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Supporting Information

Investigating the Effect of Lanthanide Radius and Diamagnetic Linker on the Framework of Metallacrown Complexes

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Table S1. Crystallographic data for complexes **1**- **8** (La-Ho).

Complexes	**1**	**2**	**3**	**4**
Empirical formula	$C_{30}H_{72}Cu_{10}Fe_2La_2N_{34}O_{52}$	$C_{30}H_{72}Cu_{10}Fe_2Pr_2N_{34}O_{52}$	$C_{30}H_{72}Cu_{10}Fe_2Nd_2N_{34}O_{52}$	$C_{20}H_{40}Cu_5Fe_2SmN_{22}NaO_{22}$
Formula weight	2766.14	2770.14	2776.80	1543.48
Temperature (K)	298(2)	298(2) K	293(2) K	293(2) K
Wavelength (A)	0.71073	0.71073 A	0.71073 A	1.54184 A
Crystal system	Triclinic,	Triclinic,	Triclinic,	Monoclinic,
Space group	$P\bar{1}$	$P\bar{1}$	$P\bar{1}$	P 1 21/n1
a (Å)	10.4309(11)	10.5279(8)	10.4494(4)	16.9804(7)
b (Å)	13.2702(15)	13.3813(11)	13.3443(7)	14.2037(5)
c (Å)	16.2883(13)	16.3388(13)	16.2694(7)	20.7567(10)
V (Å^3)	2071.9(4)	2117.0(3)	2083.72(16)	4997.1(9)
Z	1	1	1	4
D (g/cm^3)	2.217	2.173	2.213	2.052
Absorption coefficient (mm^{-1})	3.973	4.031	4.172	16.394
F(000)	1362	1366	1368	3040
Crystal size (mm)	0.17×0.15× 0.12	0.44× 0.38 × 0.36	0.25× 0.19× 0.17	0.30× 0.20 × 0.16
Theta range(°)	2.83-25.02	2.37-25.02	2.44-25.02	3.27-67.24
Limiting indices	-10≤h≤12, -15≤k≤15, -19≤l≤19	-7≤h≤12, -15≤k≤15, -17≤l≤19	-11≤h≤12, -15≤k≤15, -19≤l≤19	-20≤h≤19, -16≤k≤14, -22≤l≤24
Reflections collected / unique	13220/ 7279 [*R*(int) = 0.0461]	10557/ 7272 [*R*(int) = 0.0299]	15437/ 7345 [*R*(int) = 0.0680]	31360/ 8957 [*R*(int) = 0.1166]
Completeness to theta	99.4%	97.2%	99.9%	100.0%
Max. and min. transmission	0.6471 and 0.5515	0.3248 and 0.2701	0.5374 and 0.4219	0.1790 and 0.0838
Data / restraints / parameters	7279/ 0/ 586	7272/ 1830/ 586	7345/ 1794/ 586	8957/ 1/ 658
Goodness-of-fit on F^2	1.104	1.047	1.041	1.031
R[I>2σ(I)]	R_1 = 0.0519, wR_2 = 0.1328	R_1 = 0.0471, wR_2 = 0.1149	R_1 = 0.0558, wR_2 = 0.1182	R_1 = 0.0634, wR_2 = 0.1497
R indices (all data)	R_1 = 0.0739, wR_2 = 0.1533	R_1 = 0.0775, wR_2 = 0.1332	R_1 = 0.0884, wR_2 = 0.1402	R_1 = 0.0927, wR_2 = 0.1713
Complexes	**5**	**6**	**7**	**8**
Empirical formula	$C_{20}H_{32}Cu_5Fe_2GdN_{22}NaO_{18}$	$C_{20}H_{40}Cu_5Fe_2TbN_{22}NaO_{22}$	$C_{20}H_{40}Cu_5DyFe_2N_{22}NaO_{22}$	$C_{20}H_{38}Cu_5HoFe_2N_{22}NaO_{21}$
Formula weight	1478.32	1552.05	1555.63	1540.04
Temperature (K)	298(2) K	293(2) K	293(2)	298(2) K
Wavelength (A)	0.71073 A	1.54184 A	1.54184	0.71073 A
Crystal system	Monoclinic,	Monoclinic,	Monoclinic,	Monoclinic,
Space group	P2(1)/c	P1 21/n 1	P1 21/n 1	P2(1)/c
a (Å)	17.2009(18)	17.0246(7)	17.073(2)	17.3041(15)
b (Å)	14.2590(14)	14.1494(7)	14.1119(16)	14.2770(12)

c (Å)	26.185(3)	20.7518(8)	20.651(3)	26.341(2)
V (Å^3)	5071.1(9)	4990.4(4)	4966.6(11)	5133.4(8)
Z	4	4	4	4
D (g/cm^3)	1.936	2.066	2.080	1.993
Absorption coefficient (mm^{-1})	3.988	14.549	15.665	4,197
F(000)	2888	3052	3056	3020
Crystal size (mm)	0.11×0.09 × 0.04	0.20× 0.17 × 0.14	0.20×0.17 × 0.14	0.15× 0.12× 0.05
Theta range(°)	2.13-25.02	3.27-67.25	3.26-71.47	2.36-25,02
Limiting indices	-13≤h≤20, -16≤k≤14, -31≤l≤29	-19≤h≤20, -8≤k≤16, -24≤l≤20	-20≤h≤19,-17≤k≤16,-25≤l≤20	-17≤h≤20, -16≤k≤16, -31≤l≤31
Reflections collected / unique	24505/ 8933 [*R*(int) = 0.1656]	17935/ 8943 [*R*(int) = 0.0748]	21361/9425 [*R*(int) = 0.1367]	25459/ 9032 [*R*(int) = 0.0962]
Completeness to theta	99.8%	99.8%	97.5%	99.8%
Max. and min. transmission	0.8568 and 0.6681	0.2352 and 0.1589	0.2177 and 0.1457	0.811 and 0.552
Data / restraints / parameters	8933/ 1902/ 622	8943/ 1986/ 658	9425/ 2049/ 658	9032/ 7/ 649
Goodness-of-fit on F^2	0.949	1.024	1.018	1.001
R[I>2σ(I)]	R_1 = 0.0771, wR_2 = 0.1333	R_1 = 0.0747, wR_2 = 0.1874	R_1 = 0.0955, wR_2 = 0.2014	R_1 = 0.0480, wR_2 = 0.0787
R indices (all data)	R_1 = 0.1346, wR_2 = 0.1458	R_1 = 0.1017, wR_2 = 0.2118	R_1 = 0.1654, wR_2 = 0.2526	R_1 = 0.0951, wR_2 = 0.0862

Table S2. Selected bond lengths (Å) and angles (°) for complex **1-8**.

Complex 1					
La(1)-O(6)	2.442(6)	Cu(1)-N(1)	2.008(7)	Cu(4)-O(5)	1.966(6)
La(1)-O(8)	2.466(5)	Cu(2)-N(4)	1.907(7)	Cu(4)-N(7)	2.031(7)
La(1)-O(2)	2.478(5)	Cu(2)-O(1)	1.949(6)	Cu(5)-N(10)	1.908(7)
La(1)-O(15)	2.518(6)	Cu(2)-O(2)	1.961(5)	Cu(5)-O(8)	1.918(6)
La(1)-O(13)	2.536(5)	Cu(2)-N(3)	2.006(7)	Cu(5)-O(7)	1.934(6)
La(1)-O(4)	2.543(6)	Cu(2)-O(14)	2.409(8)	Cu(5)-N(9)	2.003(7)
La(1)-O(10)	2.580(6)	Cu(3)-N(6)	1.908(7)	Fe(1)-N(12)	1.656(7)
La(1)-N(11)	2.592(9)	Cu(3)-O(4)	1.935(6)	Fe(1)-C(13)	1.919(9)
La(1)-O(12)	2.645(7)	Cu(3)-O(3)	1.936(6)	Fe(1)-C(11)	1.925(10)
Cu(1)-N(2)	1.898(7)	Cu(3)-N(5)	2.015(7)	Fe(1)-C(15)	1.936(11)
Cu(1)-O(9)	1.931(6)	Cu(4)-N(8)	1.919(7)	Fe(1)-C(14)	1.944(10)
Cu(1)-O(10)	1.944(6)	Cu(4)-O(6)	1.950(5)	Fe(1)-C(12)	1.955(11)
O(6)-La(1)-O(8)	73.09(18)	O(6)-La(1)-O(4)	68.97(18)	O(4)-La(1)-O(10)	129.65(18)
O(6)-La(1)-O(2)	136.16(19)	O(8)-La(1)-O(4)	135.44(19)	O(6)-La(1)-N(11)	141.1(2)
O(8)-La(1)-O(2)	136.15(18)	O(2)-La(1)-O(4)	68.67(18)	O(8)-La(1)-N(11)	100.6(2)
O(6)-La(1)-O(15)	72.8(2)	O(15)-La(1)-O(4)	72.47(18)	O(2)-La(1)-N(11)	74.8(2)
O(8)-La(1)-O(15)	74.74(19)	O(13)-La(1)-O(4)	66.96(19)	O(15)-La(1)-N(11)	143.9(2)
O(2)-La(1)-O(15)	84.19(19)	O(6)-La(1)-O(10)	135.71(17)	O(13)-La(1)-N(11)	69.0(2)
O(6)-La(1)-O(13)	87.7(2)	O(8)-La(1)-O(10)	68.39(18)	O(4)-La(1)-N(11)	123.6(2)
O(8)-La(1)-O(13)	134.08(19)	O(2)-La(1)-O(10)	69.52(17)	O(10)-La(1)-N(11)	68.7(2)
O(2)-La(1)-O(13)	85.97(18)	O(15)-La(1)-O(10)	76.62(19)	O(6)-La(1)-O(12)	76.7(2)
O(15)-La(1)-O(13)	139.1(2)	O(13)-La(1)-O(10)	135.3(2)	O(8)-La(1)-O(12)	67.25(19)
O(2)-La(1)-O(12)	138.3(2)	O(13)-La(1)-O(12)	67.9(2)	O(10)-La(1)-O(12)	106.6(2)
O(15)-La(1)-O(12)	136.64(19)	O(4)-La(1)-O(12)	123.2(2)	N(11)-La(1)-O(12)	65.9(2)
N(2)-Cu(1)-O(9)	171.1(3)	N(4)-Cu(2)-O(1)	169.6(3)	N(4)-Cu(2)-O(14)	102.7(3)
N(2)-Cu(1)-O(10)	92.0(3)	N(4)-Cu(2)-O(2)	89.2(3)	O(1)-Cu(2)-O(14)	86.2(3)
O(9)-Cu(1)-O(10)	85.6(2)	O(1)-Cu(2)-O(2)	85.1(2)	O(2)-Cu(2)-O(14)	92.7(3)
N(2)-Cu(1)-N(1)	83.4(3)	N(4)-Cu(2)-N(3)	83.4(3)	N(3)-Cu(2)-O(14)	95.3(3)
O(9)-Cu(1)-N(1)	98.8(3)	O(1)-Cu(2)-N(3)	101.2(3)	N(6)-Cu(3)-O(4)	90.8(3)
O(10)-Cu(1)-N(1)	175.4(3)	O(2)-Cu(2)-N(3)	170.1(3)	N(6)-Cu(3)-O(3)	175.2(3)
O(4)-Cu(3)-O(3)	84.6(2)	O(6)-Cu(4)-O(5)	85.3(2)	O(8)-Cu(5)-O(7)	85.3(2)
N(6)-Cu(3)-N(5)	83.7(3)	N(8)-Cu(4)-N(7)	81.8(3)	N(10)-Cu(5)-N(9)	83.1(3)
O(4)-Cu(3)-N(5)	167.9(3)	O(6)-Cu(4)-N(7)	174.1(3)	O(8)-Cu(5)-N(9)	172.8(3)
O(3)-Cu(3)-N(5)	100.5(3)	O(5)-Cu(4)-N(7)	100.5(3)	O(7)-Cu(5)-N(9)	100.9(3)
N(8)-Cu(4)-O(6)	92.3(3)	N(10)-Cu(5)-O(8)	90.2(3)	N(12)-Fe(1)-C(13)	96.6(4)
N(8)-Cu(4)-O(5)	177.5(3)	N(10)-Cu(5)-O(7)	168.6(3)	N(12)-Fe(1)-C(11)	93.5(4)
C(13)-Fe(1)-C(11)	169.8(4)	C(13)-Fe(1)-C(14)	85.5(4)	C(13)-Fe(1)-C(12)	89.1(4)

