

Heterometallic $\text{Co}^{\text{III}}_4\text{Fe}^{\text{III}}_2$ Schiff base complex : structure, electron paramagnetic resonance, and alkane oxidation catalytic activity.

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The heterometallic complex $[\text{Co}_4\text{Fe}_2\text{OSae}_8]\cdot 4\text{DMF}\cdot \text{H}_2\text{O}$ (**1**) was synthesized by one-pot reaction of cobalt powder with iron chloride in a dimethylformamide solution of salicylidene-2-ethanolamine (H_2Sae) and characterized by single crystal X-ray diffraction analysis, magnetic measurements, high frequency electron paramagnetic resonance (HF-EPR), and Mössbauer spectroscopies. The exchange coupling in the $\text{Fe}(\text{III})\text{--Fe}(\text{III})$ pair is of antiferromagnetic behavior with $J/hc = -190\text{ cm}^{-1}$. The HF-EPR spectra reveal an unusual pattern with a hardly detectable triplet signal of the $\text{Fe}(\text{III})$ dimer. The magnitude of D (ca. 13.9 cm^{-1}) was found to be much larger than in related dimers. The catalytic investigations disclosed an outstanding activity of **1** toward oxidation of cycloalkanes with hydrogen peroxide, under mild conditions. The most efficient system showed a turnover number (TON) of 3.57×10^3 with the concomitant overall yield of 26% for cyclohexane, and $2.28 \times 10^3/46\%$, respectively, for cyclooctane. A remarkable turnover frequency (TOF) of $1.12 \times 10^4\text{ h}^{-1}$ (the highest initial rate $W_0 = 3.5 \times 10^{-4}\text{ M s}^{-1}$) was achieved in oxidation of cyclohexane. Kinetic experiments and selectivity parameters led to the conclusion that hydroxyl radicals are active (attacking C–H bonds) species. Kinetic and electrospray ionization mass spectrometry (ESI-MS) data allowed us to assume that the trinuclear heterometallic particle $[\text{Co}_2\text{Fe}(\text{Sae})_4]^+$, originated from **1** in solution, could be responsible for efficient generation of hydroxyl radicals from hydrogen peroxide.

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