Supporting Information

Syntheses, Structures, and Properties of A Series of Novel High-Nuclear 3d-4f Clusters with Mixed Amino Acid as Ligands: $\{Ln_6Cu_{24}\}$(Ln = Gd, Tb, Pr and Sm)

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Table S1. Crystallographic data for compounds **1-4**.

	1	**2**
Empirical formula	$C_{42}H_{188}Cl_{18}Cu_{24}N_{18}O_{175}Gd_6$	$C_{42}H_{178}Cl_{18}Cu_{24}N_{18}O_{170}Tb_6$
Formula weight	6852.66	6772.6
Crystal size (mm)	0.25× 0.22 × 0.10	0.50 × 0.30 × 0.30
Crystal appearance	Blue Prism	Blue Prism
Crystal system	Triclinic	Triclinic
Space group	*P*-1	*P*-1
a (Å)	18.2095(4)	18.701
b (Å)	18.3542(6)	18.95590(10)
c (Å)	19.668	18.9616(3)
a (˚)	91.568(9)	118.643(3)
b (˚)	106.800(7)	103.281(8)
g (˚)	119.442(6)	95.222(6)
V (Å^3)	5365.8(2)	5579.90(9)
Z	1	1
D_c (Mg/m^3)	2.142	2.195
m (mm^{-1})	4.493	4.521
F (000)	3390	3608
Temperature (K)	293 (2)	293 (2)
Wavelength (Å)	0.71073	0.71073
q range (˚)	2.34-27.49	2.15-27.49
h, *k* and *l* ranges	-23≤ *h* ≤22	-23≤ *h* ≤24
	-23≤ *k* ≤ 23	-24≤ *k* ≤ 24
	-25 ≤ *l* ≤ 24	-23 ≤ *l* ≤ 24
Reflections measured	41408	70426
Independent reflections	22876	24652
Observed reflection (*I* > 2σ(*I*))	18016	22294

R_{int}	0.0271	0.0293
Min./max. trans.	0.6984 and 1.0000	0.4632 and 1.0000
Goodness of fit on F^2	1.090	1.038
Final R* indices ($I > 2\sigma(I)$)	$R1$ = 0.0742, $wR2$ = 0.2092	$R1$ = 0.0628, $wR2$ = 0.1953
Largest diff. peak and hole (e/Å^3)	2.676 and -1.889	2.744 and -2.098
	3	**4**
Empirical formula	$C_{46}H_{200}Cl_{18}Cu_{24}N_{18}O_{177}Pr_6$	$C_{46}H_{186}Cl_{18}Cu_{24}N_{18}O_{170}Sm_6$
Formula weight	6846.76	6777.29
Crystal size (mm)	0.30 × 0.20 × 0.15	0.50 × 0.30 × 0.20
Crystal appearance	Blue Prism	Blue Prism
Crystal system	Triclinic	Triclinic
Space group	*P*-1	*P*-1
a (Å)	18.793(5)	18.802(3)
b (Å)	19.154(6)	19.104(3)
c (Å)	19.170(5)	19.128(4)
a (˚)	118.791(7)	118.688(4)
b (˚)	95.852(12)	102.919(9)
g (˚)	102.806(16)	95.555(7)
V (Å^3)	5718(3)	5704.9(17)
Z	1	1
D_c (Mg/m^3)	1.993	2.009
m (mm^{-1})	3.755	4.026
F (000)	3384	3390
Temperature (K)	293 (2)	293 (2)
Wavelength (Å)	0.71073	0.71073
q range (˚)	2.29-25.00	2.14-25.50

h, k and l ranges	$-22 \leq h \leq 22$	$-19 \leq h \leq 22$
	$-18 \leq k \leq 22$	$-23 \leq k \leq 23$
	$-22 \leq l \leq 22$	$-23 \leq l \leq 22$
Reflections measured	35850	42409
Independent reflections	19043	21067
Observed reflection ($I > 2\sigma(I)$)	13355	18840
R_{int}	0.0542	0.0352
Min./max. trans.	0.4227 and 1.0000	0.6601 and 1.0000
Goodness of fit on F^2	1.076	1.029
Final R* indices ($I > 2\sigma(I)$)	$R1$ = 0.0894, $wR2$ =0.2239	$R1$ = 0.0749, $wR2$ = 0.2107

Table S2 Bond lengths (Å) and angles (°) for **1.**

Bond	Dist.(Å)	Bond	Dist.(Å)
Gd(1)-O(3)	2.429(6)	Cu(3)-O(22)	2.296(7)
Gd(1)-O(4)	2.429(6)	Cu(3)-O(114)#1	2.43(3)
Gd(1)-O(1)	2.434(6)	Cu(4)-O(8)#1	1.963(6)
Gd(1)-O(13)	2.450(6)	Cu(4)-O(3)	1.969(6)
Gd(1)-O(39)	2.468(7)	Cu(4)-O(7)	1.983(6)
Gd(1)-O(2)#1	2.499(6)	Cu(4)-O(4)	1.995(6)
Gd(1)-O(40)	2.500(8)	Cu(4)-O(24)	2.314(7)
Gd(1)-O(23)	2.540(6)	Cu(4)-O(114)#1	2.34(3)
Gd(1)-O(21)	2.579(7)	Cu(4)-O(113)	2.34(4)
Gd(1)-Cu(3)	3.4782(11)	Cu(4)-Gd(2)#1	3.5482(12)
Gd(1)-Cu(4)	3.4903(12)	Cu(5)-O(12)#1	1.972(6)
Gd(1)-Cu(1)	3.5336(10)	Cu(5)-O(6)	1.977(6)
Gd(2)-O(6)	2.419(6)	Cu(5)-O(11)	1.980(6)
Gd(2)-O(14)	2.442(6)	Cu(5)-O(8)	1.985(6)
Gd(2)-O(8)	2.445(6)	Cu(5)-O(114)	2.29(2)
Gd(2)-O(41)	2.455(8)	Cu(5)-O(30)	2.321(7)
Gd(2)-O(42)	2.461(7)	Cu(5)-O(111)#1	2.34(2)
Gd(2)-O(5)	2.464(6)	Cu(5)-Gd(3)#1	3.5396(12)
Gd(2)-O(7)#1	2.500(6)	Cu(6)-O(4)#1	1.967(6)
Gd(2)-O(29)	2.567(7)	Cu(6)-O(12)	1.967(6)
Gd(2)-O(27)	2.570(7)	Cu(6)-O(10)	1.982(6)
Gd(2)-Cu(1)	3.4784(10)	Cu(6)-O(2)	1.986(6)
Gd(2)-Cu(5)	3.4796(11)	Cu(6)-O(36)	2.334(7)

