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SUPPORTING INFORMATION:

A High-Nuclearity Complex Containing A Decanuclear Iron (III)/Oxo Cage in Football-like Structure and Rare (R-/S)-hemiacetalate Ligands in Butterfly-like Format

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Contents

1 ^{1}H NMR for complex **1**----------1

2 The IR for complex **1**----------2

3 Synthesis of 2-(dimethoxymethyl)pyridine ----------2

4 ^{1}H NMR for 2-(dimethoxymethyl)pyridine----------3

5 Physical characterization----------3

6 Selected bond distances (Å) and angles (deg) for the complex **1**----------3

1 ^{1}H NMR for complex 1

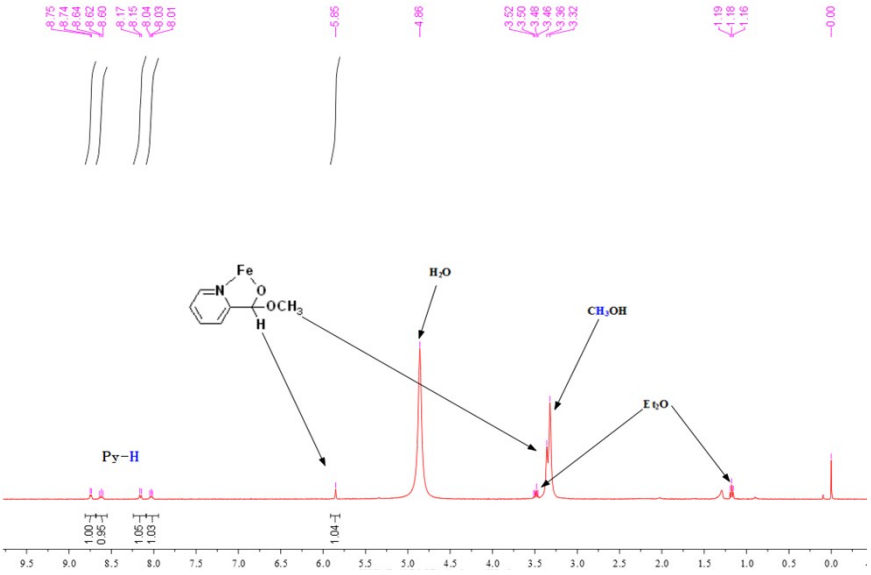

Fig. S1 ^{1}H NMR (CD_3OD) for complex **1**.

2 The IR for complex 1

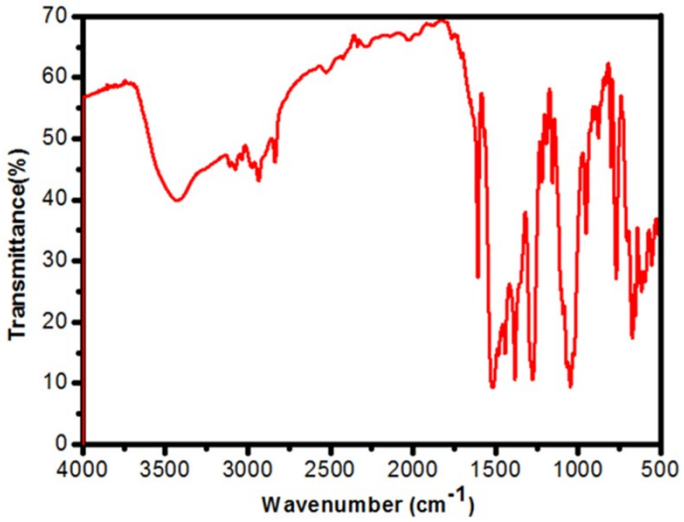

Fig. S2 The IR for complex **1**.

3 Synthesis of 2-(dimethoxymethyl)pyridine

To a solution of $Fe(NO_3)_3 \cdot 9H_2O$ (0.13 g, 0.33 mmol, 10% mmol) in 5 ml methanol was added pyridine-2-aldehyde (0.35 g, 3.26 mmol) at room temperature with stirring. The mixture was stirred for 24 h, and filtered through Celite, concentrated under reduced pressure. The resultant residue was purified by flash silica gel column chromatography with petroleum ether (60-90°C)/ethyl acetate (v/v, 5:1) as the eluent, affording desired product as a light yellow oil (363 mg, 73%). ^{1}H NMR ($CDCl_3$, 400 MHz, 23 °C) δ 8.62 (ddd, J = 4.8, 1.7, 0.9 Hz, 1H), 7.73 (td, J = 7.7, 1.8 Hz, 1H), 7.55 (d, J = 7.9 Hz, 1H), 7.26 (ddd, J = 7.5, 4.9, 1.1 Hz, 1H), 5.39 (s, 1H), 3.41 (s, 7H).

