SUPPLEMENTARY MATERIAL TO THE ARTICLE:

Ferromagnetic Heteronuclear {$Fe_4(Er, Lu)_2$} Cyclic Coordination Clusters based on Ferric Wheels

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Synthesis of $[Fe_4Er_2(teaH)_4(N_3)_4(piv)_6]$ (1)

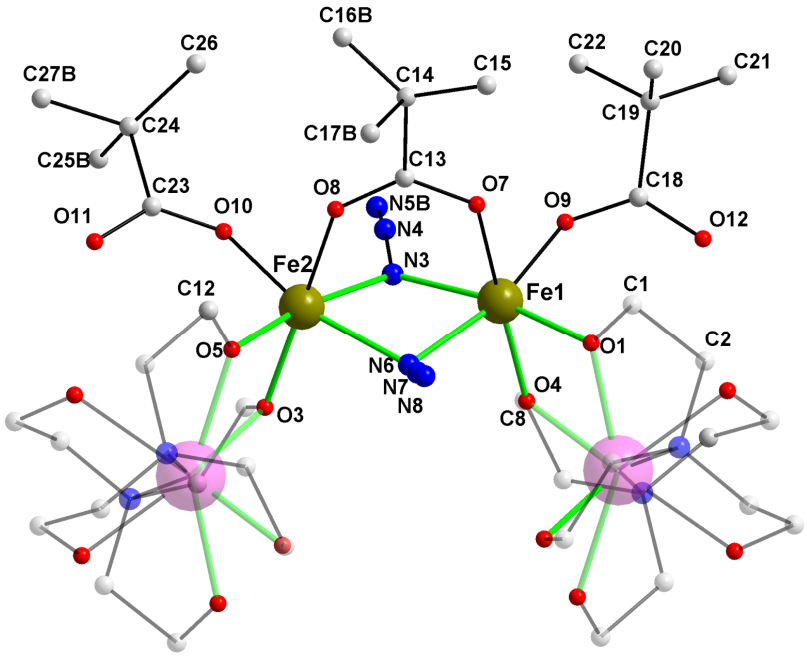
Method A: Triethanolamine (425 mg, 2.85 mmol), $[Fe^{III}_3O(Piv)_6(H_2O)_3]\cdot Piv\cdot 2PivH$ (250 mg, 0.24 mmol), $Fe(NO_3)_3\cdot 9H_2O$ (300 mg, 0.74 mmol), sodium azide (290 mg, 4.46 mmol) and $Er(NO_3)_3\cdot 6H_2O$ (343 mg, 0.74 mmol) were dissolved under stirring in 20 mL of ethanol and heated at ~ 65°C for 1 hour. The orange precipitate was filtered off from cooled solution and dried on air. Dry orange powder (~600 mg) was dissolved in 15mL of acetonitrile and insoluble white microcrystalline product was filtered off. The filtrate was kept undisturbed for slow evaporation at room temperature. After 3 days small yellow monocrystalls (thin plates) suitable for X-ray analysis were collected and air dried. Yield: ~3-4 mg (less then 1%, based on Er).

Method B: Triethanolamin (425 mg, 2.85 mmol), $[Fe^{III}_3O(Piv)_6(H_2O)_3]\cdot Piv\cdot 2PivH$ (250 mg, 0.24 mmol), $Fe(NO_3)_3\cdot 9H_2O$ (300 mg, 0.74 mmol), sodium azide (290 mg, 4.46mmol) and $Er(NO_3)_3\cdot 6H_2O$ (343 mg, 0.74 mmol) were dissolved under stirring in 20 mL of ethanol and heated at 80°C for 30 minutes. The cooled solution was filtered off (from the precipitate) and left undisturbed in a sealed vial. After 1 hour yellow monocrystalls suitable for X-ray analysis were collected and air dried. Yield: ~200 mg (15% based on Ln).