Gd(2)-Cu(2)	3.5357(11)	Cu(6)-O(113)#1	2.34(3)
Gd(3)-O(10)	2.418(6)	Cu(6)-O(111)	2.35(2)
Gd(3)-O(15)	2.441(7)	Cu(6)-Gd(1)#1	3.5373(11)
Gd(3)-O(12)	2.449(6)	Cu(7)-O(25)	1.936(9)
Gd(3)-O(9)	2.455(6)	Cu(7)-O(13)	1.966(8)
Gd(3)-O(44)	2.458(7)	Cu(7)-N(1)	1.971(14)
Gd(3)-O(43)	2.464(8)	Cu(7)-O(21)	1.973(6)
Gd(3)-O(11)#1	2.496(6)	Cu(7)-Cu(8)	2.999(2)
Gd(3)-O(33)	2.550(7)	Cu(8)-O(26)	1.925(9)
Gd(3)-O(35)	2.579(7)	Cu(8)-O(23)	1.953(7)
Gd(3)-Cu(6)	3.4764(12)	Cu(8)-O(13)	1.958(7)
Gd(3)-Cu(2)	3.4780(11)	Cu(8)-N(2)	1.968(12)
Gd(3)-Cu(5)#1	3.5397(12)	Cu(9)-O(31)	1.957(10)
Cu(1)-O(6)	1.965(6)	Cu(9)-O(14)	1.963(7)
Cu(1)-O(1)	1.968(6)	Cu(9)-N(4)	1.983(15)
Cu(1)-O(2)#1	1.971(6)	Cu(9)-O(27)	1.988(7)
Cu(1)-O(5)	1.991(6)	Cu(9)-Cu(10)	3.055(2)
Cu(1)-O(28)	2.315(7)	Cu(10)-O(32)	1.923(9)
Cu(1)-O(112)	2.32(3)	Cu(10)-O(14)	1.949(8)
Cu(1)-O(111)#1	2.41(3)	Cu(10)-N(5)	1.964(13)
Cu(2)-O(5)	1.950(6)	Cu(10)-O(29)	1.966(6)
Cu(2)-O(10)	1.965(6)	Cu(11)-O(37)	1.947(8)
Cu(2)-O(7)#1	1.980(6)	Cu(11)-O(33)	1.983(7)
Cu(2)-O(9)	1.984(6)	Cu(11)-N(7)	1.983(11)
Cu(2)-O(113)#1	2.30(4)	Cu(11)-O(15)	1.983(7)
Cu(2)-O(34)	2.306(8)	Cu(11)-Cu(12)	3.0173(19)
Cu(3)-O(9)	1.964(6)	Cu(12)-N(8)	1.940(11)
Cu(3)-O(3)	1.965(6)	Cu(12)-O(38)	1.956(8)
Cu(3)-O(11)#	1.970(6)	Cu(12)-O(15)	1.959(7)
Cu(3)-O(1)	1.972(6)	Cu(12)-O(35)	1.967(7)
Cu(3)-O(112)	2.23(3)		
Angle	(º)	Angle	(º)
Cu(1)-O(1)-Cu(3)	120.2(3)	Cu(6)-O(10)-Gd(3)	104.0(2)
Cu(1)-O(1)-Gd(1)	106.3(3)	Cu(3)#1-O(11)-Cu(5)	115.5(3)
Cu(3)-O(1)-Gd(1)	103.8(2)	Cu(3)#1-O(11)-Gd(3)#1	104.3(2)
Cu(1)#1-O(2)-Cu(6)	114.1(3)	Cu(5)-O(11)-Gd(3)#1	103.9(2)
Cu(1)#1-O(2)-Gd(1)#1	103.9(3)	Cu(6)-O(12)-Cu(5)#1	117.2(3)
Cu(6)-O(2)-Gd(1)#1	103.6(2)	Cu(6)-O(12)-Gd(3)	103.3(2)
Cu(3)-O(3)-Cu(4)	118.8(3)	Cu(5)#1-O(12)-Gd(3)	105.9(2)
Cu(3)-O(3)-Gd(1)	104.2(2)	Cu(8)-O(13)-Cu(7)	99.7(3)
Cu(4)-O(3)-Gd(1)	104.6(3)	Cu(8)-O(13)-Gd(1)	107.3(3)
Cu(6)#1-O(4)-Cu(4)	117.8(3)	Cu(7)-O(13)-Gd(1)	107.9(3)
Cu(6)#1-O(4)-Gd(1)	106.7(2)	Cu(10)-O(14)-Cu(9)	102.7(3)
Cu(4)-O(4)-Gd(1)	103.7(3)	Cu(10)-O(14)-Gd(2)	109.1(3)