N(12)-Fe(1)-C(15)	95.7(4)	C(11)-Fe(1)-C(14)	84.4(4)	C(11)-Fe(1)-C(12)	91.3(4)
C(13)-Fe(1)-C(15)	87.9(4)	C(15)-Fe(1)-C(14)	84.3(4)	C(15)-Fe(1)-C(12)	170.4(4)
C(11)-Fe(1)-C(15)	90.0(4)	N(12)-Fe(1)-C(12)	93.7(4)	C(14)-Fe(1)-C(12)	86.4(4)
N(12)-Fe(1)-C(14)	177.9(4)				
Complex 2					
Pr(1)-O(10)	2.449(5)	Cu(1)-N(9)	2.012(6)	Cu(4)-O(7)	1.921(5)
Pr(1)-O(8)	2.475(5)	Cu(2)-N(2)	1.906(6)	Cu(4)-N(5)	2.004(6)
Pr(1)-O(4)	2.491(5)	Cu(2)-O(4)	1.938(5)	Cu(5)-N(8)	1.924(6)
Pr(1)-O(25)	2.548(5)	Cu(2)-O(3)	1.943(5)	Cu(5)-O(10)	1.943(5)
Pr(1)-O(2)	2.550(4)	Cu(2)-N(1)	2.000(6)	Cu(5)-O(9)	1.965(5)
Pr(1)-O(13)	2.571(5)	Cu(2)-O(14)	2.495(7)	Cu(5)-N(7)	2.016(7)
Pr(1)-O(6)	2.567(5)	Cu(3)-N(4)	1.897(6)	Fe(1)-N(11)	1.648(7)
Pr(1)-N(16)	2.619(6)	Cu(3)-O(5)	1.932(5)	Fe(1)-C(15)	1.919(8)
Pr(1)-O(12)	2.655(6)	Cu(3)-O(6)	1.937(5)	Fe(1)-C(14)	1.935(9)
Cu(1)-N(10)	1.897(6)	Cu(3)-N(3)	2.015(6)	Fe(1)-C(13)	1.946(8)
Cu(1)-O(2)	1.920(5)	Cu(4)-N(6)	1.896(6)	Fe(1)-C(12)	1.943(9)
Cu(1)-O(1)	1.930(5)	Cu(4)-O(8)	1.919(5)	Fe(1)-C(11)	1.951(9)
O(10)-Pr(1)-O(8)	72.89(15)	O(10)-Pr(1)-O(6)	135.73(16)	O(4)-Pr(1)-O(12)	138.84(17)
O(10)-Pr(1)-O(4)	136.03(15)	O(8)-Pr(1)-O(6)	68.00(15)	O(25)-Pr(1)-O(12)	136.90(18)
O(8)-Pr(1)-O(4)	135.71(16)	O(4)-Pr(1)-O(6)	69.91(15)	O(2)-Pr(1)-O(12)	123.05(17)
O(10)-Pr(1)-O(25)	73.86(18)	O(25)-Pr(1)-O(6)	76.08(16)	O(13)-Pr(1)-O(12)	67.16(18)
O(8)-Pr(1)-O(25)	73.88(17)	O(2)-Pr(1)-O(6)	130.11(16)	O(6)-Pr(1)-O(12)	106.35(17)
O(4)-Pr(1)-O(25)	83.36(17)	O(13)-Pr(1)-O(6)	136.95(17)	N(16)-Pr(1)-O(12)	66.4(2)
O(10)-Pr(1)-O(2)	68.99(15)	O(10)-Pr(1)-N(16)	140.64(19)	N(10)-Cu(1)-O(2)	91.3(2)
O(8)-Pr(1)-O(2)	134.75(15)	O(8)-Pr(1)-N(16)	102.90(19)	N(10)-Cu(1)-O(1)	175.4(2)
O(4)-Pr(1)-O(2)	68.54(15)	O(4)-Pr(1)-N(16)	74.47(19)	O(2)-Cu(1)-O(1)	84.5(2)
O(25)-Pr(1)-O(2)	72.88(16)	O(25)-Pr(1)-N(16)	144.0(2)	N(10)-Cu(1)-N(9)	83.2(2)
O(10)-Pr(1)-O(13)	85.80(18)	O(2)-Pr(1)-N(16)	121.99(19)	O(2)-Cu(1)-N(9)	168.8(2)
O(8)-Pr(1)-O(13)	133.68(18)	O(13)-Pr(1)-N(16)	68.9(2)	O(1)-Cu(1)-N(9)	100.6(2)
O(4)-Pr(1)-O(13)	87.65(18)	O(6)-Pr(1)-N(16)	69.87(18)	N(2)-Cu(2)-O(4)	89.8(2)
O(25)-Pr(1)-O(13)	138.97(17)	O(10)-Pr(1)-O(12)	76.31(17)	N(2)-Cu(2)-O(3)	170.5(2)
O(2)-Pr(1)-O(13)	66.59(16)	O(8)-Pr(1)-O(12)	68.02(18)	O(4)-Cu(2)-O(3)	84.6(2)
N(2)-Cu(2)-N(1)	83.1(2)	O(6)-Cu(3)-N(3)	174.8(2)	O(9)-Cu(5)-N(7)	100.5(2)
O(4)-Cu(2)-N(1)	170.5(2)	N(6)-Cu(4)-O(8)	89.6(2)	N(11)-Fe(1)-C(15)	93.0(3)
O(3)-Cu(2)-N(1)	101.6(2)	N(6)-Cu(4)-O(7)	169.4(2)	N(11)-Fe(1)-C(14)	92.9(4)
N(2)-Cu(2)-O(14)	102.7(3)	O(8)-Cu(4)-O(7)	85.2(2)	C(15)-Fe(1)-C(14)	91.4(3)
O(4)-Cu(2)-O(14)	92.1(2)	N(6)-Cu(4)-N(5)	83.3(3)	N(11)-Fe(1)-C(13)	97.3(3)
O(3)-Cu(2)-O(14)	85.2(3)	O(8)-Cu(4)-N(5)	172.3(2)	C(15)-Fe(1)-C(13)	169.6(3)
N(1)-Cu(2)-O(14)	95.6(3)	O(7)-Cu(4)-N(5)	101.4(2)	C(14)-Fe(1)-C(13)	89.2(3)
N(4)-Cu(3)-O(5)	171.6(3)	N(8)-Cu(5)-O(10)	92.6(2)	N(11)-Fe(1)-C(12)	177.6(4)
N(4)-Cu(3)-O(6)	92.4(2)	N(8)-Cu(5)-O(9)	177.5(2)	C(15)-Fe(1)-C(12)	84.7(3)
O(5)-Cu(3)-O(6)	85.4(2)	O(10)-Cu(5)-O(9)	84.9(2)	C(14)-Fe(1)-C(12)	86.3(4)
N(4)-Cu(3)-N(3)	82.4(3)	N(8)-Cu(5)-N(7)	82.0(3)	C(13)-Fe(1)-C(12)	85.0(3)

O(5)-Cu(3)-N(3)	99.7(2)	O(10)-Cu(5)-N(7)	174.6(2)	N(11)-Fe(1)-C(11)	96.4(4)
C(15)-Fe(1)-C(11)	89.3(3)	C(13)-Fe(1)-C(11)	88.4(3)	C(12)-Fe(1)-C(11)	84.6(4)
C(14)-Fe(1)-C(11)	170.7(4)				
Complex **3**					
Nd(1)-O(4)	2.497(6)	Cu(1)-N(3)	2.008(7)	Cu(4)-O(5)	1.943(6)
Nd(1)-O(6)	2.503(6)	Cu(2)-N(2)	1.925(7)	Cu(4)-N(7)	2.005(7)
Nd(1)-O(10)	2.526(6)	Cu(2)-O(10)	1.936(6)	Cu(5)-N(6)	1.923(7)
Nd(1)-O(2)	2.561(6)	Cu(2)-O(9)	1.946(6)	Cu(5)-O(4)	1.933(6)
Nd(1)-O(18)	2.591(6)	Cu(2)-N(1)	1.989(7)	Cu(5)-O(3)	1.975(6)
Nd(1)-O(15)	2.601(6)	Cu(2)-O(17)	2.406(6)	Cu(5)-N(5)	2.024(7)
Nd(1)-O(8)	2.600(5)	Cu(3)-N(10)	1.901(7)	Fe(1)-N(14)	1.655(8)
Nd(1)-N(17)	2.637(7)	Cu(3)-O(7)	1.930(6)	Fe(1)-C(13)	1.925(9)
Nd(1)-O(16)	2.710(6)	Cu(3)-O(8)	1.948(6)	Fe(1)-C(15)	1.931(9)
Cu(1)-N(4)	1.904(7)	Cu(3)-N(9)	1.996(7)	Fe(1)-C(14)	1.941(10)
Cu(1)-O(2)	1.927(6)	Cu(4)-O(6)	1.911(6)	Fe(1)-C(12)	1.946(10)
Cu(1)-O(1)	1.932(6)	Cu(4)-N(8)	1.921(7)	Fe(1)-C(11)	1.952(10)
O(4)-Nd(1)-O(6)	72.88(18)	O(6)-Nd(1)-O(8)	67.92(17)	N(4)-Cu(1)-O(2)	91.7(3)
O(4)-Nd(1)-O(10)	135.26(19)	O(10)-Nd(1)-O(8)	69.79(18)	N(4)-Cu(1)-O(1)	176.0(3)
O(6)-Nd(1)-O(10)	135.48(18)	O(2)-Nd(1)-O(8)	129.50(18)	O(2)-Cu(1)-O(1)	84.4(2)
O(4)-Nd(1)-O(2)	68.96(18)	O(18)-Nd(1)-O(8)	76.39(18)	N(4)-Cu(1)-N(3)	82.2(3)
O(6)-Nd(1)-O(2)	134.88(18)	O(15)-Nd(1)-O(8)	136.58(19)	O(2)-Cu(1)-N(3)	168.0(3)
O(10)-Nd(1)-O(2)	68.08(18)	O(4)-Nd(1)-N(17)	141.8(2)	O(1)-Cu(1)-N(3)	101.5(3)
O(4)-Nd(1)-O(18)	72.10(18)	O(6)-Nd(1)-N(17)	102.0(2)	N(2)-Cu(2)-O(10)	89.4(3)
O(6)-Nd(1)-O(18)	73.46(19)	O(10)-Nd(1)-N(17)	75.1(2)	N(2)-Cu(2)-O(9)	169.6(3)
O(10)-Nd(1)-O(18)	83.80(19)	O(2)-Nd(1)-N(17)	122.8(2)	O(10)-Cu(2)-O(9)	84.4(2)
O(2)-Nd(1)-O(18)	72.64(18)	O(18)-Nd(1)-N(17)	144.2(2)	N(2)-Cu(2)-N(1)	83.4(3)
O(4)-Nd(1)-O(15)	87.24(19)	O(15)-Nd(1)-N(17)	69.5(2)	O(10)-Cu(2)-N(1)	170.0(3)
O(6)-Nd(1)-O(15)	134.77(19)	O(8)-Nd(1)-N(17)	69.4(2)	O(9)-Cu(2)-N(1)	101.6(3)
O(10)-Nd(1)-O(15)	86.82(19)	O(4)-Nd(1)-O(16)	77.05(19)	N(2)-Cu(2)-O(17)	102.3(3)
O(2)-Nd(1)-O(15)	66.39(19)	O(6)-Nd(1)-O(16)	67.36(18)	O(10)-Cu(2)-O(17)	93.2(2)
O(18)-Nd(1)-O(15)	138.53(19)	O(10)-Nd(1)-O(16)	139.65(18)	O(9)-Cu(2)-O(17)	86.4(2)
O(4)-Nd(1)-O(8)	135.06(18)	O(2)-Nd(1)-O(16)	123.91(18)	N(1)-Cu(2)-O(17)	95.2(3)
N(10)-Cu(3)-O(7)	171.2(3)	O(6)-Cu(4)-N(8)	90.1(3)	N(6)-Cu(5)-O(4)	93.4(3)
N(10)-Cu(3)-O(8)	92.9(3)	O(6)-Cu(4)-O(5)	84.4(2)	N(6)-Cu(5)-O(3)	177.0(3)
O(7)-Cu(3)-O(8)	84.8(2)	N(8)-Cu(4)-O(5)	168.4(3)	O(4)-Cu(5)-O(3)	83.8(2)
N(10)-Cu(3)-N(9)	82.6(3)	O(6)-Cu(4)-N(7)	172.5(3)	N(6)-Cu(5)-N(5)	81.5(3)
O(7)-Cu(3)-N(9)	99.5(3)	N(8)-Cu(4)-N(7)	82.9(3)	O(4)-Cu(5)-N(5)	174.9(3)
O(8)-Cu(3)-N(9)	175.6(3)	O(5)-Cu(4)-N(7)	102.0(3)	O(3)-Cu(5)-N(5)	101.2(3)
N(14)-Fe(1)-C(13)	96.8(4)	N(14)-Fe(1)-C(12)	96.2(4)	C(13)-Fe(1)-C(11)	85.9(4)
N(14)-Fe(1)-C(15)	93.7(4)	C(13)-Fe(1)-C(12)	89.0(4)	C(15)-Fe(1)-C(11)	83.5(4)
C(13)-Fe(1)-C(15)	169.4(4)	C(15)-Fe(1)-C(12)	89.6(4)	C(14)-Fe(1)-C(11)	86.7(4)
N(14)-Fe(1)-C(14)	93.2(4)	C(14)-Fe(1)-C(12)	170.4(4)	C(12)-Fe(1)-C(11)	84.0(4)
C(13)-Fe(1)-C(14)	88.3(4)	N(14)-Fe(1)-C(11)	177.3(4)	N(14)-Fe(1)-C(11)	177.3(4)

