

Supporting Informations

The yields and elemental analysis data

Anal. Caclcd for **2a**, $C_{32}H_{32}N_4O_{34}CuNd_2$ (1368.64): C 28.08%; H 2.36%; N 4.09%.
Found: C 27.91%; H 2.80%; N 3.67%. The yield of **2a** is 60%.

Anal. Caclcd for **2b**, $C_{32}H_{16}N_4O_{26}CuNd_2$ (1224.52): C 31.39%; H 1.32%; N 4.58%.
Found: C 31.04%; H 1.76%; N 4.16%.

Anal. Caclcd for **3a**, $C_{32}H_{32}N_4O_{34}CuSm_2$ (1380.86): C 27.83%; H 2.34%; N 4.06%.
Found: C 27.44%; H 2.68%; N 3.67%. The yield of **3a** is 55%.

Anal. Caclcd for **3b**, $C_{32}H_{16}N_4O_{26}CuSm_2$ (1236.76): C 31.08%; H 1.30%; N 4.53%.
Found: C 30.85%; H 1.66%; N 4.28%.

Anal. Caclcd for **4a**, $C_{32}H_{32}N_4O_{34}CuEu_2$ (1384.088): C 27.77%; H 2.33%; N 4.05%.
Found: C 27.39%; H 2.86%; N 3.72%. The yield of **4a** is 65%.

Anal. Caclcd for **4b**, $C_{32}H_{16}N_4O_{26}CuEu_2$ (1239.96): C 30.96%; H 1.29%; N 4.52%.
Found: C 30.74%; H 1.75%; N 4.08%.

Anal. Caclcd for **5a**, $C_{32}H_{32}N_4O_{34}CuTb_2$ (1398.00): C 27.49%; H 2.31%; N 4.01 %.
Found: C 27.64%; H 2.68%; N 3.85%. The yield of **5a** is 65%.

Anal. Caclcd for **5b**, $C_{32}H_{16}N_4O_{26}CuTb_2$ (1253.90): C 30.65%; H 1.29%; N 4.47%.
Found: C 30.44%; H 1.61%; N 4.18%.

Anal. Caclcd for **6a**, $C_{32}H_{32}N_4O_{34}CuDy_2$ (1405.16): C 27.35%; H 2.30%; N 3.99 %.
Found: C 27.04%; H 2.78%; N 3.68%. The yield of **6a** is 60%.

Anal. Caclcd for **6b**, $C_{32}H_{16}N_4O_{26}CuDy_2$ (1261.04): C 30.45%; H 1.27%; N 4.44%.
Found: C 30.34%; H 1.63%; N 4.27%.

Anal. Caclcd for **7a**, $C_{32}H_{32}N_4O_{34}CuHo_2$ (1410.02): C 27.26%; H 2.29%; N 3.97%.
Found: C 26.84%; H 1.96%; N 3.54%. The yield of **7a** is 70%.

Anal. Caclcd for **7b**, $C_{32}H_{16}N_4O_{26}CuHo_2$ (1265.89): C 30.36%; H 1.27%; N 4.43%.
Found: C 29.42%; H 1.62%; N 4.09%.

Anal. Caclcd for **8a**, $C_{32}H_{32}N_4O_{34}CuEr_2$ (1414.69): C 27.17%; H 2.28%; N 3.96%.
Found: C 26.84%; H 2.72%; N 3.64%. The yield of **8a** is 65%.

Anal. Calcd for **8b**, $C_{32}H_{16}N_4O_{26}CuEr_2$ (1270.56): C 30.25%; H 1.27%; N 4.41%. Found: C 30.04%; H 1.66%; N 4.09%.

Anal. Calcd for **La-1**, $C_{24}H_{18}N_3O_{22}CuLa$ (902.86): C 31.93%; H 1.99%; N 4.65%. Found: C 32.16%; H 1.84%; N 4.53%. The yield of **La-1** is 45%.

