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Enantiopure Tetranuclear Iron(III) Complexes using Chiral Reduced Schiff Base Ligands: Synthesis, Structure, Spectroscopy, Magnetic Properties and DFT studies

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Table S1: Crystal Data and Structure Refinement Parameters for $[\{Fe(L^2)_2\}_3Fe].2CH_3OH$

	$[\{Fe(L^2)_2\}_3Fe]. 2CH_3OH$
formula	$C_{80}H_{122}N_6O_{14}Fe_4$
fw	1615.24
cyst system	Trigonal
space group	$P6_522$
a (Å)	13.2290(19)
b (Å)	13.2290(19)
c (Å)	84.354(17)
α (deg)	90.00
β (deg)	90.00
γ (deg)	120.00
V (Å^3)	12785(4)
Z	6
D_{calcd} (mg m^{-3})	1.259
μ (mm^{-1})	0.729
θ (deg)	1.45 – 25.00
T (K)	293(2)
R1,[a] wR2[b] [$I > 2\sigma(I)$]	0.1035, 0.2114
GOF on F^2	1.184

[a] $R1 = \sum |F_o| - |F_c| / \sum |F_o|$. [b] $wR2 = [\sum w(F_o^2 - F_c^2)^2 / \sum w(F_o^2)^2]^{1/2}$

Table S2: Selected Bond Distances (Å) and Angles (deg) for $[Fe(L^2)_2]^-$ and FeO_6 core

Distances			
Fe1 – O1	1.908(8)	Fe2 – O2	1.982(6)
Fe1 – O2	1.991(6)	Fe2 – O4	1.995(6)
Fe1 – O3	1.933(7)	Fe2 – O6	1.978(6)
Fe1 – O4	2.005(6)	Fe1 ···· Fe2	3.213(8)
Fe1 – N1	2.277(9)	Fe2 ···· Fe3	3.224(7)
Fe1 – N2	2.292(7)		
Angles			
O1 – Fe1 – O2	109.5(3)	O2 – Fe2 – O2#1	99.1(4)
O1 – Fe1 – O3	135.3(3)	O2 – Fe2 – O4	72.8(2)
O1 – Fe1 – O4	105.9(3)	O2 – Fe2 – O4#1	94.0(2)
O1 – Fe1 – N1	83.4(3)	O2 – Fe2 – O6	164.0(3)
O1 – Fe1 – N2	79.5(3)	O2 – Fe2 – O6#1	94.9(3)
O2 – Fe1 – O3	105.2(3)	O4 – Fe2 – O4#1	160.0(4)
O2 – Fe1 – O4	72.4(2)	O4 – Fe2 – O6	98.6(2)
O2 – Fe1 – N1	75.5(3)	O4 – Fe2 – O6#1	97.5(3)
O2 – Fe1 – N2	147.7(3)	Fe1 – O2 – Fe2	107.9(2)
O3 – Fe1 – O4	110.8(3)	Fe1 – O4 – Fe2	106.9(2)
O3 – Fe1 – N1	79.0(3)	Fe1 ····Fe2 ···· Fe3	121.1(6)
O3 – Fe1 – N2	86.0(3)	Fe1 ····Fe2 ···· Fe1#1	117.8(7)
O4 – Fe1 – N1	147.8(3)		
O4 – Fe1 – N2	75.3(3)		
N1 – Fe1 – N2	136.8(3)		