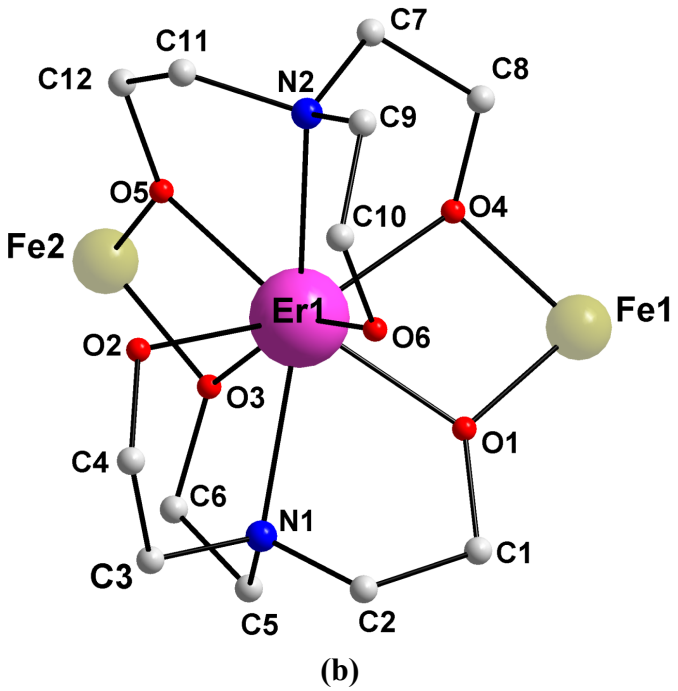
Anal. calc. for $[Fe_4Er_2(teaH)_4(N_3)_4(piv)_6]$ (1): C, 33.76; H, 5.56; N, 11.66; Found: C, 33.65; H, 5.61; N, 11.80. IR (KBr), /cm^{-1}: 3356 (b, vs), 3152 (mw), 2962 (m), 2903 (w), 2868 (mw), 1567 (s), 1398 (s), 1486 (s), 1459 (w), 1427 (vs), 1384 (vs), 1292 (w), 1229 (ms), 1082 (b, s), 1031 (mw), 918 (mw), 897 (m), 785 (w), 626 (m), 597 (m), 523 (mw), 438 (mw).

Synthesis of $[Fe_4Lu_2(teaH)_4(N_3)_4(piv)_6]$ (2)

The same procedure as **1** was adopted using $Lu(NO_3)_3\cdot 6H_2O$ (347 mg, 0.74mmol). Yellowish thin plate crystals were obtained (yield: ~8 mg, less then 1%, based on Lu). Anal. calc. for $[Fe_4Lu_2(teaH)_4(N_3)_4(piv)_6]$ (2): C, 33.49; H, 5.52; N, 11.57; Found: C, 33.58; H, 5.58; N, 11.71. IR (KBr), /cm^{-1}: 3356 (b, vs), 3152 (mw), 2962 (m), 2903 (w), 2868 (mw), 1567 (s), 1398 (s), 1486 (s), 1459 (w), 1427 (vs), 1384 (vs), 1292 (w), 1229 (ms), 1082 (b, s), 1031 (mw), 918 (mw), 897 (m), 785 (w), 626 (m), 597 (m), 523 (mw), 438 (mw).



(a)



(b)

Figure S1: The coordination geometry around: a) iron(III) atoms; b) lanthanide (erbium) atom. Hydrogen atoms were omitted for clarity.

Physical measurements: Magnetic susceptibility data (1.8-300K) were collected on powdered samples of a SQUID-based sample magnetometer on Quantum Design model MPMS-XL instrument in a 0.1 T applied magnetic field. Magnetisation isotherm was collected at 2, 3 - 5K between 0 and 7.0T. All data were corrected for the contribution of the sample holder and diamagnetism of the samples estimated from Pascal's constants.[1, 2] Magnetic data analyses were carried out by calculations of energy levels associated with the spin Hamiltonians presented in the text, and with the MAGPACK program package.[3] Analysis of magnetisation data M versus applied field H were carried out by MAGPACK program package.

1. Kahn, O., *Molecular Magnetism*. VCH Publishers, Inc.: New York, Weinheim, Cambridge, 1993
2. P. Pascal, *Ann. Chim. Phys.,* 1910**, 19**, 5.
3. Borras-Almenar, J. J.; Clemente-Juan, J. M.; Coronado, E.; Tsukerblat, B. S., *J. Comp. Chem.,* **2001,** *22*, 985-991.