Anal. Calcd for **La-2**, $C_{32}H_{16}N_4O_{26}CuLa_2$ (1213.85): C 31.66%; H 1.33%; N 4.62%. Found: C 31.84%; H 1.17%; N 4.29%. The yield of **La-2** is 25%.

Anal. Calcd for **Ce-1**, $C_{32}H_{24}N_4O_{30}CuCe_2$ (1288.33): C 29.83%; H 1.88%; N 4.35%. Found: C 29.54%; H 2.03%; N 4.18%. The yield of **Ce-1** is 60%.

Anal. Calcd for **Pr-a**, $C_{32}H_{32}N_4O_{34}CuPr_2$ (1361.98): C 28.22%; H 2.37%; N 4.11%. Found: C 27.84%; H 2.75%; N 3.92%. The yield of **Pr-a** is 60%.

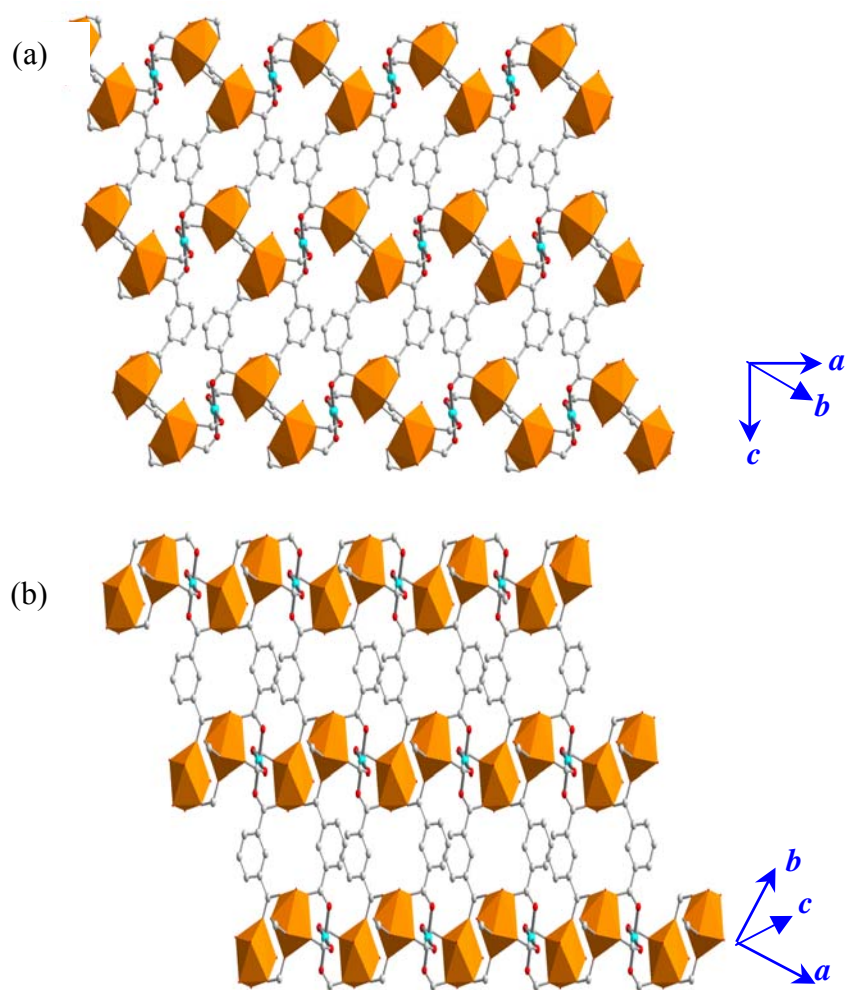


Fig. S1. Perspective views of the different two-dimensional layers in **1a**; the nitryl groups are omitted for clarity. Gd: yellow; Cu: pale blue; O red; C: grey.