Cu(2)-O(5)-Cu(1)	120.8(3)	Cu(9)-O(14)-Gd(2)	108.3(3)
Cu(2)-O(5)-Gd(2)	105.9(2)	Cu(12)-O(15)-Cu(11)	99.9(3)
Cu(1)-O(5)-Gd(2)	102.1(3)	Cu(12)-O(15)-Gd(3)	109.7(3)
Cu(1)-O(6)-Cu(5)	117.7(3)	Cu(11)-O(15)-Gd(3)	107.9(3)
Cu(1)-O(6)-Gd(2)	104.5(3)	Cu(7)-O(21)-Gd(1)	103.0(3)
Cu(5)-O(6)-Gd(2)	104.2(2)	Cu(8)-O(23)-Gd(1)	104.2(3)
Cu(2)#1-O(7)-Cu(4)	114.0(3)	Cu(9)-O(27)-Gd(2)	102.8(3)
Cu(2)#1-O(7)-Gd(2)#1	103.6(2)	Cu(10)-O(29)-Gd(2)	103.8(3)
Cu(4)-O(7)-Gd(2)#1	104.0(3)	Cu(11)-O(33)-Gd(3)	104.0(3)
Cu(4)#1-O(8)-Cu(5)	117.7(3)	Cu(12)-O(35)-Gd(3)	104.3(3)
Cu(4)#1-O(8)-Gd(2)	106.7(3)	Cu(7)-O(51)-Cu(8)	11.99(3)
Cu(5)-O(8)-Gd(2)	103.0(2)	Cu(5)#1-O(111)-Cu(6)	91.5(6)
Cu(4)#1-O(8)-Cu(5)	117.7(3)	Cu(5)#1-O(111)-Cu(1)#1	90.4(6)
Cu(4)#1-O(8)-Gd(2)	106.7(3)	Cu(6)-O(111)-Cu(1)#1	88.5(7)
Cu(5)-O(8)-Gd(2)	103.0(2)	Cu(3)-O(112)-Cu(1)	97.4(9)
Cu(3)-O(9)-Cu(2)	119.4(3)	Cu(2)#1-O(113)-Cu(4)	91.5(10)
Cu(3)-O(9)-Gd(3)	106.0(3)	Cu(2)#1-O(113)-Cu(6)#1	94.5(10)
Cu(2)-O(9)-Gd(3)	102.7(2)	Cu(4)-O(113)-Cu(6)#1	92.9(10)
Cu(2)-O(10)-Cu(6)	119.7(3)	Cu(5)-O(114)-Cu(4)#1	93.7(7)
Cu(2)-O(10)-Gd(3)	104.6(2)	Cu(5)-O(114)-Cu(3)#1	90.0(7)

Symmetry transformations used to generate equivalent atoms: #1 -x+1, -y+1, -z+1.

Table S3 Bond lengths (Å) and angles (°) for **2.**

Bond	Dist.(Å)	Bond	Dist.(Å)
Tb(1)-O(1)	2.398(5)	Cu(3)-O(9)#1	1.974(5)
Tb(1)-O(34)	2.402(6)	Cu(3)-O(18)	2.293(6)
Tb(1)-O(35)	2.407(6)	Cu(3)-O(111)	2.342(18)
Tb(1)-O(9)#1	2.416(5)	Cu(3)-O(113)#1	2.41(3)
Tb(1)-O(13)	2.416(5)	Cu(4)-O(4)	1.956(5)
Tb(1)-O(4)	2.424(5)	Cu(4)-O(10)	1.956(5)
Tb(1)-O(5)	2.451(5)	Cu(4)-O(12)	1.975(5)
Tb(1)-O(17)	2.517(5)	Cu(4)-O(5)	1.980(5)
Tb(1)-O(19)	2.528(6)	Cu(4)-O(112)#1	2.07(3)
Tb(1)-Cu(3)	3.4554(9)	Cu(4)-O(22)#1	2.279(6)
Tb(1)-Cu(1)	3.4557(8)	Cu(4)-Tb(3)#1	3.4611(9)
Tb(1)-Cu(5)#1	3.5104(10)	Cu(5)-O(7)	1.961(5)
Tb(2)-O(7)	2.397(5)	Cu(5)-O(9)	1.961(5)
Tb(2)-O(14)	2.399(5)	Cu(5)-O(6)	1.971(5)
Tb(2)-O(37)	2.405(6)	Cu(5)-O(5)#1	1.975(5)
Tb(2)-O(36)	2.417(6)	Cu(5)-O(114)#1	2.21(4)
Tb(2)-O(11)#1	2.418(5)	Cu(5)-O(24)	2.296(5)