C(15)-Fe(1)-C(14)	91.3(4)				
Complex **4**					
Na(1)-O(16)	2.398(9)	Cu(5)-N(8)	1.898(8)	Cu(1)-N(17)	2.427(9)
Na(1)-O(18)	2.409(8)	Cu(5)-O(10)	1.931(7)	Cu(4)-N(6)	1.913(8)
Na(1)-O(7)#1	2.414(8)	Cu(5)-O(9)	1.953(7)	Cu(4)-O(8)	1.943(6)
Na(1)-N(13)	2.449(10)	Cu(5)-N(7)	2.008(8)	Cu(4)-O(7)	2.000(7)
Na(1)-N(21)#2	2.472(10)	Cu(5)-H(20C)	1.9269	Cu(4)-N(5)	2.011(8)
Sm(1)-O(2)	2.404(7)	Cu(3)-N(4)	1.908(8)	Cu(4)-N(11)	2.255(9)
Sm(1)-O(10)	2.406(6)	Cu(3)-O(6)	1.922(7)	Cu(2)-N(2)	1.884(8)
Sm(1)-O(13)	2.430(7)	Cu(3)-O(5)	1.957(7)	Cu(2)-O(4)	1.925(6)
Sm(1)-O(15)	2.426(7)	Cu(3)-N(3)	1.996(8)	Cu(2)-O(3)	1.924(7)
Sm(1)-O(14)	2.438(7)	Cu(1)-N(10)	1.905(8)	Cu(2)-N(1)	1.998(8)
Sm(1)-O(8)	2.445(7)	Cu(1)-O(2)	1.942(7)	Fe(1)-N(12)	1.667(9)
Sm(1)-O(6)	2.454(7)	Cu(1)-O(1)	1.958(6)	Fe(1)-C(13)	1.928(10)
Sm(1)-O(4)	2.470(7)	Cu(1)-N(9)	2.035(8)	Fe(1)-C(14)	1.927(11)
Fe(1)-C(11)	1.934(10)	Fe(2)-N(20)	1.638(9)	Fe(2)-C(18)	1.930(11)
Fe(1)-C(12)	1.945(11)	Fe(2)-C(17)	1.924(10)	Fe(2)-C(16)	1.947(11)
Fe(1)-C(15)	1.949(11)	Fe(2)-C(19)	1.926(11)	Fe(2)-C(20)	1.953(10)
O(16)-Na(1)-O(18)	161.0(3)	O(13)-Sm(1)-O(15)	141.6(2)	O(8)-Sm(1)-O(6)	68.3(2)
O(16)-Na(1)-O(7)#1	91.7(3)	O(2)-Sm(1)-O(14)	88.9(2)	O(2)-Sm(1)-O(4)	72.6(2)
O(18)-Na(1)-O(7)#1	107.4(3)	O(10)-Sm(1)-O(14)	136.1(2)	O(10)-Sm(1)-O(4)	133.2(2)
O(16)-Na(1)-N(13)	80.2(3)	O(13)-Sm(1)-O(14)	67.4(2)	O(13)-Sm(1)-O(4)	134.3(2)
O(18)-Na(1)-N(13)	97.8(3)	O(15)-Sm(1)-O(14)	150.2(2)	O(15)-Sm(1)-O(4)	78.5(2)
O(7)#1-Na(1)-N(13)	92.2(3)	O(2)-Sm(1)-O(8)	145.8(2)	O(14)-Sm(1)-O(4)	72.3(2)
O(16)-Na(1)-N(21)#2	92.8(3)	O(10)-Sm(1)-O(8)	73.6(2)	O(8)-Sm(1)-O(4)	136.1(2)
O(18)-Na(1)-N(21)#2	86.1(3)	O(13)-Sm(1)-O(8)	81.9(2)	O(6)-Sm(1)-O(4)	72.4(2)
O(7)#1-Na(1)-N(21)#2	96.4(3)	O(15)-Sm(1)-O(8)	82.7(2)	N(10)-Cu(1)-O(2)	90.4(3)
N(13)-Na(1)-N(21)#2	169.1(4)	O(14)-Sm(1)-O(8)	114.9(2)	N(10)-Cu(1)-O(1)	172.3(3)
O(2)-Sm(1)-O(10)	72.3(2)	O(2)-Sm(1)-O(6)	144.7(2)	O(2)-Cu(1)-O(1)	84.2(3)
O(2)-Sm(1)-O(13)	85.8(2)	O(10)-Sm(1)-O(6)	139.0(2)	N(10)-Cu(1)-N(9)	82.3(3)
O(10)-Sm(1)-O(13)	71.8(2)	O(13)-Sm(1)-O(6)	116.0(2)	O(2)-Cu(1)-N(9)	167.1(3)
O(2)-Sm(1)-O(15)	87.7(2)	O(15)-Sm(1)-O(6)	90.1(2)	O(1)-Cu(1)-N(9)	102.0(3)
O(10)-Sm(1)-O(15)	70.1(2)	O(14)-Sm(1)-O(6)	76.0(2)	N(10)-Cu(1)-N(17)	89.6(3)
O(2)-Cu(1)-N(17)	101.4(3)	N(4)-Cu(3)-O(6)	91.4(3)	N(6)-Cu(4)-N(5)	82.7(3)
O(1)-Cu(1)-N(17)	96.7(3)	N(4)-Cu(3)-O(5)	175.2(3)	O(8)-Cu(4)-N(5)	167.0(3)
N(9)-Cu(1)-N(17)	89.2(3)	O(6)-Cu(3)-O(5)	84.3(3)	O(7)-Cu(4)-N(5)	102.5(3)
N(2)-Cu(2)-O(4)	92.7(3)	N(4)-Cu(3)-N(3)	83.9(3)	N(6)-Cu(4)-N(11)	114.3(3)
N(2)-Cu(2)-O(3)	175.9(3)	O(6)-Cu(3)-N(3)	173.9(3)	O(8)-Cu(4)-N(11)	97.6(3)
O(4)-Cu(2)-O(3)	84.9(3)	O(5)-Cu(3)-N(3)	100.6(3)	O(7)-Cu(4)-N(11)	87.5(3)
N(2)-Cu(2)-N(1)	83.1(3)	N(6)-Cu(4)-O(8)	87.1(3)	N(5)-Cu(4)-N(11)	93.9(3)
O(4)-Cu(2)-N(1)	163.9(3)	N(6)-Cu(4)-O(7)	157.4(3)	N(8)-Cu(5)-O(10)	92.9(3)
O(3)-Cu(2)-N(1)	100.1(3)	O(8)-Cu(4)-O(7)	84.0(3)	N(8)-Cu(5)-O(9)	176.8(3)
O(10)-Cu(5)-O(9)	84.0(3)	C(13)-Fe(1)-C(11)	171.3(4)	C(14)-Fe(1)-C(15)	85.2(4)

N(8)-Cu(5)-N(7)	82.4(3)	C(14)-Fe(1)-C(11)	85.7(4)	C(11)-Fe(1)-C(15)	90.7(4)
O(10)-Cu(5)-N(7)	167.6(3)	N(12)-Fe(1)-C(12)	95.8(4)	C(12)-Fe(1)-C(15)	167.8(4)
O(9)-Cu(5)-N(7)	100.4(3)	C(13)-Fe(1)-C(12)	91.6(4)	N(20)-Fe(2)-C(17)	97.9(4)
N(12)-Fe(1)-C(13)	93.4(4)	C(14)-Fe(1)-C(12)	82.7(4)	N(20)-Fe(2)-C(19)	93.9(4)
N(12)-Fe(1)-C(14)	178.2(5)	C(11)-Fe(1)-C(12)	88.2(4)	C(17)-Fe(2)-C(19)	168.2(4)
C(13)-Fe(1)-C(14)	85.7(5)	N(12)-Fe(1)-C(15)	96.3(4)	N(20)-Fe(2)-C(18)	93.7(5)
N(12)-Fe(1)-C(11)	95.3(4)	C(13)-Fe(1)-C(15)	87.7(4)	C(17)-Fe(2)-C(18)	90.2(4)
C(19)-Fe(2)-C(18)	88.3(4)	C(19)-Fe(2)-C(16)	84.4(4)	C(17)-Fe(2)-C(20)	89.4(4)
N(20)-Fe(2)-C(16)	178.2(5)	C(18)-Fe(2)-C(16)	85.7(4)	C(19)-Fe(2)-C(20)	90.3(4)
C(17)-Fe(2)-C(16)	83.8(4)	N(20)-Fe(2)-C(20)	94.8(4)	C(18)-Fe(2)-C(20)	171.5(4)
C(16)-Fe(2)-C(20)	85.8(4)				
Complex **5**					
Gd(1)-O(15)	2.386(8)	Cu(2)-N(17)	2.428(10)	Fe(1)-C(13)	1.917(15)
Gd(1)-O(2)	2.398(7)	Cu(5)-N(8)	1.936(9)	Fe(1)-C(14)	1.947(15)
Gd(1)-O(4)	2.408(7)	Cu(5)-O(10)	1.936(7)	Fe(1)-C(15)	1.945(14)
Gd(1)-O(14)	2.424(8)	Cu(5)-O(9)	2.026(8)	Fe(1)-C(11)	1.950(14)
Gd(1)-O(13)	2.438(7)	Cu(5)-N(7)	2.037(9)	Fe(2)-N(20)	1.598(11)
Gd(1)-O(10)	2.440(7)	Cu(5)-N(11)	2.244(11)	Fe(2)-C(17)	1.898(15)
Gd(1)-O(8)	2.439(7)	Cu(4)-N(6)	1.905(9)	Fe(2)-C(18)	1.897(14)
Gd(1)-O(6)	2.449(7)	Cu(4)-O(8)	1.921(8)	Fe(2)-C(20)	1.931(13)
Cu(1)-N(10)	1.912(10)	Cu(4)-O(7)	1.931(7)	Fe(2)-C(16)	1.927(13)
Cu(1)-O(2)	1.932(7)	Cu(4)-N(5)	2.003(9)	Fe(2)-C(19)	1.941(15)
Cu(1)-O(1)	1.939(7)	Cu(3)-N(4)	1.886(9)	Na(1)-O(17)	2.420(10)
Cu(1)-N(9)	2.012(9)	Cu(3)-O(5)	1.922(8)	Na(1)-O(9)#1	2.432(9)
Cu(2)-N(2)	1.927(9)	Cu(3)-O(6)	1.938(7)	Na(1)-O(18)	2.444(10)
Cu(2)-O(4)	1.957(7)	Cu(3)-N(3)	2.001(8)	Na(1)-N(12)	2.465(12)
Cu(2)-O(3)	1.966(7)	Fe(1)-N(13)	1.620(11)	Na(1)-N(22)#2	2.519(13)
Cu(2)-N(1)	2.014(10)	Fe(1)-C(12)	1.915(14)		
O(15)-Gd(1)-O(2)	71.3(3)	N(10)-Cu(1)-O(2)	92.0(4)	O(8)-Cu(4)-O(7)	84.7(3)
O(15)-Gd(1)-O(4)	87.9(3)	N(10)-Cu(1)-O(1)	176.2(4)	N(6)-Cu(4)-N(5)	82.1(4)
O(2)-Gd(1)-O(4)	72.6(2)	O(2)-Cu(1)-O(1)	84.4(3)	O(8)-Cu(4)-N(5)	172.6(4)
O(15)-Gd(1)-O(14)	148.0(3)	N(10)-Cu(1)-N(9)	83.6(4)	O(7)-Cu(4)-N(5)	102.0(3)
O(2)-Gd(1)-O(14)	136.4(3)	O(2)-Cu(1)-N(9)	168.0(4)	N(4)-Cu(3)-O(5)	175.7(4)
O(4)-Gd(1)-O(14)	87.5(3)	O(1)-Cu(1)-N(9)	99.8(3)	N(4)-Cu(3)-O(6)	92.2(4)
O(15)-Gd(1)-O(13)	141.5(3)	N(2)-Cu(2)-O(4)	89.8(4)	O(5)-Cu(3)-O(6)	84.8(3)
O(2)-Gd(1)-O(13)	70.5(3)	N(2)-Cu(2)-O(3)	169.1(4)	N(4)-Cu(3)-N(3)	82.9(4)
O(4)-Gd(1)-O(13)	85.7(2)	O(4)-Cu(2)-O(3)	83.7(3)	O(5)-Cu(3)-N(3)	100.8(4)
O(14)-Gd(1)-O(13)	69.6(3)	N(2)-Cu(2)-N(1)	82.0(4)	O(6)-Cu(3)-N(3)	165.6(4)
O(15)-Gd(1)-O(10)	84.5(3)	O(4)-Cu(2)-N(1)	165.1(4)	N(13)-Fe(1)-C(12)	96.7(6)
O(2)-Gd(1)-O(10)	73.7(2)	O(3)-Cu(2)-N(1)	102.3(3)	N(13)-Fe(1)-C(13)	92.9(5)
O(4)-Gd(1)-O(10)	146.2(2)	N(2)-Cu(2)-N(17)	93.3(4)	C(12)-Fe(1)-C(13)	89.2(6)
O(14)-Gd(1)-O(10)	115.4(3)	O(4)-Cu(2)-N(17)	103.5(3)	N(13)-Fe(1)-C(14)	94.9(6)
O(13)-Gd(1)-O(10)	80.1(3)	O(3)-Cu(2)-N(17)	96.6(3)	C(12)-Fe(1)-C(14)	168.3(6)