4 ^{1}H NMR for 2-(dimethoxymethyl)pyridine

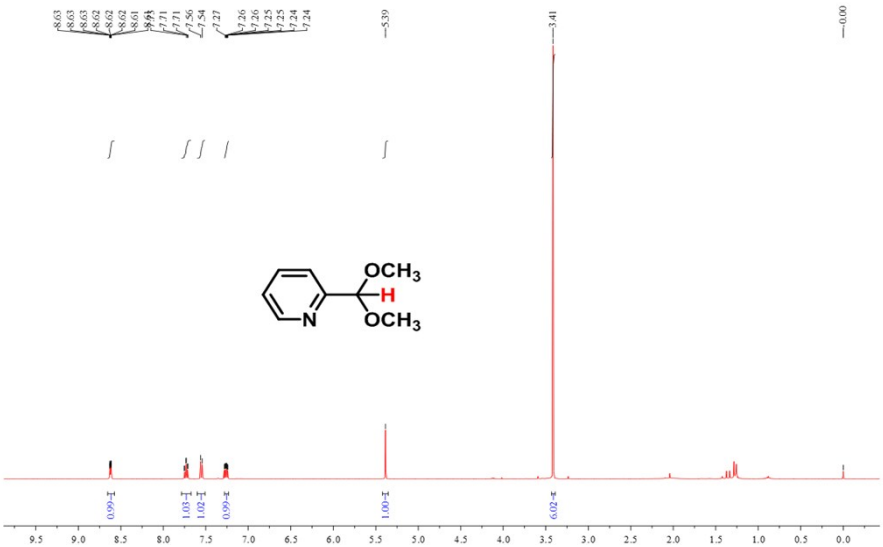

Fig. S3 ^{1}H NMR ($CDCl_3$) for 2-(dimethoxymethyl)pyridine.

5 Physical characterization

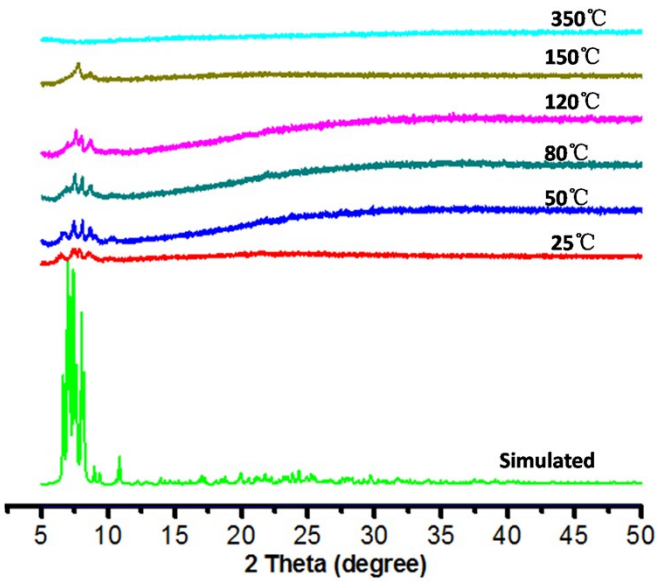

Fig. S4 The varied-temperature PXRD patterns of complex **1** from room temperature to 350 °C.