Tb(2)-O(6)	2.425(5)	Cu(5)-Tb(1)#1	3.5104(10)
Tb(2)-O(2)	2.461(5)	Cu(6)-O(7)#1	1.956(5)
Tb(2)-O(25)	2.524(5)	Cu(6)-O(12)#1	1.957(5)
Tb(2)-O(27)	2.556(6)	Cu(6)-O(11)	1.978(5)
Tb(2)-Cu(6)#1	3.4478(9)	Cu(6)-O(8)	1.979(5)
Tb(2)-Cu(5)	3.4540(10)	Cu(6)-O(113)#1	2.10(4)
Tb(2)-Cu(2)	3.5023(9)	Cu(6)-O(26)#1	2.295(6)
Tb(3)-O(10)#1	2.391(5)	Cu(6)-Tb(2)#1	3.4478(9)
Tb(3)-O(38)	2.402(6)	Cu(7)-O(28)	1.958(7)
Tb(3)-O(15)	2.414(5)	Cu(7)-O(13)	1.964(6)
Tb(3)-O(3)	2.420(5)	Cu(7)-N(1)	1.971(10)
Tb(3)-O(12)#1	2.423(5)	Cu(7)-O(17)	1.983(5)
Tb(3)-O(39)	2.439(6)	Cu(7)-Cu(8)	3.0119(17)
Tb(3)-O(8)	2.471(5)	Cu(8)-O(29)	1.959(7)
Tb(3)-O(23)	2.529(5)	Cu(8)-O(13)	1.961(6)
Tb(3)-O(21)	2.540(6)	Cu(8)-O(19)	1.978(5)
Tb(3)-Cu(2)	3.4479(9)	Cu(8)-N(2)	1.980(10)
Tb(3)-Cu(4)#1	3.4611(9)	Cu(9)-O(32)	1.935(6)
Tb(3)-Cu(6)	3.5084(9)	Cu(9)-O(14)	1.963(5)
Cu(1)-O(11)#1	1.948(5)	Cu(9)-O(25)	1.964(5)
Cu(1)-O(1)	1.955(5)	Cu(9)-N(5)	1.966(9)
Cu(1)-O(2)	1.970(5)	Cu(9)-Cu(10)	3.0196(14)
Cu(1)-O(4)	1.974(5)	Cu(10)-O(14)	1.955(6)
Cu(1)-O(16)	2.294(6)	Cu(10)-N(6)	1.987(13)
Cu(1)-O(111)	2.338(18)	Cu(10)-O(33)	1.986(7)
Cu(1)-O(112)#1	2.40(4)	Cu(10)-O(27)	1.991(6)
Cu(2)-O(6)	1.953(5)	Cu(11)-O(31)	1.955(7)
Cu(2)-O(10)#1	1.958(5)	Cu(11)-O(15)	1.963(6)
Cu(2)-O(2)	1.973(5)	Cu(11)-O(23)	1.977(6)
Cu(2)-O(3)	1.975(5)	Cu(11)-N(4)	1.982(9)
Cu(2)-O(20)	2.279(6)	Cu(11)-Cu(12)	3.0173(16)
Cu(2)-O(114)#1	2.32(3)	Cu(12)-O(15)	1.961(6)
Cu(2)-O(111)	2.347(18)	Cu(12)-O(30)	1.965(6)
Cu(3)-O(3)	1.948(5)	Cu(12)-O(21)	1.996(5)
Cu(3)-O(1)	1.959(5)	Cu(12)-N(3)	2.002(12)
Cu(3)-O(8)	1.970(5)	Cu(12)-O(131)	2.388(12)
Angle	(º)	Angle	(º)
Cu(1)-O(1)-Cu(3)	119.7(2)	Cu(2)#1-O(10)-Tb(3)#1	104.5(2)
Cu(1)-O(1)-Tb(1)	104.6(2)	Cu(1)#1-O(11)-Cu(6)	120.1(3)
Cu(3)-O(1)-Tb(1)	104.5(2)	Cu(1)#1-O(11)-Tb(2)#1	106.3(2)
Cu(1)-O(2)-Cu(2)	115.5(2)	Cu(6)-O(11)-Tb(2)#1	102.86(19)
Cu(1)-O(2)-Tb(2)	104.0(2)	Cu(6)#1-O(12)-Cu(4)	120.2(3)
Cu(2)-O(2)-Tb(2)	103.82(19)	Cu(6)#1-O(12)-Tb(3)#1	106.0(2)
Cu(3)-O(3)-Cu(2)	119.2(3)	Cu(4)-O(12)-Tb(3)#1	103.3(2)

Cu(3)-O(3)-Tb(3)	106.5(2)	Cu(8)-O(13)-Cu(7)	100.2(3)
Cu(2)-O(3)-Tb(3)	102.9(2)	Cu(8)-O(13)-Tb(1)	108.5(2)
Cu(4)-O(4)-Cu(1)	120.1(2)	Cu(7)-O(13)-Tb(1)	108.5(2)
Cu(4)-O(4)-Tb(1)	106.2(2)	Cu(10)-O(14)-Cu(9)	100.8(3)
Cu(1)-O(4)-Tb(1)	103.1(2)	Cu(10)-O(14)-Tb(2)	110.0(2)
Cu(5)#1-O(5)-Cu(4)	115.1(2)	Cu(9)-O(14)-Tb(2)	108.0(2)
Cu(5)#1-O(5)-Tb(1)	104.5(2)	Cu(12)-O(15)-Cu(11)	100.5(2)
Cu(4)-O(5)-Tb(1)	104.4(2)	Cu(12)-O(15)-Tb(3)	108.9(2)
Cu(2)-O(6)-Cu(5)	119.8(2)	Cu(11)-O(15)-Tb(3)	108.6(2)
Cu(2)-O(6)-Tb(2)	105.7(2)	Cu(7)-O(17)-Tb(1)	104.2(2)
Cu(5)-O(6)-Tb(2)	103.1(2)	Cu(8)-O(19)-Tb(1)	103.8(2)
Cu(6)#1-O(7)-Cu(5)	120.2(2)	Cu(12)-O(21)-Tb(3)	103.1(2)
Cu(6)#1-O(7)-Tb(2)	104.3(2)	Cu(11)-O(23)-Tb(3)	103.9(2)
Cu(5)-O(7)-Tb(2)	104.4(2)	Cu(9)-O(25)-Tb(2)	103.3(2)
Cu(3)-O(8)-Cu(6)	115.6(3)	Cu(10)-O(27)-Tb(2)	103.0(2)
Cu(3)-O(8)-Tb(3)	103.9(2)	Cu(1)-O(111)-Cu(3)	92.6(6)
Cu(6)-O(8)-Tb(3)	103.5(2)	Cu(1)-O(111)-Cu(2)	90.7(5)
Cu(5)-O(9)-Cu(3)#1	118.5(2)	Cu(3)-O(111)-Cu(2)	92.3(6)
Cu(5)-O(9)-Tb(1)#1	106.2(2)	Cu(4)#1-O(112)-Cu(1)#1	99.1(7)
Cu(3)#1-O(9)-Tb(1)#1	103.4(2)	Cu(6)#1-O(113)-Cu(3)#1	95.4(8)
Cu(4)-O(10)-Cu(2)#1	119.5(3)	Cu(5)#1-O(114)-Cu(2)#1	97.1(6)
Cu(4)-O(10)-Tb(3)#1	105.1(2)		

Symmetry transformations used to generate equivalent atoms: #1 -x, -y+1, -z+1.