O(15)-Gd(1)-O(8)	89.9(3)	N(1)-Cu(2)-N(17)	89.5(4)	C(13)-Fe(1)-C(14)	88.4(6)
O(2)-Gd(1)-O(8)	139.3(3)	N(8)-Cu(5)-O(10)	87.5(4)	N(13)-Fe(1)-C(15)	178.8(6)
O(4)-Gd(1)-O(8)	144.3(2)	N(8)-Cu(5)-O(9)	155.8(4)	C(12)-Fe(1)-C(15)	82.2(6)
O(14)-Gd(1)-O(8)	75.9(3)	O(10)-Cu(5)-O(9)	83.3(3)	C(13)-Fe(1)-C(15)	87.0(6)
O(13)-Gd(1)-O(8)	116.3(3)	N(8)-Cu(5)-N(7)	81.9(4)	C(14)-Fe(1)-C(15)	86.3(6)
O(10)-Gd(1)-O(8)	68.7(2)	O(10)-Cu(5)-N(7)	166.4(4)	N(13)-Fe(1)-C(11)	95.0(5)
O(15)-Gd(1)-O(6)	76.9(3)	O(9)-Cu(5)-N(7)	103.1(4)	C(12)-Fe(1)-C(11)	90.1(6)
O(2)-Gd(1)-O(6)	133.3(2)	N(8)-Cu(5)-N(11)	114.9(4)	C(13)-Fe(1)-C(11)	172.1(5)
O(4)-Gd(1)-O(6)	72.8(2)	O(10)-Cu(5)-N(11)	97.5(3)	C(14)-Fe(1)-C(11)	90.7(6)
O(14)-Gd(1)-O(6)	71.4(3)	O(9)-Cu(5)-N(11)	88.5(4)	C(15)-Fe(1)-C(11)	85.1(5)
O(13)-Gd(1)-O(6)	135.9(3)	N(7)-Cu(5)-N(11)	94.7(4)	N(20)-Fe(2)-C(17)	94.9(6)
O(10)-Gd(1)-O(6)	136.3(2)	N(6)-Cu(4)-O(8)	91.3(4)	N(20)-Fe(2)-C(18)	97.6(6)
O(8)-Gd(1)-O(6)	72.1(2)	N(6)-Cu(4)-O(7)	175.7(3)	C(17)-Fe(2)-C(18)	90.3(6)
N(20)-Fe(2)-C(20)	95.6(6)	C(17)-Fe(2)-C(19)	171.9(6)	O(17)-Na(1)-N(12)	84.5(4)
C(17)-Fe(2)-C(20)	88.6(6)	C(18)-Fe(2)-C(19)	89.9(6)	O(9)#1-Na(1)-N(12)	92.9(4)
C(18)-Fe(2)-C(20)	166.8(6)	C(20)-Fe(2)-C(19)	89.4(6)	O(18)-Na(1)-N(12)	96.1(4)
N(20)-Fe(2)-C(16)	179.2(6)	C(16)-Fe(2)-C(19)	87.1(5)	O(17)-Na(1)-N(22)#2	90.2(4)
C(17)-Fe(2)-C(16)	84.9(6)	O(17)-Na(1)-O(9)#1	95.0(3)	O(9)#1-Na(1)-N(22)#2	96.2(4)
C(18)-Fe(2)-C(16)	83.2(5)	O(17)-Na(1)-O(18)	159.1(4)	O(18)-Na(1)-N(22)#2	85.7(4)
C(20)-Fe(2)-C(16)	83.6(5)	O(9)#1-Na(1)-O(18)	105.8(3)	N(12)-Na(1)-N(22)#2	169.9(4)
N(20)-Fe(2)-C(19)	93.1(6)				
Complex **6**					
Tb(1)-O(15)	2.370(7)	Cu(2)-N(2)	1.904(8)	Cu(4)-N(6)	1.897(8)
Tb(1)-O(4)	2.374(7)	Cu(2)-O(4)	1.933(7)	Cu(4)-O(8)	1.925(7)
Tb(1)-O(6)	2.377(6)	Cu(2)-O(3)	1.949(7)	Cu(4)-O(7)	1.926(7)
Tb(1)-O(14)	2.381(7)	Cu(2)-N(1)	2.008(8)	Cu(4)-N(5)	2.007(8)
Tb(1)-O(13)	2.392(7)	Cu(5)-N(8)	1.902(8)	Fe(1)-N(12)	1.663(9)
Tb(1)-O(2)	2.421(7)	Cu(5)-O(10)	1.928(7)	Fe(1)-C(11)	1.915(10)
Tb(1)-O(10)	2.437(6)	Cu(5)-O(9)	1.951(7)	Fe(1)-C(15)	1.930(11)
Tb(1)-O(8)	2.458(7)	Cu(5)-N(7)	2.010(8)	Fe(1)-C(13)	1.934(11)
Cu(1)-N(10)	1.914(8)	Cu(3)-N(4)	1.913(8)	Fe(1)-C(12)	1.957(12)
Cu(1)-O(2)	1.950(6)	Cu(3)-O(6)	1.950(6)	Fe(1)-C(14)	1.960(12)
Cu(1)-O(1)	1.998(7)	Cu(3)-O(5)	1.958(7)	Fe(2)-N(20)	1.652(8)
Cu(1)-N(9)	2.007(8)	Cu(3)-N(3)	2.024(8)	Fe(2)-C(17)	1.941(11)
Cu(1)-N(11)	2.259(9)	Cu(3)-N(17)	2.422(9)	Fe(2)-C(18)	1.945(10)
Fe(2)-C(19)	1.945(11)	Na(1)-O(20)	2.392(8)	Na(1)-N(13)	2.456(11)
Fe(2)-C(20)	1.952(11)	Na(1)-O(1)#1	2.408(8)	Na(1)-N(21)#2	2.487(10)
Fe(2)-C(16)	1.957(10)	Na(1)-O(19)	2.426(8)	Na(1)-O(21)	2.567(13)
O(15)-Tb(1)-O(4)	70.6(2)	N(10)-Cu(1)-O(2)	86.7(3)	N(4)-Cu(3)-N(17)	91.0(3)
O(15)-Tb(1)-O(6)	88.4(2)	N(10)-Cu(1)-O(1)	157.0(3)	O(6)-Cu(3)-N(17)	102.1(3)
O(4)-Tb(1)-O(6)	72.6(2)	O(2)-Cu(1)-O(1)	84.1(3)	O(5)-Cu(3)-N(17)	96.9(3)
O(15)-Tb(1)-O(14)	147.9(2)	N(10)-Cu(1)-N(9)	82.9(3)	N(3)-Cu(3)-N(17)	89.3(3)
O(4)-Tb(1)-O(14)	137.4(2)	O(2)-Cu(1)-N(9)	166.7(3)	N(6)-Cu(4)-O(8)	91.8(3)

O(6)-Tb(1)-O(14)	87.7(2)	O(1)-Cu(1)-N(9)	102.4(3)	N(6)-Cu(4)-O(7)	175.4(3)
O(15)-Tb(1)-O(13)	140.8(2)	N(10)-Cu(1)-N(11)	114.5(3)	O(8)-Cu(4)-O(7)	85.3(3)
O(4)-Tb(1)-O(13)	70.6(2)	O(2)-Cu(1)-N(11)	97.6(3)	N(6)-Cu(4)-N(5)	83.2(3)
O(6)-Tb(1)-O(13)	85.5(2)	O(1)-Cu(1)-N(11)	87.7(3)	O(8)-Cu(4)-N(5)	164.0(4)
O(14)-Tb(1)-O(13)	70.4(2)	N(9)-Cu(1)-N(11)	94.3(3)	O(7)-Cu(4)-N(5)	100.5(3)
O(15)-Tb(1)-O(2)	83.2(2)	N(2)-Cu(2)-O(4)	91.3(3)	N(12)-Fe(1)-C(11)	94.4(4)
O(4)-Tb(1)-O(2)	73.4(2)	N(2)-Cu(2)-O(3)	175.6(3)	N(12)-Fe(1)-C(15)	178.3(5)
O(6)-Tb(1)-O(2)	145.9(2)	O(4)-Cu(2)-O(3)	84.7(3)	C(11)-Fe(1)-C(15)	84.8(5)
O(14)-Tb(1)-O(2)	116.1(2)	N(2)-Cu(2)-N(1)	83.1(3)	N(12)-Fe(1)-C(13)	94.4(5)
O(13)-Tb(1)-O(2)	80.6(2)	O(4)-Cu(2)-N(1)	168.3(3)	C(11)-Fe(1)-C(13)	171.1(5)
O(15)-Tb(1)-O(10)	89.5(2)	O(3)-Cu(2)-N(1)	100.6(3)	C(15)-Fe(1)-C(13)	86.3(5)
O(4)-Tb(1)-O(10)	138.6(2)	N(8)-Cu(5)-O(10)	91.2(3)	N(12)-Fe(1)-C(12)	95.1(5)
O(6)-Tb(1)-O(10)	144.9(2)	N(8)-Cu(5)-O(9)	175.6(3)	C(11)-Fe(1)-C(12)	87.9(5)
O(14)-Tb(1)-O(10)	75.9(2)	O(10)-Cu(5)-O(9)	84.6(3)	C(15)-Fe(1)-C(12)	83.3(5)
O(13)-Tb(1)-O(10)	116.6(2)	N(8)-Cu(5)-N(7)	84.0(3)	C(13)-Fe(1)-C(12)	90.2(5)
O(2)-Tb(1)-O(10)	68.3(2)	O(10)-Cu(5)-N(7)	174.4(3)	N(12)-Fe(1)-C(14)	97.0(5)
O(15)-Tb(1)-O(8)	77.1(2)	O(9)-Cu(5)-N(7)	100.3(3)	C(11)-Fe(1)-C(14)	91.5(4)
O(4)-Tb(1)-O(8)	132.7(2)	N(4)-Cu(3)-O(6)	89.9(3)	C(15)-Fe(1)-C(14)	84.6(5)
O(6)-Tb(1)-O(8)	72.9(2)	N(4)-Cu(3)-O(5)	171.1(3)	C(13)-Fe(1)-C(14)	88.5(5)
O(14)-Tb(1)-O(8)	71.3(2)	O(6)-Cu(3)-O(5)	84.4(3)	C(12)-Fe(1)-C(14)	167.9(5)
O(13)-Tb(1)-O(8)	136.4(2)	N(4)-Cu(3)-N(3)	82.5(3)	N(20)-Fe(2)-C(17)	94.4(4)
O(2)-Tb(1)-O(8)	136.0(2)	O(6)-Cu(3)-N(3)	166.4(3)	N(20)-Fe(2)-C(18)	97.1(4)
O(10)-Tb(1)-O(8)	72.5(2)	O(5)-Cu(3)-N(3)	101.7(3)	C(17)-Fe(2)-C(18)	90.5(5)
N(20)-Fe(2)-C(19)	93.5(4)	C(19)-Fe(2)-C(20)	89.6(4)	N(13)-Na(1)-N(21)#2	168.6(3)
C(17)-Fe(2)-C(19)	172.0(4)	N(20)-Fe(2)-C(16)	178.6(4)	O(20)-Na(1)-O(19)	161.3(3)
C(18)-Fe(2)-C(19)	89.4(5)	C(17)-Fe(2)-C(16)	86.4(4)	O(1)#1-Na(1)-O(19)	106.0(3)
N(20)-Fe(2)-C(20)	94.9(4)	C(18)-Fe(2)-C(16)	84.1(4)	O(20)-Na(1)-N(13)	82.0(3)
C(17)-Fe(2)-C(20)	88.8(5)	C(19)-Fe(2)-C(16)	85.7(4)	O(1)#1-Na(1)-N(13)	93.0(3)
C(18)-Fe(2)-C(20)	168.0(4)	C(20)-Fe(2)-C(16)	84.0(4)	O(19)-Na(1)-N(13)	96.4(3)
O(20)-Na(1)-N(21)#2	91.5(3)	O(20)-Na(1)-O(1)#1	92.6(3)	O(19)-Na(1)-O(21)	77.0(4)
O(1)#1-Na(1)-N(21)#2	96.7(3)	O(20)-Na(1)-O(21)	84.3(4)	N(13)-Na(1)-O(21)	82.6(4)
O(19)-Na(1)-N(21)#2	86.7(3)	O(1)#1-Na(1)-O(21)	175.0(4)	N(21)#2-Na(1)-O(21)	87.4(4)
Complex **7**					
Dy(1)-O(15)	2.357(11)	Fe(2)-C(17)	1.946(17)	O(6)-Cu(3)	1.939(10)
Dy(1)-O(13)	2.365(11)	Na(1)-O(17)	2.373(13)	O(7)-Cu(4)	1.950(11)
Dy(1)-O(10)	2.372(10)	Na(1)-O(5)#1	2.401(12)	O(8)-Cu(4)	1.916(11)
Dy(1)-O(8)	2.401(11)	Na(1)-O(16)	2.430(13)	O(9)-Cu(5)	1.946(11)
Dy(1)-O(6)	2.423(11)	Na(1)-N(13)	2.431(16)	O(10)-Cu(5)	1.955(11)
Dy(1)-O(4)	2.425(10)	Na(1)-N(21)#2	2.459(15)	Cu(1)-N(10)	1.865(13)
Dy(1)-O(14)	2.439(11)	O(5)-Na(1)#1	2.401(12)	Cu(1)-N(9)	1.996(12)
Dy(1)-O(2)	2.443(10)	N(21)-Na(1)#3	2.459(15)	Cu(2)-N(2)	1.900(12)
Fe(1)-N(12)	1.661(14)	O(1)-Cu(1)	1.918(11)	Cu(2)-N(1)	2.027(13)
Fe(1)-C(15)	1.905(17)	O(2)-N(2)	1.397(15)	Cu(3)-N(4)	1.922(13)