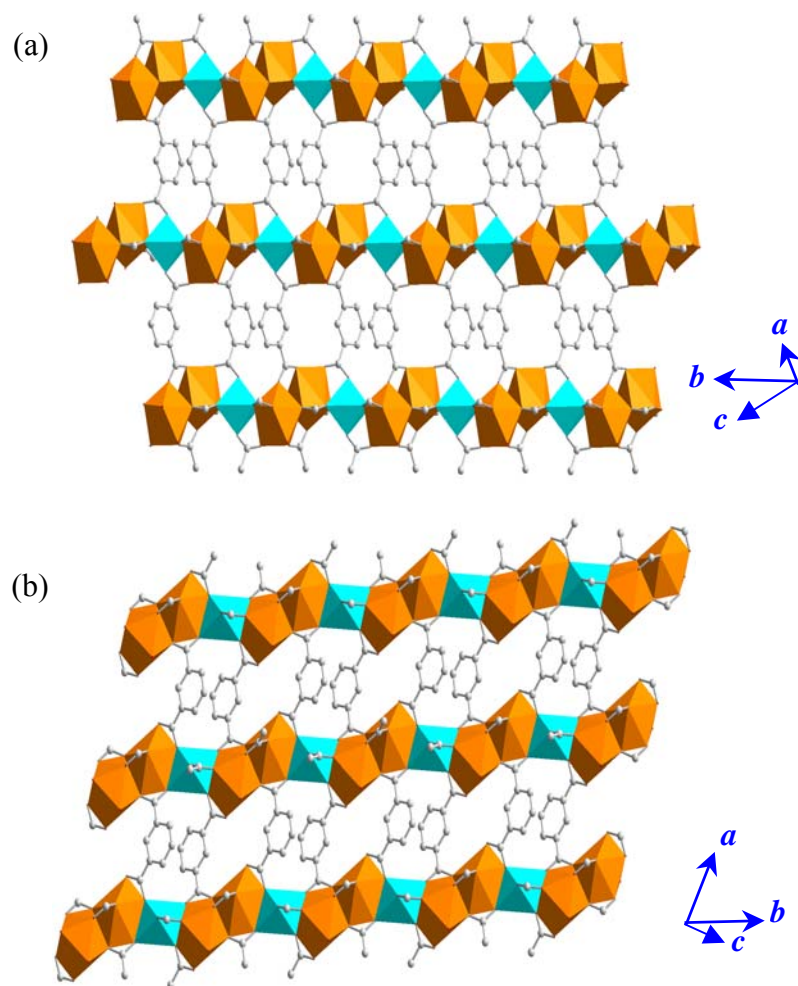


Fig. S2. Perspective views of the different two-dimensional layers in **1b**; the nitril groups are omitted for clarity. Gd: yellow; Cu: pale blue; O red; C: grey.

