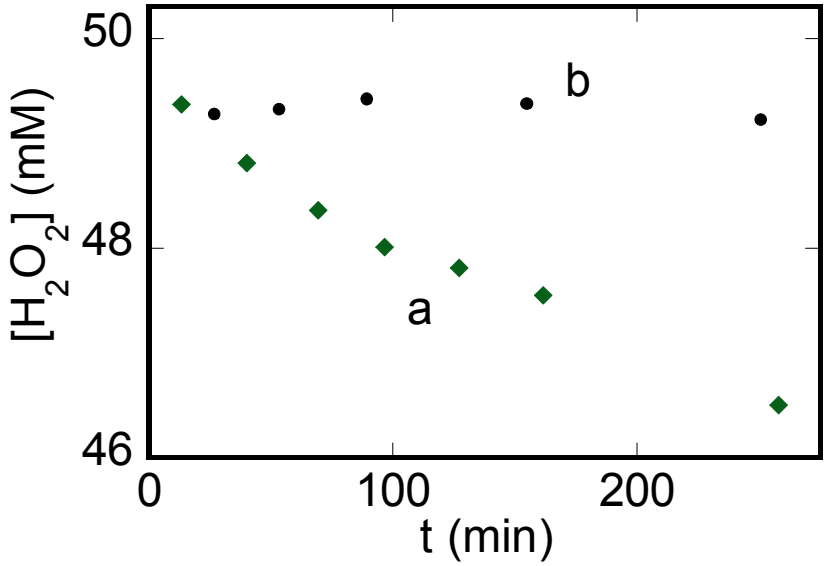

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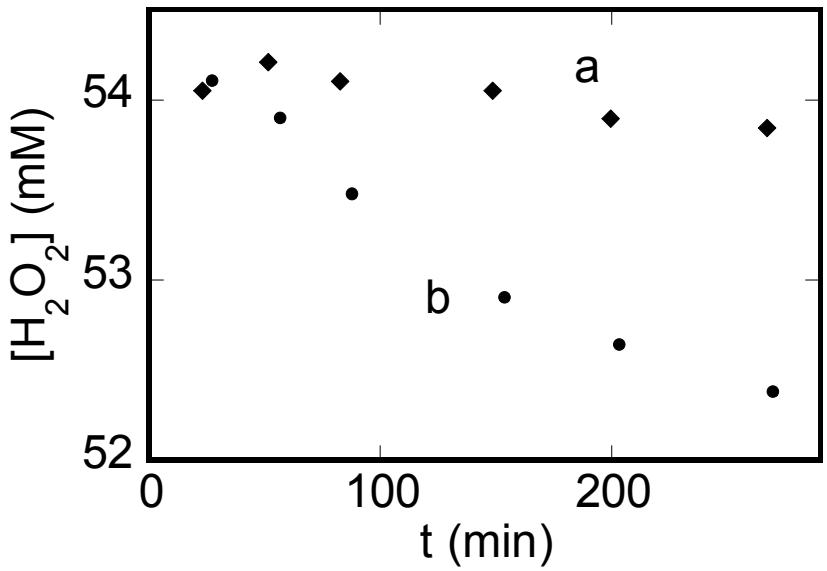

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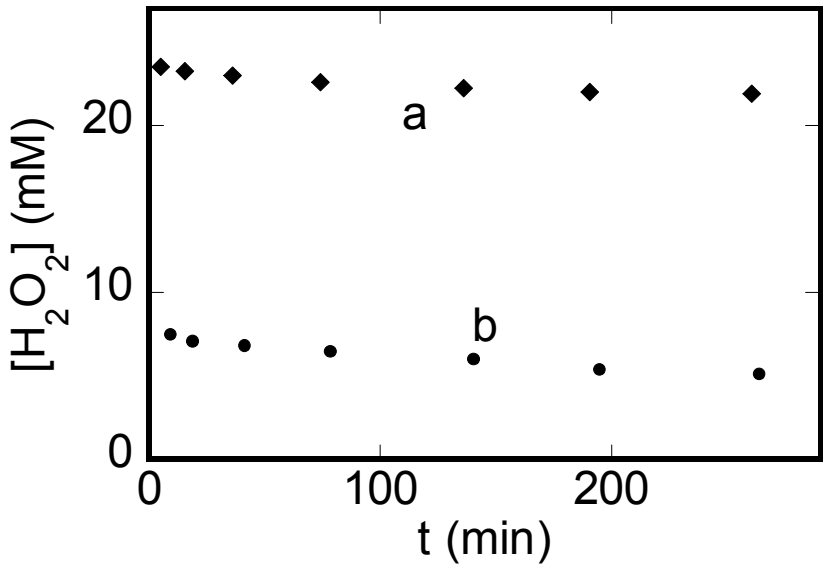

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