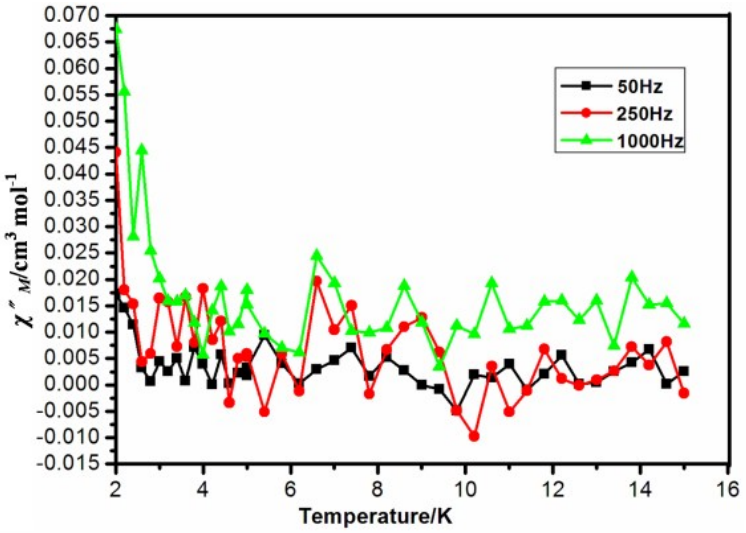

Fig. S5 Temperature dependence of the out-of-phase components (χ'') of ac magnetic susceptibility for **1** in a 3.5 Oe ac field at various ac frequencies.

6 Selected bond distances (Å) and angles (deg) for the complex 1.

Table S1 Selected bond distances (Å) and angles (deg) for the complex 1.

Bond	Bondlength	Bond	Bondlength
Fe(1)-N(12)	2.149(4)	Fe(1)-N(15)	2.153(4)
Fe(2)-Fe(9)	2.9764(12)	Fe(3)-O(3)	1.930(3)
Fe(3)-N(14)	2.140(4)	Fe(3)-N(11)	2.160(4)
Fe(6)-N(10)	2.132(5)	Fe(6)-N(9)	2.143(4)
Fe(8)-Fe(9)	2.9407(13)	Fe(9)-N(8)	2.146(5)
Fe(9)-N(13)	2.143(5)		

Bond	Bondangle	Bond	Bondangle
O(26)-Fe(1)-O(29)	92.22(14)	O(26)-Fe(1)-O(12)	81.67(14)
O(29)-Fe(1)-O(12)	109.58(15)	O(26)-Fe(1)-O(9)	101.84(16)
O(29)-Fe(1)-O(9)	80.71(15)	O(12)-Fe(1)-O(9)	169.14(15)
O(26)-Fe(1)-N(12)	157.37(16)	O(29)-Fe(1)-N(12)	87.97(17)
O(12)-Fe(1)-N(12)	76.97(17)	O(9)-Fe(1)-N(12)	100.52(18)
O(26)-Fe(1)-N(15)	93.35(16)	O(29)-Fe(1)-N(15)	156.64(16)
O(12)-Fe(1)-N(15)	93.67(16)	O(9)-Fe(1)-N(15)	75.95(16)
N(12)-Fe(1)-N(15)	95.39(17)	O(26)-Fe(1)-Fe(8)	90.74(10)
O(29)-Fe(1)-Fe(8)	40.02(11)	O(12)-Fe(1)-Fe(8)	148.66(11)
O(9)-Fe(1)-Fe(8)	42.13(11)	N(12)-Fe(1)-Fe(8)	103.63(13)
N(15)-Fe(1)-Fe(8)	117.20(12)	O(26)-Fe(1)-Fe(7)	40.10(10)
O(29)-Fe(1)-Fe(7)	92.39(10)	O(12)-Fe(1)-Fe(7)	44.31(10)
O(9)-Fe(1)-Fe(7)	141.38(12)	N(12)-Fe(1)-Fe(7)	117.27(13)
N(15)-Fe(1)-Fe(7)	106.35(13)	Fe(8)-Fe(1)-Fe(7)	115.66(3)
O(3)-Fe(2)-O(21)	102.11(15)	O(3)-Fe(2)-O(17)	99.30(14)
O(21)-Fe(2)-O(17)	102.92(16)	O(3)-Fe(2)-O(22)	90.12(14)