Table S4 Bond lengths (Å) and angles (°) for **3.**

Bond	Dist.(Å)	Bond	Dist.(Å)
Pr(1)-O(1)	2.457(8)	Cu(3)-O(113)#1	2.29(3)
Pr(1)-O(13)	2.460(8)	Cu(3)-O(22)	2.293(9)
Pr(1)-O(3)	2.482(8)	Cu(3)-O(114)	2.35(4)
Pr(1)-O(2)#1	2.496(8)	Cu(4)-O(3)#1	1.949(9)
Pr(1)-O(41)	2.513(10)	Cu(4)-O(8)	1.964(8)
Pr(1)-O(42)	2.531(9)	Cu(4)-O(7)	1.977(9)
Pr(1)-O(4)#1	2.532(8)	Cu(4)-O(4)	1.986(8)
Pr(1)-O(23)	2.605(10)	Cu(4)-O(26)	2.301(9)
Pr(1)-O(21)	2.647(8)	Cu(4)-O(114)#1	2.31(3)
Pr(1)-Cu(3)	3.4859(16)	Cu(4)-O(111)#1	2.359(18)
Pr(1)-Cu(1)	3.5068(17)	Cu(4)-Pr(1)#1	3.5588(18)
Pr(1)-Cu(4)#1	3.5588(18)	Cu(5)-O(12)	1.951(8)
Pr(2)-O(8)	2.445(8)	Cu(5)-O(8)	1.956(8)
Pr(2)-O(14)	2.464(8)	Cu(5)-O(11)	1.959(8)
Pr(2)-O(7)	2.471(8)	Cu(5)-O(6)	1.989(9)
Pr(2)-O(6)	2.496(8)	Cu(5)-O(28)	2.294(9)

Pr(2)-O(43)	2.508(10)	Cu(5)-O(114)#1	2.33(5)
Pr(2)-O(5)	2.514(8)	Cu(5)-O(112)	2.39(5)
Pr(2)-O(44)	2.523(10)	Cu(5)-Pr(3)#1	3.5574(18)
Pr(2)-O(27)	2.584(9)	Cu(6)-O(2)	1.957(8)
Pr(2)-O(25)	2.605(9)	Cu(6)-O(10)	1.959(8)
Pr(2)-Cu(4)	3.4962(18)	Cu(6)-O(12)#1	1.970(8)
Pr(2)-Cu(5)	3.4991(18)	Cu(6)-O(4)	1.980(8)
Pr(2)-Cu(2)	3.5588(18)	Cu(6)-O(112)#1	2.28(3)
Pr(3)-O(10)	2.439(7)	Cu(6)-O(30)	2.308(9)
Pr(3)-O(15)	2.459(8)	Cu(6)-O(111)	2.371(18)
Pr(3)-O(12)#	2.472(8)	Cu(6)-Pr(1)#1	3.5616(19)
Pr(3)-O(9)	2.473(7)	Cu(7)-O(33)	1.912(10)
Pr(3)-O(45)	2.504(9)	Cu(7)-O(13)	1.956(9)
Pr(3)-O(11)#1	2.518(8)	Cu(7)-N(1)	1.965(16)
Pr(3)-O(46)	2.522(9)	Cu(7)-O(23)	1.968(9)
Pr(3)-O(31)	2.578(10)	Cu(7)-Cu(8)	3.051(3)
Pr(3)-O(29)	2.648(9)	Cu(8)-N(2)	1.942(13)
Pr(3)-Cu(6)	3.4917(19)	Cu(8)-O(13)	1.951(8)
Pr(3)-Cu(2)	3.4962(18)	Cu(8)-O(34)	1.956(10)
Pr(3)-Cu(3)	3.5570(17)	Cu(8)-O(21)	2.003(8)
Cu(1)-O(1)	1.942(8)	Cu(9)-O(39)	1.930(15)
Cu(1)-O(6)	1.950(8)	Cu(9)-O(14)	1.968(9)
Cu(1)-O(2)#1	1.973(8)	Cu(9)-N(3)	1.97(2)
Cu(1)-O(5)	1.993(9)	Cu(9)-O(27)	1.981(9)
Cu(1)-O(112)	2.32(4)	Cu(9)-Cu(10)	3.044(3)
Cu(1)-O(24)	2.326(10)	Cu(10)-O(14)	1.954(10)
Cu(1)-O(113)#1	2.39(3)	Cu(10)-O(25)	1.982(9)
Cu(2)-O(7)	1.959(8)	Cu(10)-O(40)	2.030(16)
Cu(2)-O(9)	1.972(8)	Cu(10)-N(4)	2.11(2)
Cu(2)-O(5)	1.977(8)	Cu(11)-N(5)	1.87(2)
Cu(2)-O(10)	1.977(8)	Cu(11)-O(15)	1.942(9)
Cu(2)-O(32)	2.313(10)	Cu(11)-O(37)	1.945(12)
Cu(2)-O(113)#1	2.32(2)	Cu(11)-O(31)	1.988(9)
Cu(2)-O(111)	2.358(17)	Cu(11)-Cu(12)	3.037(3)
Cu(3)-O(9)	1.964(8)	Cu(12)-O(38)	1.956(12)
Cu(3)-O(1)	1.964(8)	Cu(12)-O(15)	1.971(9)
Cu(3)-O(11)#1	1.977(8)	Cu(12)-N(6)	1.972(15)
Cu(3)-O(3)	1.982(8)	Cu(12)-O(29)	2.008(9)
Angle	(º)	Angle	(º)
Cu(1)-O(1)-Cu(3)	119.9(4)	Cu(3)#1-O(11)-Pr(3)#1	103.9(4)
Cu(1)-O(1)-Pr(1)	105.1(3)	Cu(5)-O(12)-Cu(6)#1	119.6(4)
Cu(3)-O(1)-Pr(1)	103.5(3)	Cu(5)-O(12)-Pr(3)#1	106.5(3)
Cu(6)-O(2)-Cu(1)#1	119.1(4)	Cu(6)#1-O(12)-Pr(3)#1	103.0(3)
Cu(6)-O(2)-Pr(1)#1	105.6(4)	Cu(8)-O(13)-Cu(7)	102.7(4)