Fe(1)-C(12)	1.933(18)	O(2)-Cu(1)	1.942(10)	Cu(3)-N(3)	2.000(12)
Fe(1)-C(13)	1.934(17)	O(3)-C(4)	1.301(18)	Cu(3)-N(11)	2.250(14)
Fe(1)-C(14)	1.945(18)	O(3)-Cu(2)	1.963(10)	Cu(4)-N(6)	1.901(13)
Fe(1)-C(11)	1.954(17)	O(4)-N(4)	1.385(15)	Cu(4)-N(5)	2.017(13)
Fe(2)-N(20)	1.629(13)	O(4)-Cu(2)	1.930(11)	Cu(5)-N(8)	1.879(13)
Fe(2)-C(18)	1.907(16)	O(5)-C(6)	1.280(18)	Cu(5)-N(7)	2.022(13)
Fe(2)-C(20)	1.919(17)	O(5)-Cu(3)	1.998(11)	Cu(5)-N(17)	2.424(14)
Fe(2)-C(16)	1.929(16)	Fe(2)-C(19)	1.940(17)		
Cu(3)-N(11)	2.250	Na(1)-N(13)	2.431	Cu(2)-N(18)	2.694
Cu(5)-N(17)	2.423	Na(1)-N(21)	2.459		
O(15)-Dy(1)-O(13)	148.9(4)	N(12)-Fe(1)-C(15)	179.0(8)	C(16)-Fe(2)-C(17)	86.4(7)
O(15)-Dy(1)-O(10)	88.3(4)	N(12)-Fe(1)-C(12)	95.0(7)	C(19)-Fe(2)-C(17)	171.6(7)
O(13)-Dy(1)-O(10)	87.4(4)	C(15)-Fe(1)-C(12)	83.9(7)	O(17)-Na(1)-O(5)#1	91.9(4)
O(15)-Dy(1)-O(8)	136.9(4)	N(12)-Fe(1)-C(13)	93.5(7)	O(17)-Na(1)-O(16)	161.3(5)
O(13)-Dy(1)-O(8)	70.2(4)	C(15)-Fe(1)-C(13)	86.6(7)	O(5)#1-Na(1)-O(16)	106.8(4)
O(10)-Dy(1)-O(8)	73.0(4)	C(12)-Fe(1)-C(13)	90.4(7)	O(17)-Na(1)-N(13)	83.7(5)
O(15)-Dy(1)-O(6)	114.9(4)	N(12)-Fe(1)-C(14)	96.0(7)	O(5)#1-Na(1)-N(13)	94.1(5)
O(13)-Dy(1)-O(6)	83.9(4)	C(15)-Fe(1)-C(14)	85.0(7)	O(16)-Na(1)-N(13)	95.0(5)
O(10)-Dy(1)-O(6)	146.5(4)	C(12)-Fe(1)-C(14)	168.9(7)	O(17)-Na(1)-N(21)#2	92.4(5)
O(8)-Dy(1)-O(6)	73.6(3)	C(13)-Fe(1)-C(14)	88.6(7)	O(5)#1-Na(1)-N(21)#2	97.9(5)
O(15)-Dy(1)-O(4)	75.6(4)	N(12)-Fe(1)-C(11)	95.1(7)	O(16)-Na(1)-N(21)#2	84.9(5)
O(13)-Dy(1)-O(4)	90.5(4)	C(15)-Fe(1)-C(11)	84.7(7)	N(13)-Na(1)-N(21)#2	167.5(5)
O(10)-Dy(1)-O(4)	144.5(4)	C(12)-Fe(1)-C(11)	88.3(7)	N(10)-Cu(1)-O(1)	175.6(5)
O(8)-Dy(1)-O(4)	138.6(4)	C(13)-Fe(1)-C(11)	171.3(7)	N(10)-Cu(1)-O(2)	91.9(5)
O(6)-Dy(1)-O(4)	68.1(3)	C(14)-Fe(1)-C(11)	91.1(7)	O(1)-Cu(1)-O(2)	85.9(4)
O(15)-Dy(1)-O(14)	64.5(3)	N(20)-Fe(2)-C(18)	96.7(7)	N(10)-Cu(1)-N(9)	83.2(5)
O(13)-Dy(1)-O(14)	145.8(3)	N(20)-Fe(2)-C(20)	94.9(7)	O(1)-Cu(1)-N(9)	99.9(5)
O(10)-Dy(1)-O(14)	87.2(4)	C(18)-Fe(2)-C(20)	168.3(7)	O(2)-Cu(1)-N(9)	164.3(5)
O(8)-Dy(1)-O(14)	75.9(3)	N(20)-Fe(2)-C(16)	178.7(7)	N(2)-Cu(2)-O(4)	91.8(5)
O(6)-Dy(1)-O(14)	82.2(3)	C(18)-Fe(2)-C(16)	84.2(7)	N(2)-Cu(2)-O(3)	176.6(5)
O(4)-Dy(1)-O(14)	112.7(3)	C(20)-Fe(2)-C(16)	84.3(7)	O(4)-Cu(2)-O(3)	85.0(4)
O(15)-Dy(1)-O(2)	71.8(4)	N(20)-Fe(2)-C(19)	93.6(7)	N(2)-Cu(2)-N(1)	83.4(5)
O(13)-Dy(1)-O(2)	77.6(4)	C(18)-Fe(2)-C(19)	90.9(7)	O(4)-Cu(2)-N(1)	174.5(5)
O(10)-Dy(1)-O(2)	72.8(3)	C(20)-Fe(2)-C(19)	89.4(7)	O(3)-Cu(2)-N(1)	99.9(5)
O(8)-Dy(1)-O(2)	133.4(3)	C(16)-Fe(2)-C(19)	85.4(7)	N(4)-Cu(3)-O(6)	86.9(5)
O(6)-Dy(1)-O(2)	135.6(3)	N(20)-Fe(2)-C(17)	94.6(7)	N(4)-Cu(3)-O(5)	156.6(5)
O(4)-Dy(1)-O(2)	72.1(3)	C(18)-Fe(2)-C(17)	89.7(7)	O(6)-Cu(3)-O(5)	83.6(5)
O(14)-Dy(1)-O(2)	132.2(3)	C(20)-Fe(2)-C(17)	88.4(7)	N(4)-Cu(3)-N(3)	83.2(5)
O(6)-Cu(3)-N(3)	166.2(5)	O(8)-Cu(4)-O(7)	87.6(4)	N(8)-Cu(5)-N(7)	81.9(6)
O(5)-Cu(3)-N(3)	102.0(5)	N(6)-Cu(4)-N(5)	82.8(5)	O(9)-Cu(5)-N(7)	101.4(5)
N(4)-Cu(3)-N(11)	115.0(5)	O(8)-Cu(4)-N(5)	168.3(5)	O(10)-Cu(5)-N(7)	165.7(5)
O(6)-Cu(3)-N(11)	97.8(5)	O(7)-Cu(4)-N(5)	97.0(5)	N(8)-Cu(5)-N(17)	91.3(5)
O(5)-Cu(3)-N(11)	87.6(5)	N(8)-Cu(5)-O(9)	171.1(5)	O(9)-Cu(5)-N(17)	96.9(5)

N(3)-Cu(3)-N(11)	95.1(5)	N(8)-Cu(5)-O(10)	90.5(5)	O(10)-Cu(5)-N(17)	102.4(5)
N(6)-Cu(4)-O(8)	92.6(5)	O(9)-Cu(5)-O(10)	84.5(4)	N(7)-Cu(5)-N(17)	90.0(5)
N(6)-Cu(4)-O(7)	179.7(5)				
Complex **8**					
Ho(1)-O(15)	2.362(6)	Cu(1)-N(1)	2.037(7)	Cu(4)-N(8)	1.892(7)
Ho(1)-O(14)	2.368(7)	Cu(1)-N(17)	2.415(9)	Cu(4)-O(5)	1.943(6)
Ho(1)-O(2)	2.386(5)	Cu(2)-N(4)	1.919(7)	Cu(4)-O(6)	1.946(6)
Ho(1)-O(10)	2.389(5)	Cu(2)-O(2)	1.929(6)	Cu(4)-N(7)	2.010(7)
Ho(1)-O(13)	2.411(6)	Cu(2)-O(1)	1.981(6)	Cu(5)-N(10)	1.894(7)
Ho(1)-O(4)	2.427(6)	Cu(2)-N(3)	2.029(7)	Cu(5)-O(8)	1.940(6)
Ho(1)-O(6)	2.435(5)	Cu(3)-N(6)	1.926(7)	Cu(5)-O(7)	1.953(6)
Ho(1)-O(8)	2.452(6)	Cu(3)-O(4)	1.952(6)	Cu(5)-N(9)	1.996(7)
Cu(1)-N(2)	1.914(7)	Cu(3)-N(5)	2.015(7)	Fe(1)-N(12)	1.655(9)
Cu(1)-O(9)	1.968(6)	Cu(3)-O(3)	2.016(6)	Fe(1)-C(15)	1.934(12)
Cu(1)-O(10)	1.975(6)	Cu(3)-N(11)	2.263(8)	Fe(1)-C(12)	1.936(12)
Fe(1)-C(13)	1.944(11)	Fe(2)-N(20)	1.638(9)	Fe(2)-C(16)	1.963(11)
Fe(1)-C(14)	1.975(12)	Fe(2)-C(17)	1.952(12)	Fe(2)-C(20)	1.961(12)
Fe(1)-C(11)	1.991(11)	Fe(2)-C(19)	1.957(12)	Fe(2)-C(18)	1.967(11)
N(2)-Cu(1)-O(9)	170.3(3)	O(8)-Cu(5)-N(9)	165.9(3)	C(12)-Fe(1)-C(13)	90.1(4)
N(2)-Cu(1)-O(10)	90.1(3)	O(7)-Cu(5)-N(9)	100.4(3)	N(12)-Fe(1)-C(14)	179.4(5)
O(9)-Cu(1)-O(10)	84.4(2)	O(15)-Ho(1)-O(14)	148.5(2)	C(15)-Fe(1)-C(14)	84.2(5)
N(2)-Cu(1)-N(1)	82.1(3)	O(15)-Ho(1)-O(2)	71.5(2)	C(12)-Fe(1)-C(14)	84.1(4)
O(9)-Cu(1)-N(1)	101.6(3)	O(14)-Ho(1)-O(2)	136.5(2)	C(13)-Fe(1)-C(14)	85.8(4)
O(10)-Cu(1)-N(1)	166.0(3)	O(15)-Ho(1)-O(10)	88.3(2)	N(12)-Fe(1)-C(11)	94.6(4)
N(2)-Cu(1)-N(17)	91.7(3)	O(14)-Ho(1)-O(10)	88.1(2)	C(15)-Fe(1)-C(11)	91.3(4)
O(9)-Cu(1)-N(17)	97.4(3)	O(2)-Ho(1)-O(10)	73.30(19)	C(12)-Fe(1)-C(11)	88.7(4)
O(10)-Cu(1)-N(17)	103.6(3)	O(15)-Ho(1)-O(13)	141.0(2)	C(13)-Fe(1)-C(11)	171.7(4)
N(1)-Cu(1)-N(17)	88.4(3)	O(14)-Ho(1)-O(13)	69.8(2)	C(14)-Fe(1)-C(11)	85.9(4)
N(4)-Cu(2)-O(2)	91.4(3)	O(2)-Ho(1)-O(13)	69.8(2)	N(20)-Fe(2)-C(17)	95.4(4)
N(4)-Cu(2)-O(1)	175.8(3)	O(10)-Ho(1)-O(13)	85.6(2)	N(20)-Fe(2)-C(19)	93.6(4)
O(2)-Cu(2)-O(1)	85.0(2)	O(15)-Ho(1)-O(4)	84.5(2)	C(17)-Fe(2)-C(19)	170.8(4)
N(4)-Cu(2)-N(3)	83.3(3)	O(14)-Ho(1)-O(4)	114.3(2)	N(20)-Fe(2)-C(16)	178.3(4)
O(2)-Cu(2)-N(3)	168.4(3)	O(2)-Ho(1)-O(4)	73.39(19)	C(17)-Fe(2)-C(16)	85.6(4)
O(1)-Cu(2)-N(3)	99.9(3)	O(10)-Ho(1)-O(4)	146.50(19)	C(19)-Fe(2)-C(16)	85.4(4)
N(6)-Cu(3)-O(4)	86.7(3)	O(13)-Ho(1)-O(4)	79.8(2)	N(20)-Fe(2)-C(20)	97.5(4)
N(6)-Cu(3)-N(5)	82.3(3)	O(15)-Ho(1)-O(6)	89.6(2)	C(17)-Fe(2)-C(20)	91.1(4)
O(4)-Cu(3)-N(5)	165.5(3)	O(14)-Ho(1)-O(6)	75.8(2)	C(19)-Fe(2)-C(20)	89.1(4)
N(6)-Cu(3)-O(3)	154.8(3)	O(2)-Ho(1)-O(6)	138.4(2)	C(16)-Fe(2)-C(20)	83.9(4)
O(4)-Cu(3)-O(3)	83.9(3)	O(10)-Ho(1)-O(6)	144.7(2)	N(20)-Fe(2)-C(18)	94.9(4)
N(5)-Cu(3)-O(3)	102.2(3)	O(13)-Ho(1)-O(6)	116.5(2)	C(17)-Fe(2)-C(18)	88.8(5)
N(6)-Cu(3)-N(11)	116.6(3)	O(4)-Ho(1)-O(6)	68.10(19)	C(19)-Fe(2)-C(18)	89.1(4)
O(4)-Cu(3)-N(11)	97.5(3)	O(15)-Ho(1)-O(8)	76.8(2)	C(16)-Fe(2)-C(18)	83.7(4)
N(5)-Cu(3)-N(11)	95.9(3)	O(14)-Ho(1)-O(8)	72.2(2)	C(20)-Fe(2)-C(18)	167.6(4)