O(21)-Fe(2)-O(22)	80.48(15)	O(17)-Fe(2)-O(22)	168.96(14)
O(3)-Fe(2)-O(30)	100.82(15)	O(21)-Fe(2)-O(30)	150.91(14)
O(17)-Fe(2)-O(30)	90.73(16)	O(22)-Fe(2)-O(30)	81.82(15)
O(3)-Fe(2)-O(31)	159.94(15)	O(21)-Fe(2)-O(31)	95.56(14)
O(17)-Fe(2)-O(31)	85.76(15)	O(22)-Fe(2)-O(31)	83.45(14)
O(30)-Fe(2)-O(31)	59.52(15)	O(3)-Fe(2)-Fe(9)	88.11(10)
O(21)-Fe(2)-Fe(9)	41.06(11)	O(17)-Fe(2)-Fe(9)	143.77(12)
O(22)-Fe(2)-Fe(9)	41.47(11)	O(30)-Fe(2)-Fe(9)	122.86(11)
O(31)-Fe(2)-Fe(9)	99.29(10)	O(3)-Fe(3)-O(47)	82.23(14)
O(3)-Fe(3)-O(4)	104.82(14)	O(47)-Fe(3)-O(4)	172.09(15)
O(3)-Fe(3)-O(25)	90.36(14)	O(47)-Fe(3)-O(25)	104.41(14)
O(4)-Fe(3)-O(25)	79.43(14)	O(3)-Fe(3)-N(14)	94.56(16)
O(47)-Fe(3)-N(14)	99.12(16)	O(4)-Fe(3)-N(14)	77.00(16)
O(25)-Fe(3)-N(14)	156.40(15)	O(3)-Fe(3)-N(11)	159.24(15)
O(47)-Fe(3)-N(11)	77.38(15)	O(4)-Fe(3)-N(11)	95.78(16)
O(25)-Fe(3)-N(11)	90.92(15)	N(14)-Fe(3)-N(11)	92.52(18)
O(26)-Fe(4)-O(23)	103.57(15)	O(26)-Fe(4)-O(3)	101.76(14)
O(23)-Fe(4)-O(3)	103.78(14)	O(26)-Fe(4)-O(47)	87.81(14)
O(23)-Fe(4)-O(47)	167.62(14)	O(3)-Fe(4)-O(47)	78.17(13)
O(26)-Fe(4)-O(27)	105.78(15)	O(23)-Fe(4)-O(27)	86.65(15)
O(3)-Fe(4)-O(27)	147.30(15)	O(47)-Fe(4)-O(27)	85.55(15)
O(26)-Fe(4)-O(28)	161.52(14)	O(23)-Fe(4)-O(28)	86.46(15)
O(3)-Fe(4)-O(28)	90.60(14)	O(47)-Fe(4)-O(28)	81.28(14)
O(27)-Fe(4)-O(28)	58.74(15)	O(21)-Fe(5)-O(29)	103.08(16)
O(21)-Fe(5)-O(19)	100.79(15)	O(29)-Fe(5)-O(19)	102.88(14)
O(21)-Fe(5)-O(20)	89.03(16)	O(29)-Fe(5)-O(20)	167.34(16)
O(19)-Fe(5)-O(20)	78.04(14)	O(21)-Fe(5)-O(46)	102.5(2)