Cu(1)#1-O(2)-Pr(1)#1	102.8(3)	Cu(8)-O(13)-Pr(1)	110.2(3)
Cu(4)#1-O(3)-Cu(3)	118.0(4)	Cu(7)-O(13)-Pr(1)	109.0(4)
Cu(4)#1-O(3)-Pr(1)	106.2(3)	Cu(10)-O(14)-Cu(9)	101.8(4)
Cu(3)-O(3)-Pr(1)	102.1(3)	Cu(10)-O(14)-Pr(2)	109.3(4)
Cu(6)-O(4)-Cu(4)	115.2(4)	Cu(9)-O(14)-Pr(2)	108.5(4)
Cu(6)-O(4)-Pr(1)#1	103.6(3)	Cu(11)-O(15)-Cu(12)	101.8(4)
Cu(4)-O(4)-Pr(1)#1	103.3(3)	Cu(11)-O(15)-Pr(3)	108.7(4)
Cu(2)-O(5)-Cu(1)	114.8(4)	Cu(12)-O(15)-Pr(3)	109.0(3)
Cu(2)-O(5)-Pr(2)	104.2(3)	Cu(8)-O(21)-Pr(1)	101.7(3)
Cu(1)-O(5)-Pr(2)	104.2(3)	Cu(7)-O(23)-Pr(1)	103.3(4)
Cu(1)-O(6)-Cu(5)	118.8(4)	Cu(10)-O(25)-Pr(2)	103.2(4)
Cu(1)-O(6)-Pr(2)	106.2(4)	Cu(9)-O(27)-Pr(2)	103.6(4)
Cu(5)-O(6)-Pr(2)	102.0(3)	Cu(12)-O(29)-Pr(3)	101.0(4)
Cu(2)-O(7)-Cu(4)	118.0(4)	Cu(11)-O(31)-Pr(3)	102.9(4)
Cu(2)-O(7)-Pr(2)	106.4(3)	Cu(2)-O(111)-Cu(4)	91.3(5)
Cu(4)-O(7)-Pr(2)	103.1(3)	Cu(2)-O(111)-Cu(6)	91.9(5)
Cu(5)-O(8)-Cu(4)	119.2(4)	Cu(4)-O(111)-Cu(6)	90.1(5)
Cu(5)-O(8)-Pr(2)	104.8(3)	Cu(6)#1-O(112)-Cu(1)	95.0(10)
Cu(4)-O(8)-Pr(2)	104.4(3)	Cu(6)#1-O(112)-Cu(5)	93.1(12)
Cu(3)-O(9)-Cu(2)	118.6(4)	Cu(1)-O(112)-Cu(5)	92.2(12)
Cu(3)-O(9)-Pr(3)	106.0(3)	Cu(3)#1-O(113)-Cu(2)#1	94.4(8)
Cu(2)-O(9)-Pr(3)	103.2(3)	Cu(3)#1-O(113)-Cu(1)#1	92.3(8)
Cu(6)-O(10)-Cu(2)	119.3(4)	Cu(2)#1-O(113)-Cu(1)#1	90.3(8)
Cu(6)-O(10)-Pr(3)	104.6(3)	Cu(4)#1-O(114)-Cu(5)#1	93.5(11)
Cu(2)-O(10)-Pr(3)	104.2(3)	Cu(4)#1-O(114)-Cu(3)	92.7(11)
Cu(5)-O(11)-Cu(3)#1	116.3(4)	Cu(5)#1-O(114)-Cu(3)	91.1(11)
Cu(5)-O(11)-Pr(3)#1	104.5(3)		

Symmetry transformations used to generate equivalent atoms: #1 -x, -y−1, -z+1.

Table S5 Bond lengths (Å) and angles (°) for **4.**

Bond	Dist.(Å)	Bond	Dist.(Å)
Sm(1)-O(13)	2.427(7)	Cu(3)-O(14)	1.985(7)
Sm(1)-O(10)	2.442(7)	Cu(3)-O(23)	2.304(8)
Sm(1)-O(6)	2.447(7)	Cu(3)-O(113)	2.32(3)
Sm(1)-O(4)	2.448(7)	Cu(3)-O(111)#1	2.37(2)
Sm(1)-O(16)	2.464(8)	Cu(3)-Sm(3)#1	3.5372(13)
Sm(1)-O(17)	2.475(8)	Cu(4)-O(5)	1.953(7)
Sm(1)-O(2)	2.492(6)	Cu(4)-O(7)#1	1.972(7)
Sm(1)-O(24)	2.565(7)	Cu(4)-O(14)	1.978(6)
Sm(1)-O(22)	2.569(7)	Cu(4)-O(15)#1	1.983(7)
Sm(1)-Cu(2)	3.4749(13)	Cu(4)-O(27)	2.289(8)
Sm(1)-Cu(3)	3.4756(13)	Cu(4)-O(114)#1	2.34(4)