O(3)-Cu(3)-N(11)	87.9(3)	O(2)-Ho(1)-O(8)	133.62(19)	O(20)-Na(1)-O(3)#1	94.5(3)
N(8)-Cu(4)-O(5)	175.4(3)	O(10)-Ho(1)-O(8)	72.80(18)	O(20)-Na(1)-O(21)	159.1(3)
N(8)-Cu(4)-O(6)	90.5(3)	O(13)-Ho(1)-O(8)	136.6(2)	O(3)#1-Na(1)-O(21)	106.3(2)
O(5)-Cu(4)-O(6)	85.1(2)	O(4)-Ho(1)-O(8)	136.13(18)	O(20)-Na(1)-N(13)	85.6(3)
N(8)-Cu(4)-N(7)	83.9(3)	O(6)-Ho(1)-O(8)	72.38(19)	O(3)#1-Na(1)-N(13)	91.0(3)
O(5)-Cu(4)-N(7)	100.6(3)	N(12)-Fe(1)-C(15)	96.2(5)	O(21)-Na(1)-N(13)	96.4(3)
O(6)-Cu(4)-N(7)	173.3(3)	N(12)-Fe(1)-C(12)	95.6(4)	O(20)-Na(1)-N(21)#2	89.5(3)
N(10)-Cu(5)-O(8)	91.9(3)	C(15)-Fe(1)-C(12)	168.2(5)	O(3)#1-Na(1)-N(21)#2	97.2(3)
N(10)-Cu(5)-O(7)	176.3(3)	N(12)-Fe(1)-C(13)	93.7(4)	O(21)-Na(1)-N(21)#2	85.5(3)
O(8)-Cu(5)-O(7)	85.0(2)	C(15)-Fe(1)-C(13)	88.2(4)	N(13)-Na(1)-N(21)#2	170.8(3)
N(10)-Cu(5)-N(9)	83.0(3)				

Symmetry codes for complex **4**: #1 -x, -y+1, -z+1; #2 x-1/2, -y+3/2, z+1/2; #3 x+1/2, -y+3/2, z-1/2. Symmetry codes for complex **5**: #1 -x+2, -y+2, -z+2 ; #2 x+1, -y+5/2, z+1/2; #3 x-1, -y+5/2, z-1/2. Symmetry codes for complex **6**: #1 -x+1, -y+1, -z+1; #2 x-1/2, -y+1/2, z+1/2; #3 x+1/2, -y+1/2, z-1/2. Symmetry codes for complex **7**: #1 -x+1, -y+1, -z+1; #2 x-1/2, -y+1/2, z+1/2; #3 x+1/2, -y+1/2, z-1/2. Symmetry codes for complex **8**: #1 -x+1, -y+1, -z+1; #2 x-1/2, -y+1/2, z+1/2; #3 x+1/2, -y+1/2, z-1/2.

Table S3. LnIII geometry analysis of 1-8 by SHAPE 2.1 software

Complex 1		**Complex 2**		**Complex 3**	
Geometry (CN = 9)	**La**	**Geometry (CN = 7)**	**Pr**	**Geometry (CN = 7)**	**Nd**
EP-9	36.678	EP-9	36.679	EP-9	36.855
OPY-9	22.549	OPY-9	22.328	OPY-9	22.710
HBPY-9	18.880	HBPY-9	18.889	HBPY-9	18.587
JTC-9	15.917	JTC-9	16.068	JTC-9	15.984
JCCU-9	10.745	JCCU-9	10.914	JCCU-9	10.778
CCU-9	9.655	CCU-9	9.774	CCU-9	9.595
JCSAPR-9	1.347	JCSAPR-9	1.359	JCSAPR-9	1.441
CSAPR-9	0.394	CSAPR-9	0.370	CSAPR-9	0.409
JTCTPR-9	2.531	JTCTPR-9	2.772	JTCTPR-9	2.760
TCTPR-9	1.036	TCTPR-9	1.223	TCTPR-9	1.150
JTDIC-9	12.711	JTDIC-9	12.948	JTDIC-9	12.760
HH-9	11.337	HH-9	11.079	HH-9	11.054
MFF-9	0.635	MFF-9	0.629	MFF-9	0.656
Complex 4		**Complex 5**		**Complex 6**	
Geometry (CN = 8)	**Sm**	**Geometry (CN = 8)**	**Eu**	**Geometry (CN = 8)**	**Tb**
OP-8	32.030	OP-8	31.725	OP-8	31.464
HPY-8	23.318	HPY-8	23.712	HPY-8	23.456
HBPY-8	16.134	HBPY-8	16.020	HBPY-8	16.090
CU-8	11.518	CU-8	11.442	CU-8	11.470
SAPR-8	2.485	SAPR-8	2.347	SAPR-8	2.262
TDD-8	1.951	TDD-8	1.845	TDD-8	1.832

JGBF-8	13.851	JGBF-8	13.903	JGBF-8	13.853
JETBPY-8	27.793	JETBPY-8	27.887	JETBPY-8	27.866
JBTPY-8	1.868	JBTPY-8	1.733	JBTPY-8	1.663
BTPR-8	1.062	BTPR-8	0.901	BTPR-8	0.895
JSD-8	4.157	JSD-8	4.039	JSD-8	3.992
TT-8	12.295	TT-8	12.239	TT-8	12.258
ETBPY-8	23.604	ETBPY-8	23.683	ETBPY-8	23.761
Complex 7					
Geometry (CN = 8)	Dy	**Geometry (CN = 8)**	**Dy**	**Geometry (CN = 8)**	**Dy**
OP-8	44.659	TDD-8	25.262	BTPR-8	24.589
HPY-8	36.167	JGBF-8	30.720	JSD-8	28.815
HBPY-8	32.167	JETBPY-8	42.264	TT-8	30.565
CU-8	31.723	JBTPR-8	26.470	ETBPY-8	38.484
SAPR-8	25.787				
Complex 8					
Geometry (CN = 8)	Ho	**Geometry (CN = 8)**	**Ho**	**Geometry (CN = 8)**	**Ho**
OP-8	31.717	TDD-8	1.931	BTPR-8	0.966
HPY-8	23.830	JGBF-8	13.550	JSD-8	3.833
HBPY-8	15.923	JETBPY-8	27.775	TT-8	12.255
CU-8	1.449	JBTPR-8	1.706	ETBPY-8	23.745
SAPR-8	2.344				

Table S4 Ln^{III} geometry analysis of 1-8 by SHAPE 2.1 software

Lable	**Shape**	**Lable**	**Shape**
EP-9	Enneagon (D_{9h})	OP-8	Octagon($D8_{h)}$
OPY-9	Octagonal pyramid (C_{8v})	HPY-8	Heptagonal pyramid(C_{7v})
HBPY-9	Heptagonal bipyramid(D_{7h})	HBPY-8	Hexagonal bipyramid(D_{6h})
JTC-9	Triangular cupola (J3) = trivacant cuboctahedron (C_{3v})	CU-8	Cube(O_h)
JCCU-9	Capped cube (Elongated square pyramid, J8) (C_{4v})	SAPR-8	Square antiprism(D_{4d})
CCU-9	Capped cube(C_{4v})	TDD-8	Triangular dodecahedron(D_{2d})
JCSAPR-9	Capped sq. antiprism (Gyroelongated square pyramid J10 (C_{4v})	JGBF-8	Johnson Gyrobifastigium J26 (D_{2d})
CSAPR-9	Capped square antiprism (C_{4v})	JETBPY-8	Johnson Elongated triangular bipyramid J14 (D3h)
JTCTPR-9	Tricapped trigonal prism J51 (D_{3h})	JBTP-8	Johnson Bisugmented trigonal prism J50 C_{2v}
TCTPR-9	Tricapped trigonal prism(D_{3h})	BTPR-8	Biaugmented trigonal prism (C_{2v})
JTDIC-9	Tridiminished icosahedron J63	JSD-8	Snub disphenoid J84 (D_{2d})

	(C_{3v})		
HH-9	Hula-hoop(C_{2v})	TT-8	Triakis tetrahedron
MFF-9	Muffin(C_s)	ETBPY-8	Elongated trigonal bipyramid (D_{3h})

Table S5. Ln-N and average Ln-O/N and Ln-O (ligand) bond lengths(Å)

Ln^{III}	La	Pr	Nd	Sm	Gd	Tb	Dy	Ho
Ln- N	2.592(6)	2.619(6)	2.637(7)	2.426(7)	2.386(8)	2.370(7)	2.365(11)	2.362(6)
Ln-O/N	2.533(3)	2.547(2)	2.580	2.435(8)	2.426(8)	2.413(4)	2.412(8)	2.417(8)
Ln-O	2.501(8)	2.506(4)	2.537(4)	2.434	2.422(7)	2.401(2)	2.403(1)	2.403(7)

Table S6 Ln-Cu_5 (ring) and Ln-O_5 (ring) distances

Ln^{III}	La	Pr	Nd	Sm	Gd	Tb	Dy	Ho
Ln-Cu_5	0.516	0.534	0.543	0.269	0.274	0.224	0.136	0.273
Ln-O_5	0.602	0.609	0.632	0.348	0.334	0.346	0.342	0.329

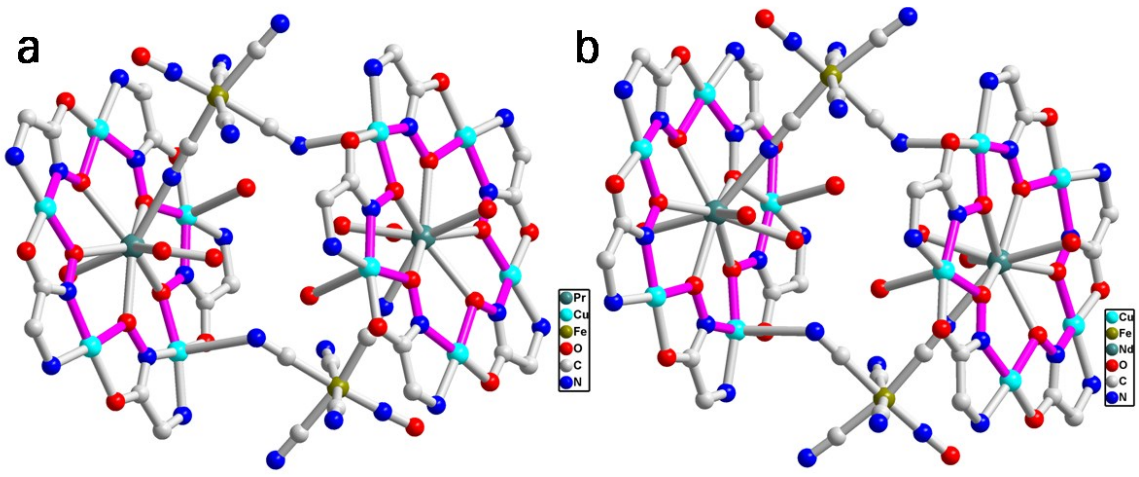

Figure S1 Crystal structures of complexes **2** (a) and **3** (b). All hydrogen atoms, non-coordinated nitrate ions and free water molecules are omitted for clarity of presentation. The coordinated water molecules are simplified as O.

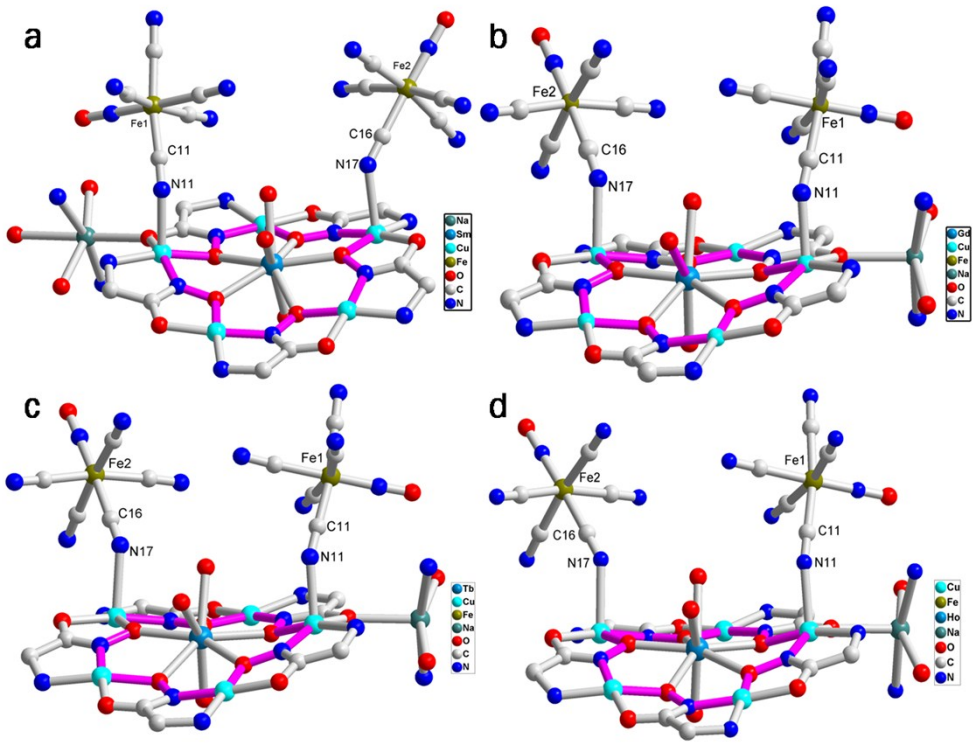

Figure S2 Crystal structures of complexes **4** - **6** (a-c) and **8** (d). All hydrogen atoms, non-coordinated nitrate ions and free water molecules are omitted for clarity of presentation. The coordinated water molecules are simplified as O.