O(29)-Fe(5)-O(46)	88.99(19)	O(19)-Fe(5)-O(46)	150.67(19)
O(20)-Fe(5)-O(46)	84.74(18)	O(21)-Fe(5)-O(34)	159.22(16)
O(29)-Fe(5)-O(34)	86.31(17)	O(19)-Fe(5)-O(34)	94.98(17)
O(20)-Fe(5)-O(34)	81.04(17)	O(46)-Fe(5)-O(34)	58.6(2)
O(19)-Fe(6)-O(20)	82.61(15)	O(19)-Fe(6)-O(18)	105.51(15)
O(20)-Fe(6)-O(18)	170.66(14)	O(19)-Fe(6)-O(17)	90.18(15)
O(20)-Fe(6)-O(17)	105.13(16)	O(18)-Fe(6)-O(17)	79.82(15)
O(19)-Fe(6)-N(10)	93.23(17)	O(20)-Fe(6)-N(10)	97.99(18)
O(18)-Fe(6)-N(10)	77.23(17)	O(17)-Fe(6)-N(10)	156.88(16)
O(19)-Fe(6)-N(9)	158.58(17)	O(20)-Fe(6)-N(9)	76.71(18)
O(18)-Fe(6)-N(9)	95.58(17)	O(17)-Fe(6)-N(9)	89.84(17)
N(10)-Fe(6)-N(9)	95.12(19)	O(19)-Fe(7)-O(26)	100.76(14)
O(19)-Fe(7)-O(25)	100.37(15)	O(26)-Fe(7)-O(25)	103.34(14)
O(19)-Fe(7)-O(12)	90.58(15)	O(26)-Fe(7)-O(12)	79.40(14)
O(25)-Fe(7)-O(12)	167.89(14)	O(19)-Fe(7)-O(15)	98.33(14)
O(26)-Fe(7)-O(15)	153.03(14)	O(25)-Fe(7)-O(15)	91.68(14)
O(12)-Fe(7)-O(15)	81.54(14)	O(19)-Fe(7)-O(44)	156.86(15)
O(26)-Fe(7)-O(44)	99.20(14)	O(25)-Fe(7)-O(44)	86.21(14)
O(12)-Fe(7)-O(44)	81.70(14)	O(15)-Fe(7)-O(44)	59.06(14)
O(19)-Fe(7)-Fe(1)	86.22(11)	O(26)-Fe(7)-Fe(1)	40.68(10)
O(25)-Fe(7)-Fe(1)	143.74(10)	O(12)-Fe(7)-Fe(1)	41.36(9)
O(23)-Fe(8)-O(9)	100.17(16)	O(29)-Fe(8)-O(9)	81.15(15)
O(23)-Fe(8)-O(24)	82.13(16)	O(29)-Fe(8)-O(24)	102.77(16)
O(9)-Fe(8)-O(24)	175.41(16)	O(23)-Fe(8)-O(43)	105.0(2)
O(29)-Fe(8)-O(43)	158.7(2)	O(9)-Fe(8)-O(43)	84.35(19)
O(24)-Fe(8)-O(43)	91.22(19)	O(23)-Fe(8)-O(42)	165.3(2)
O(29)-Fe(8)-O(42)	99.8(2)	O(9)-Fe(8)-O(42)	88.9(2)
O(24)-Fe(8)-O(42)	88.1(2)	O(43)-Fe(8)-O(42)	64.2(3)
O(23)-Fe(8)-Fe(9)	41.30(10)	O(29)-Fe(8)-Fe(9)	90.65(11)
O(9)-Fe(8)-Fe(9)	140.40(12)	O(24)-Fe(8)-Fe(9)	42.72(12)
O(43)-Fe(8)-Fe(9)	110.43(18)	O(42)-Fe(8)-Fe(9)	130.68(17)
O(23)-Fe(9)-O(22)	107.25(15)	O(23)-Fe(9)-O(21)	90.85(14)
O(22)-Fe(9)-O(21)	82.13(15)	O(23)-Fe(9)-O(24)	81.70(16)
O(22)-Fe(9)-O(24)	169.03(15)	O(21)-Fe(9)-O(24)	104.46(17)
O(23)-Fe(9)-N(13)	90.92(17)	O(22)-Fe(9)-N(13)	77.04(18)
O(21)-Fe(9)-N(13)	158.66(18)	O(24)-Fe(9)-N(13)	96.84(19)
O(23)-Fe(9)-N(8)	157.3(2)	O(22)-Fe(9)-N(8)	95.03(19)
O(21)-Fe(9)-N(8)	87.79(17)	O(24)-Fe(9)-N(8)	76.70(19)
N(13)-Fe(9)-N(8)	98.5(2)	O(18)-Fe(10)-O(4)	177.16(15)
O(18)-Fe(10)-O(17)	80.66(15)	O(4)-Fe(10)-O(17)	97.85(15)
O(18)-Fe(10)-O(25)	97.39(14)	O(4)-Fe(10)-O(25)	80.13(14)
O(17)-Fe(10)-O(25)	89.15(14)	O(18)-Fe(10)-O(13)	92.71(17)
O(4)-Fe(10)-O(13)	89.01(18)	O(17)-Fe(10)-O(13)	171.35(16)
O(25)-Fe(10)-O(13)	97.25(15)	O(18)-Fe(10)-O(6)	90.47(18)

O(4)-Fe(10)-O(6)	92.09(18)	O(17)-Fe(10)-O(6)	95.91(17)
O(25)-Fe(10)-O(6)	171.26(17)	O(13)-Fe(10)-O(6)	78.50(18)
O(48)-N(2)-O(28)	122.3(6)	Fe(3)-O(47)-Fe(4)	95.06(14)
Fe(8)-O(29)-Fe(1)	98.96(16)	Fe(5)-O(29)-Fe(1)	122.67(18)
Fe(5)-O(29)-Fe(8)	125.78(19)	Fe(4)-O(26)-Fe(1)	123.92(17)