Sm(1)-Cu(1)	3.5343(14)	Cu(4)-O(113)	2.36(3)
Sm(2)-O(5)	2.419(6)	Cu(4)-Sm(3)#1	3.5360(14)
Sm(2)-O(11)	2.422(7)	Cu(5)-O(3)	1.960(7)
Sm(2)-O(1)	2.438(6)	Cu(5)-O(1)	1.968(7)
Sm(2)-O(15)#1	2.451(6)	Cu(5)-O(9)	1.977(7)
Sm(2)-O(18)	2.462(8)	Cu(5)-O(8)	1.980(7)
Sm(2)-O(19)	2.478(7)	Cu(5)-O(33)	2.287(7)
Sm(2)-O(8)	2.491(7)	Cu(5)-O(112)#1	2.29(2)
Sm(2)-O(28)	2.576(8)	Cu(5)-O(111)	2.30(2)
Sm(2)-O(26)	2.609(7)	Cu(6)-O(6)	1.957(6)
Sm(2)-Cu(4)	3.4665(14)	Cu(6)-O(3)	1.964(6)
Sm(2)-Cu(1)	3.4728(14)	Cu(6)-O(7)	1.970(7)
Sm(2)-Cu(5)	3.5260(13)	Cu(6)-O(2)	1.992(7)
Sm(3)-O(3)	2.418(6)	Cu(6)-O(31)	2.300(7)
Sm(3)-O(12)	2.446(7)	Cu(6)-O(114)	2.31(4)
Sm(3)-O(9)	2.449(6)	Cu(6)-O(112)#1	2.42(3)
Sm(3)-O(7)	2.460(6)	Cu(7)-N(1)	1.964(14)
Sm(3)-O(20)	2.460(8)	Cu(7)-O(34)	1.977(11)
Sm(3)-O(14)#1	2.486(7)	Cu(7)-O(10)	1.977(8)
Sm(3)-O(21)	2.501(8)	Cu(7)-O(22)	1.981(7)
Sm(3)-O(30)	2.568(8)	Cu(7)-Cu(8)	3.031(2)
Sm(3)-O(32)	2.605(7)	Cu(8)-O(35)	1.934(11)
Sm(3)-Cu(5)	3.4654(13)	Cu(8)-O(10)	1.968(8)
Sm(3)-Cu(6)	3.4815(13)	Cu(8)-O(24)	1.980(7)
Sm(3)-Cu(4)#1	3.5360(14)	Cu(8)-N(2)	1.997(16)
Cu(1)-O(4)	1.959(7)	Cu(9)-O(11)	1.964(7)
Cu(1)-O(1)	1.960(7)	Cu(9)-N(3)	1.965(13)
Cu(1)-O(5)	1.965(6)	Cu(9)-O(36)	1.993(10)
Cu(1)-O(2)	1.981(7)	Cu(9)-O(26)	2.003(7)
Cu(1)-O(29)	2.308(8)	Cu(9)-Cu(10)	3.036(2)
Cu(1)-O(113)	2.33(3)	Cu(10)-N(4)	1.946(13)
Cu(1)-O(112)#1	2.34(3)	Cu(10)-O(37)	1.954(9)
Cu(2)-O(15)	1.949(7)	Cu(10)-O(11)	1.971(8)
Cu(2)-O(13)	1.957(7)	Cu(10)-O(28)	1.971(7)
Cu(2)-O(8)#1	1.975(7)	Cu(11)-O(12)	1.949(8)
Cu(2)-O(6)	1.981(7)	Cu(11)-O(38)	1.953(8)
Cu(2)-O(25)	2.307(8)	Cu(11)-N(5)	1.967(13)
Cu(2)-O(114)	2.32(4)	Cu(11)-O(30)	1.974(7)
Cu(2)-O(111)#1	2.36(3)	Cu(11)-Cu(12)	3.047(2)
Cu(2)-Sm(2)#1	3.5307(13)	Cu(12)-N(6)	1.948(11)
Cu(3)-O(9)#1	1.957(7)	Cu(12)-O(12)	1.954(7)
Cu(3)-O(13)	1.966(7)	Cu(12)-O(39)	1.976(8)
Cu(3)-O(4)	1.976(7)	Cu(12)-O(32)	1.997(7)
Angle	(º)	Angle	(º)