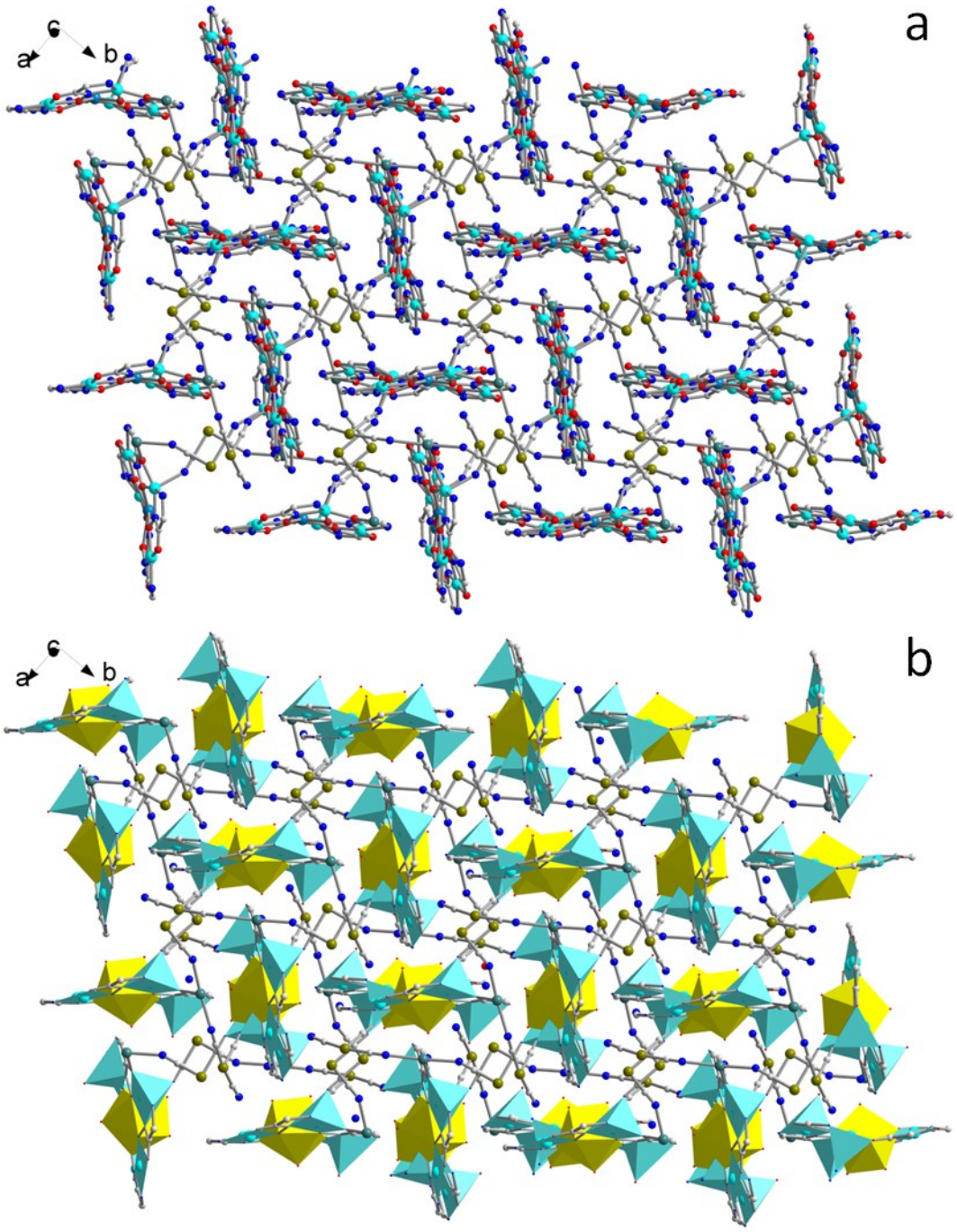

Figure S3. The two-dimensional framework (a) and polyhedron construction (b) of **7**.

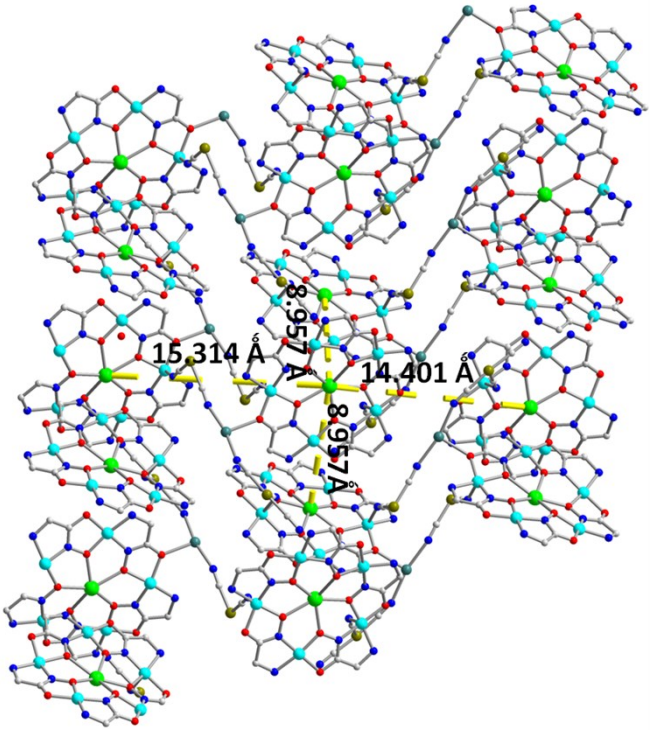

Figure S4. The Dy···Dy distances in the 2-dimensional framework.

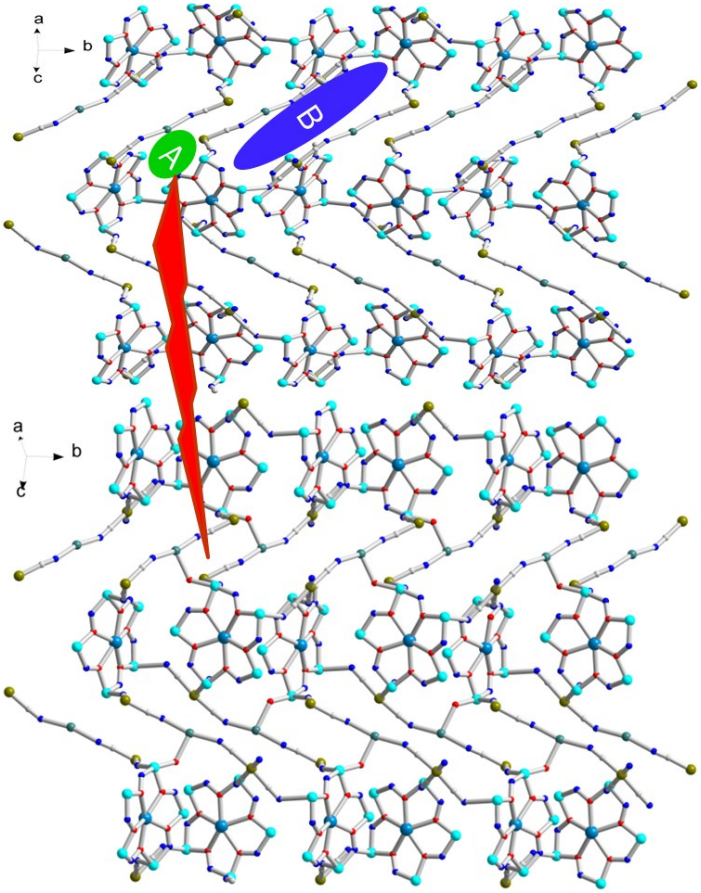

Figure S5. The pores distribution in complex **7** based on the bridging of $[Fe(CN)_5NO]^{2-}$ anions.

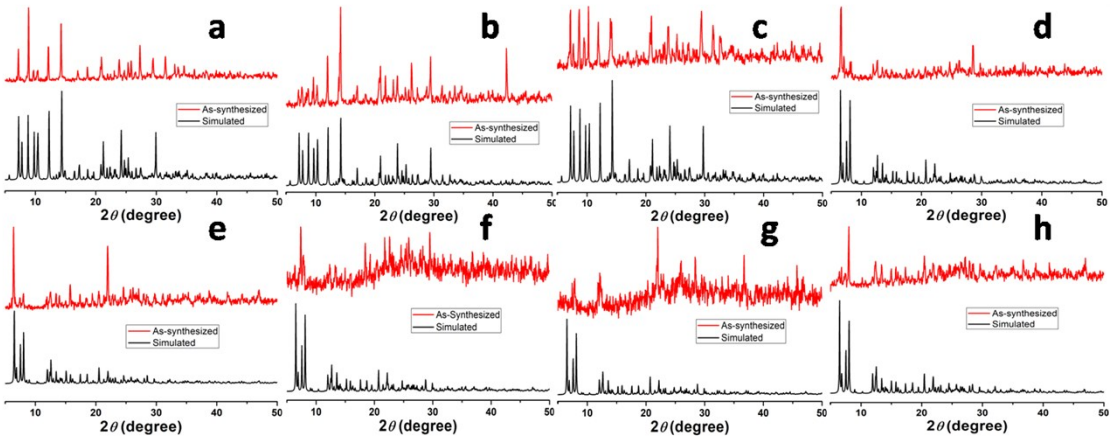

Figure S6. Powder XRD patterns of complexes **1-8** (a-h).

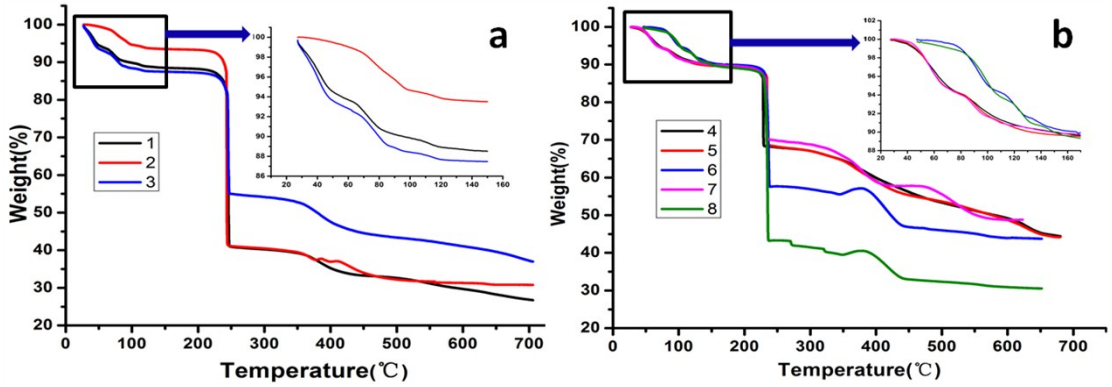

Figure S7. TGA curves for complexes **1-3** (a) and **4-8** (b).

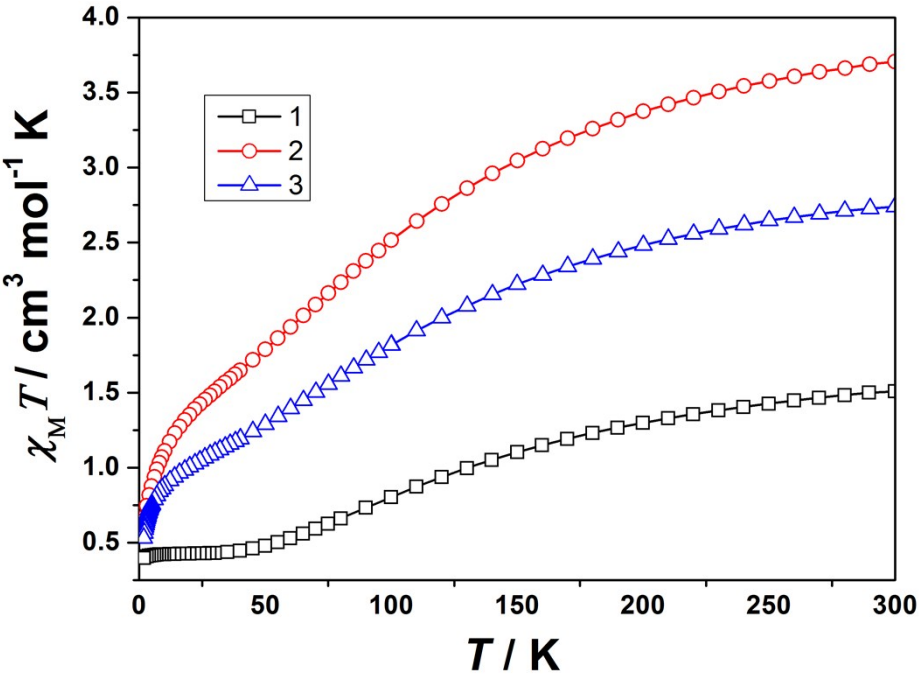

Figure S8 Temperature dependence of the $\chi_M T$ products for **1**-**3** with an applied 1 kOe

field.

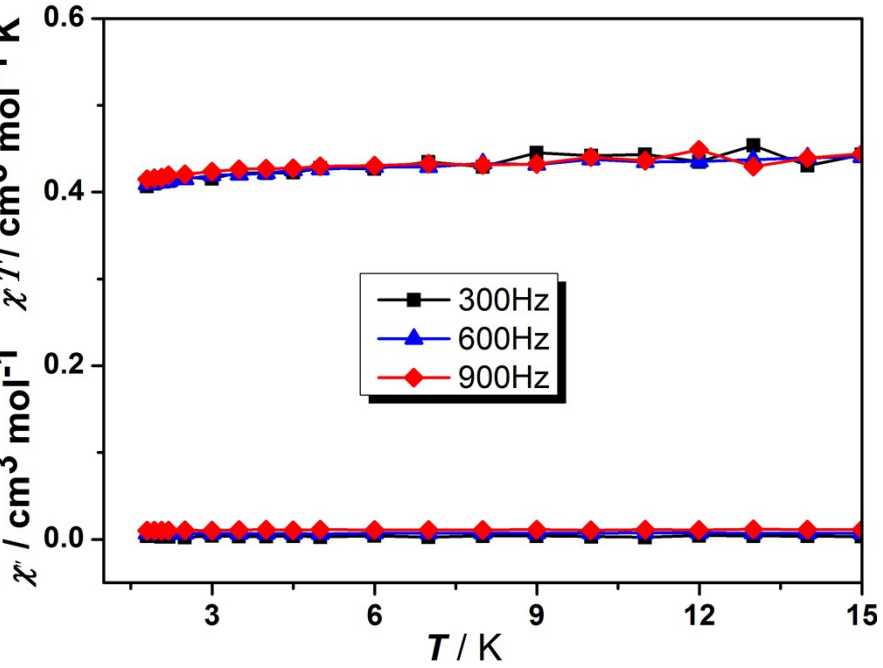

Figure S9 Temperature dependence of the in-phase χ′*T* and out-of-phase χ" ac susceptibilities between 300 and 900 Hz under zero dc field for **1**.