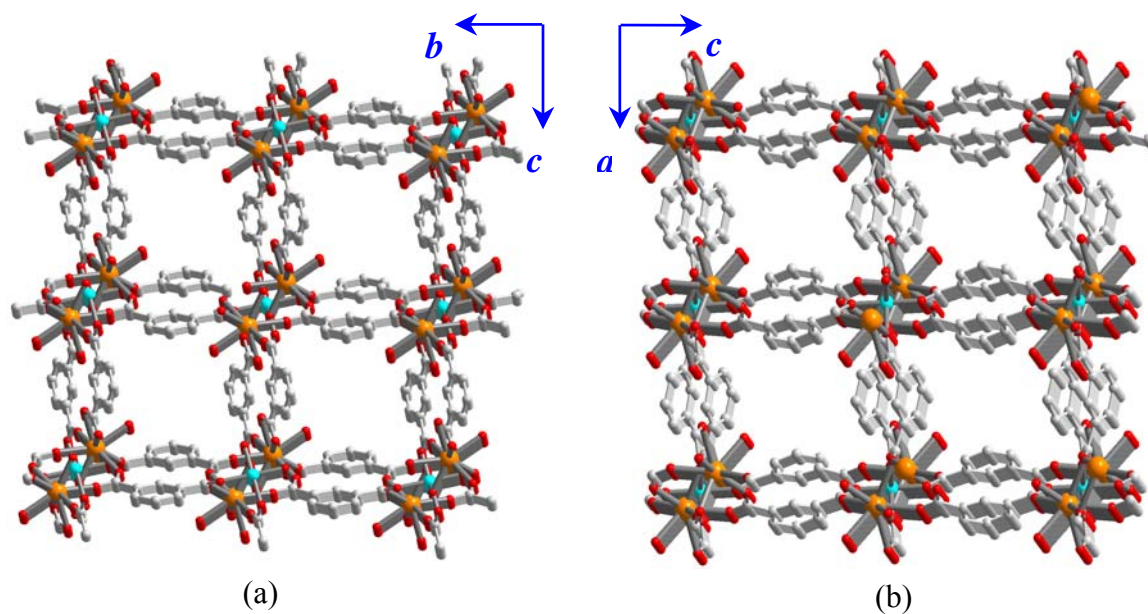


Fig. S3. Perspective views of the three-dimensional framework for **1a** (a) and **1b** (b), the guest water molecules and nitril groups are omitted for clarity. Gd: yellow; Cu: pale blue; O red; C: grey.

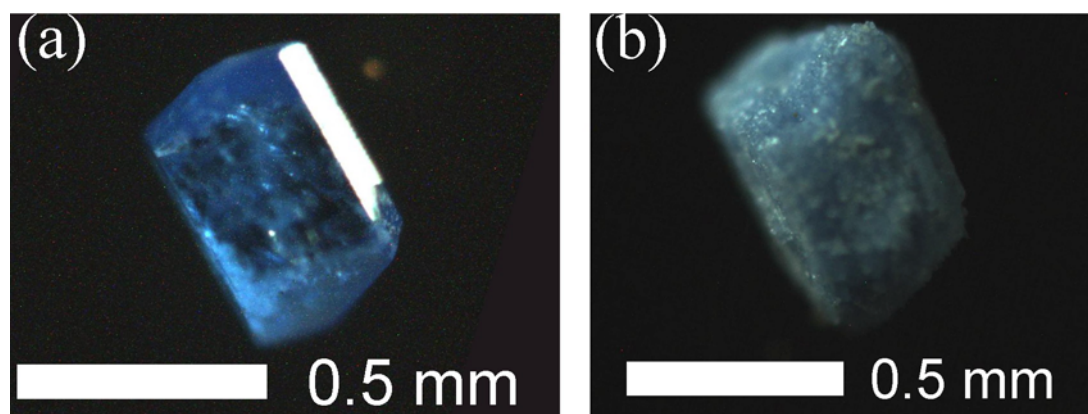


Fig. S4. Optical images of the same piece of crystal (**1a**), the original crystal (a) and after handle of crystal (b).

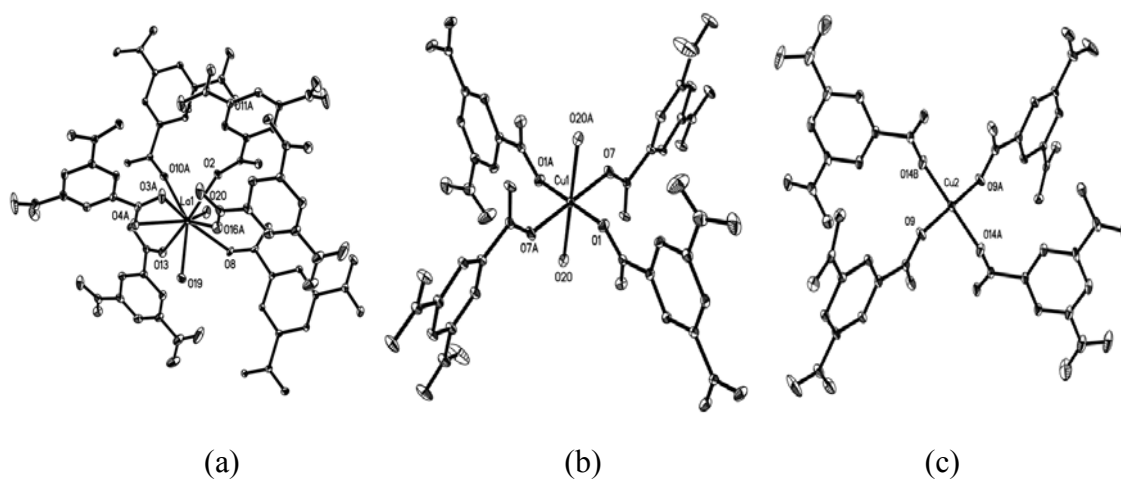


Fig. S5. Perspective views of the coordination environments of the metal centers in **La-1** with atoms represented by 30% thermal ellipsoids. Symmetry code: (A) $x+1, y, z$.