Cu(1)-O(1)-Sm(2)	103.8(3)	Cu(10)-O(11)-Sm(2)	108.3(3)
Cu(5)-O(1)-Sm(2)	105.8(3)	Cu(11)-O(12)-Cu(12)	102.7(4)
Cu(1)-O(2)-Cu(6)	114.2(3)	Cu(11)-O(12)-Sm(3)	109.1(3)
Cu(1)-O(2)-Sm(1)	103.8(3)	Cu(12)-O(12)-Sm(3)	109.5(3)
Cu(6)-O(2)-Sm(1)	103.7(3)	Cu(2)-O(13)-Cu(3)	118.6(3)
Cu(5)-O(3)-Cu(6)	118.6(3)	Cu(2)-O(13)-Sm(1)	104.4(3)
Cu(5)-O(3)-Sm(3)	104.2(3)	Cu(3)-O(13)-Sm(1)	104.1(3)
Cu(6)-O(3)-Sm(3)	104.7(3)	Cu(4)-O(14)-Cu(3)	114.9(3)
Cu(1)-O(4)-Cu(3)	118.0(3)	Cu(4)-O(14)-Sm(3)#1	104.2(3)
Cu(1)-O(4)-Sm(1)	106.1(3)	Cu(3)-O(14)-Sm(3)#1	104.0(3)
Cu(3)-O(4)-Sm(1)	103.0(3)	Cu(2)-O(15)-Cu(4)#1	119.6(3)
Cu(4)-O(5)-Cu(1)	120.0(3)	Cu(2)-O(15)-Sm(2)#1	106.2(3)
Cu(4)-O(5)-Sm(2)	104.4(3)	Cu(4)#1-O(15)-Sm(2)#1	102.3(3)
Cu(1)-O(5)-Sm(2)	104.3(3)	Cu(7)-O(22)-Sm(1)	103.6(3)
Cu(6)-O(6)-Cu(2)	119.4(3)	Cu(8)-O(24)-Sm(1)	103.7(3)
Cu(6)-O(6)-Sm(1)	106.4(3)	Cu(9)-O(26)-Sm(2)	102.0(3)
Cu(2)-O(6)-Sm(1)	102.9(3)	Cu(10)-O(28)-Sm(2)	102.7(3)
Cu(6)-O(7)-Cu(4)#1	119.6(3)	Cu(11)-O(30)-Sm(3)	103.7(3)
Cu(6)-O(7)-Sm(3)	103.0(3)	Cu(12)-O(32)-Sm(3)	102.3(3)
Cu(4)#1-O(7)-Sm(3)	105.3(3)	Cu(5)-O(111)-Cu(2)#1	91.4(7)
Cu(2)#1-O(8)-Cu(5)	115.1(3)	Cu(5)-O(111)-Cu(3)#1	92.5(7)
Cu(2)#1-O(8)-Sm(2)	103.9(3)	Cu(2)#1-O(111)-Cu(3)#1	90.9(7)
Cu(5)-O(8)-Sm(2)	103.5(3)	Cu(5)#1-O(112)-Cu(1)#1	93.5(8)
Cu(3)#1-O(9)-Cu(5)	118.0(3)	Cu(5)#1-O(112)-Cu(6)#1	91.3(7)
Cu(3)#1-O(9)-Sm(3)	106.3(3)	Cu(1)#1-O(112)-Cu(6)#1	88.8(8)
Cu(5)-O(9)-Sm(3)	102.6(3)	Cu(3)-O(113)-Cu(1)	93.0(8)
Cu(8)-O(10)-Cu(7)	100.4(3)	Cu(3)-O(113)-Cu(4)	91.1(9)
Cu(8)-O(10)-Sm(1)	108.6(3)	Cu(1)-O(113)-Cu(4)	92.5(8)
Cu(7)-O(10)-Sm(1)	108.3(3)	Cu(6)-O(114)-Cu(2)	94.6(10)
Cu(9)-O(11)-Cu(10)	101.0(3)	Cu(6)-O(114)-Cu(4)#1	94.3(11)
Cu(9)-O(11)-Sm(2)	110.1(3)	Cu(2)-O(114)-Cu(4)#1	93.8(11)
Cu(1)-O(1)-Sm(2)	103.8(3)		

Symmetry transformations used to generate equivalent atoms: #1 -x, -y, -z.

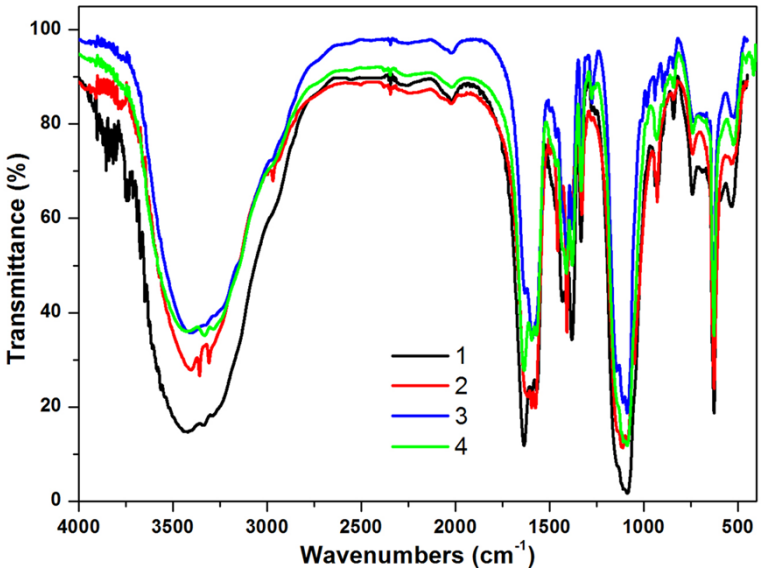

Figure S1. IR spectra of compounds **1-4**.

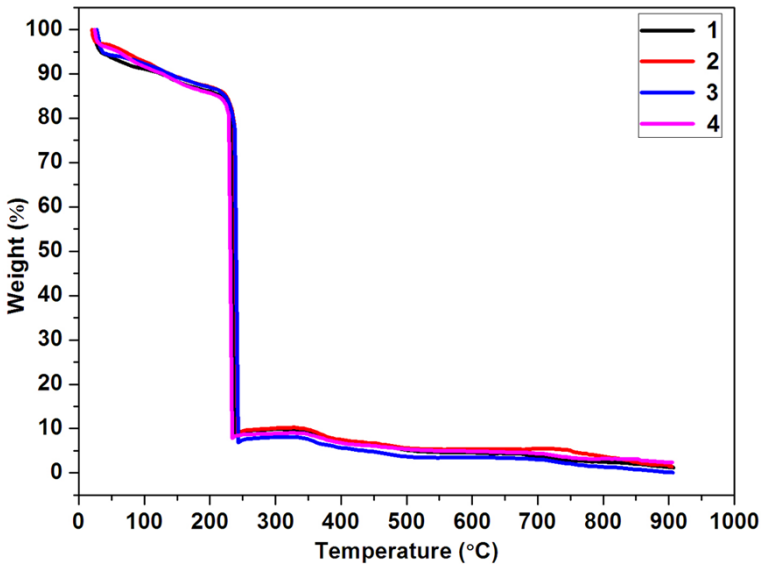

Figure S2. TGA curves of compounds **1-4**.