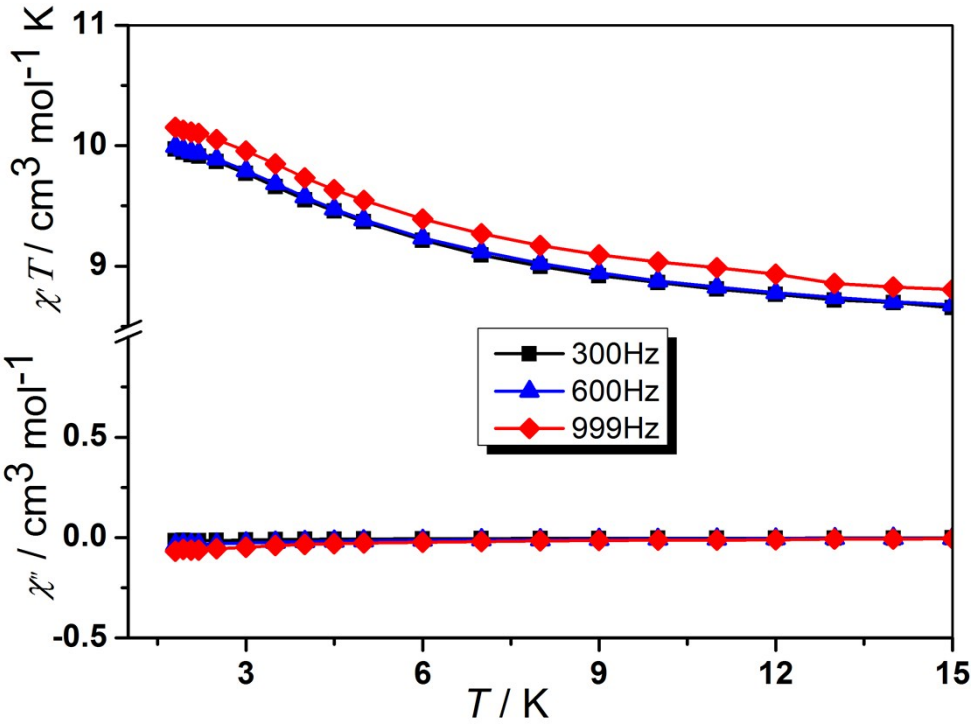

Figure S10 Temperature dependence of the in-phase χ′*T* and out-of-phase χ" ac susceptibilities

between 300 and 999 Hz under zero dc field for **5**.

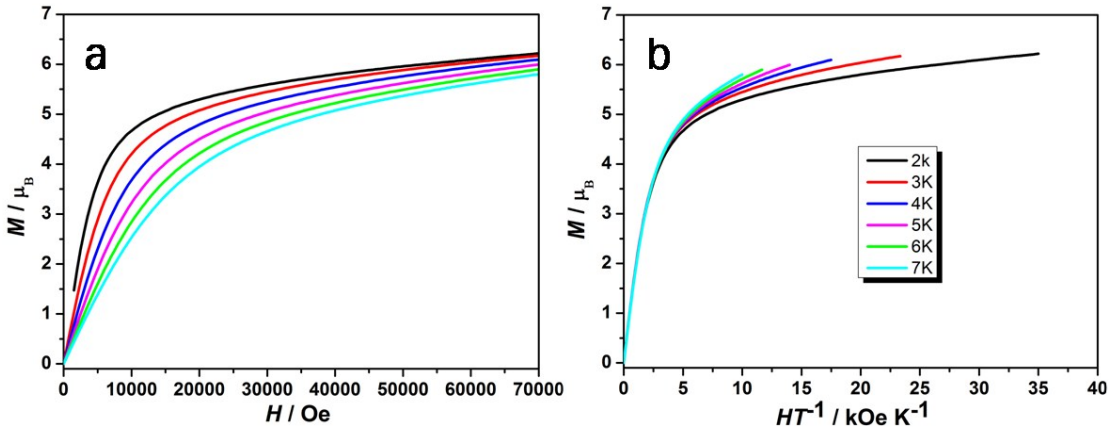

Figure S11 *M* vs. *H* plots (a) and *M vs*. *H/T* plots (b) at different temperatures between 1.8 and 8 K for **6**.

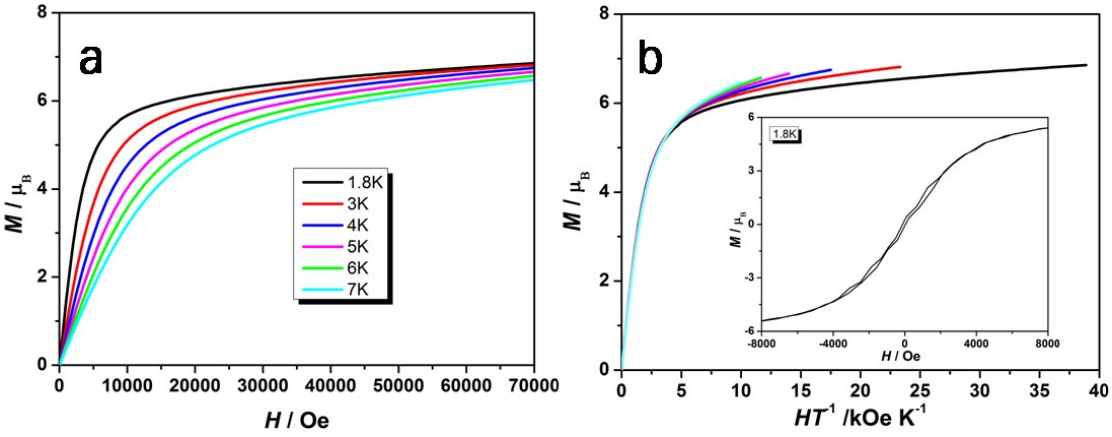

Figure S12 *M* vs. *H* plots (a) and *M vs*. *H/T* plots (b) at different temperatures between 1.8 and 8 K for **7**.

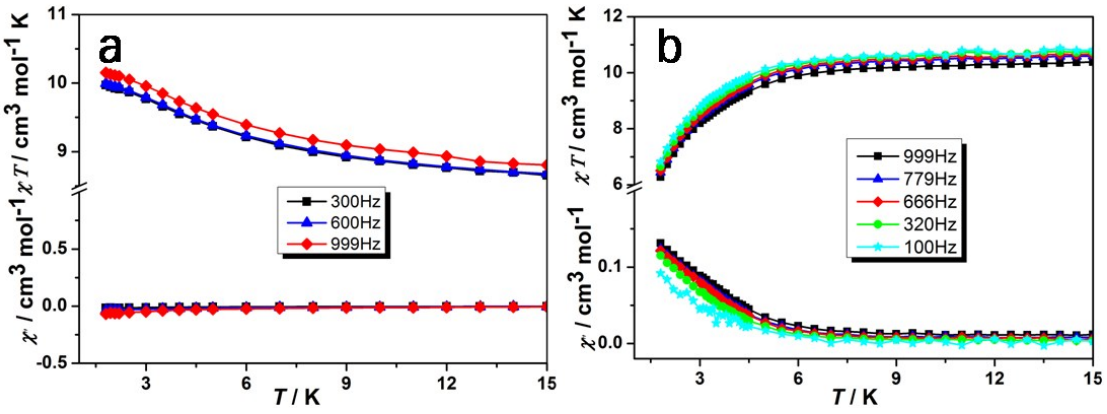

Figure S13 Temperature dependence of in-phase $\chi'T$ and out-of-phase χ" ac susceptibility between 300 and 999 Hz at H_{dc} = 0 Oe (a) and between 100 and 999 Hz at H_{dc} = 2 kOe (b) for **6**.

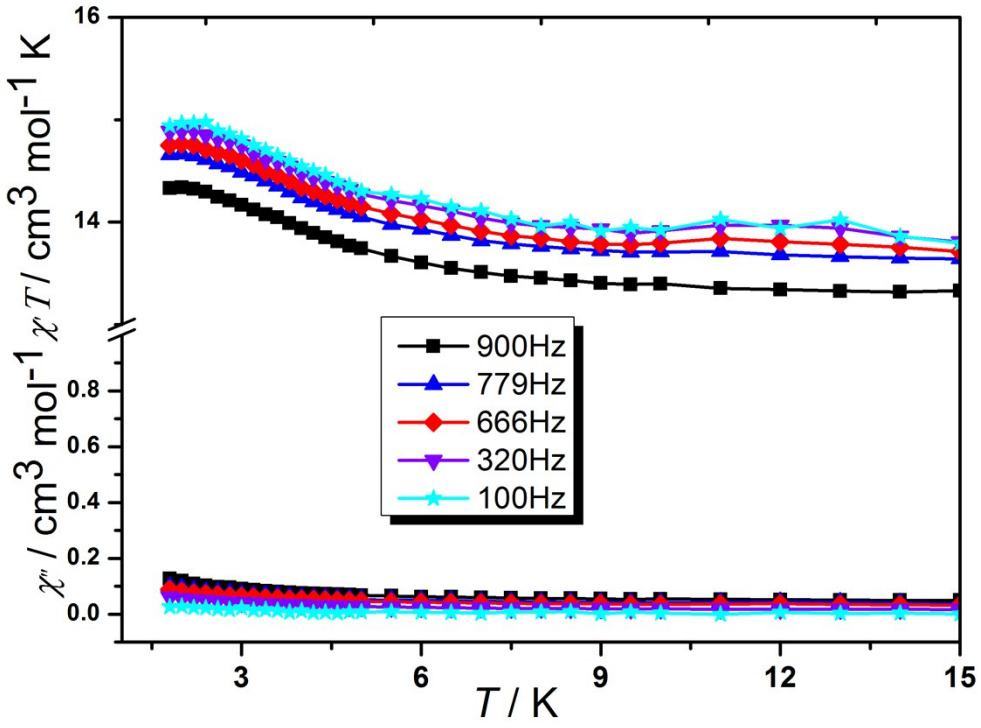

Figure S14 Temperature dependence of the in-phase χ' and out-of-phase χ" ac susceptibilities between 100 and 900 Hz at H_{dc} = 0 Oe for **7.**

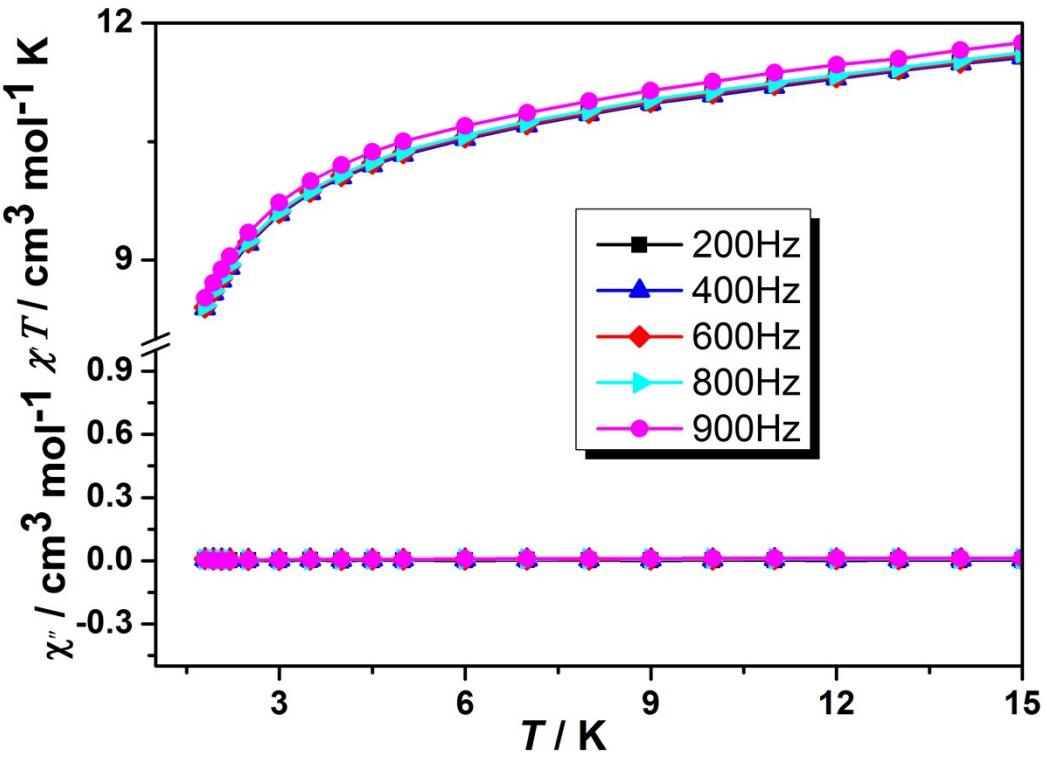

Figure S15 Temperature dependence of the in-phase χ′ and out-of-phase χ" ac susceptibilities between 200 and 900 Hz at H_{dc} = 0 Oe for **8.**