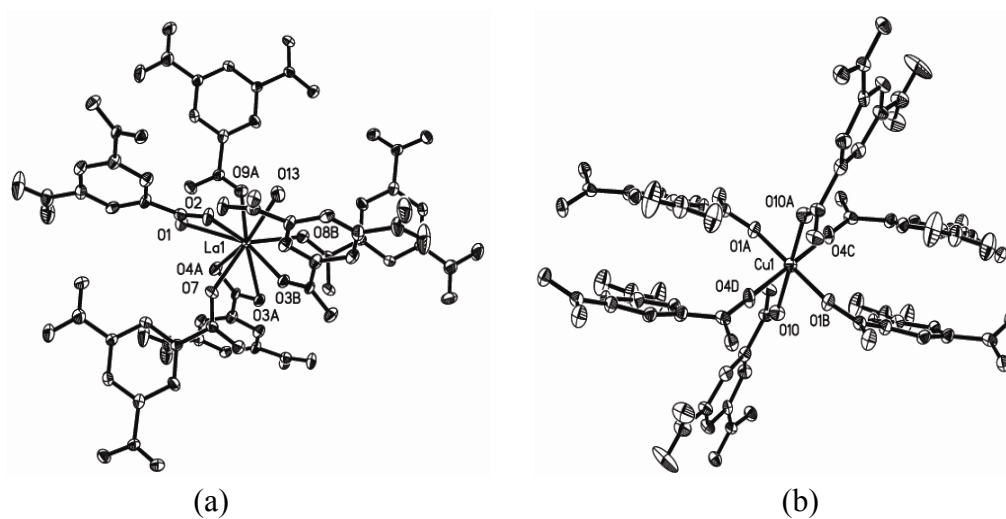


Fig. S6. Perspective views of the coordination environments of the metal centers in **La-2** with atoms represented by 30% thermal ellipsoids. Symmetry code: (A) $-x+1, -y+2, -z+1$; (B) $x, y, z-1$; (C) $-x, -y+2, -z+1$; (D) $x+1, y, z$.

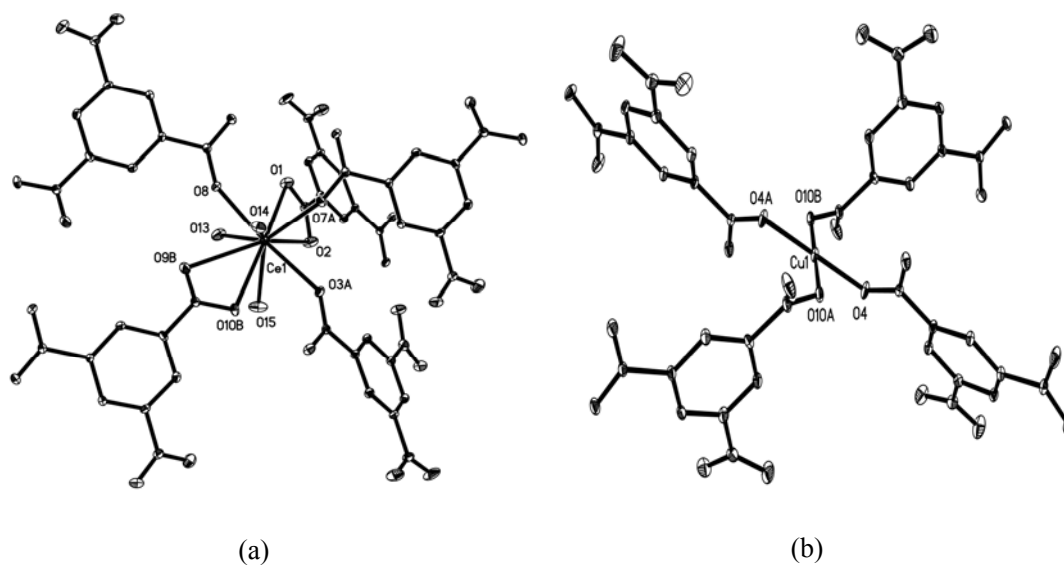


Fig. S7. Perspective views of the coordination environments of the metal centers in **Ce-1** with atoms represented by 30% thermal ellipsoids. Symmetry code: (A) $-x, -y+1, -z+1$; (B) $-x-1, -y+2, -z+1$.

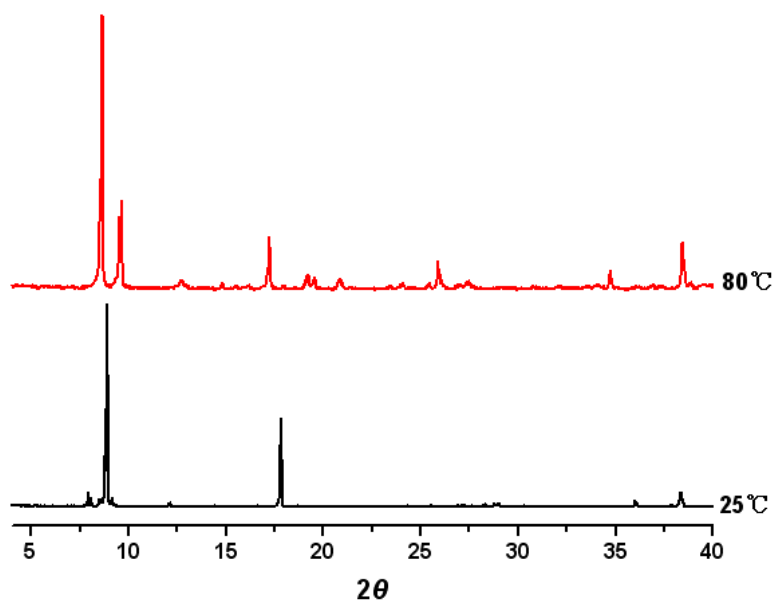
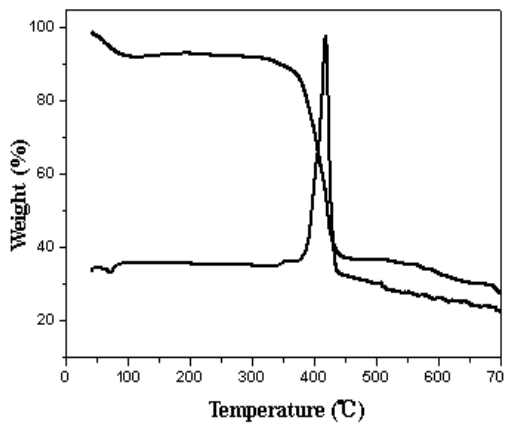
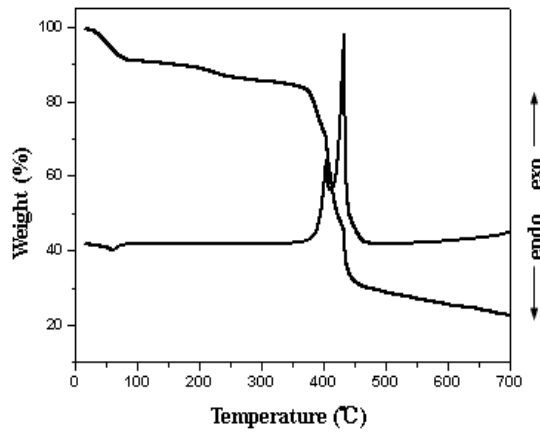


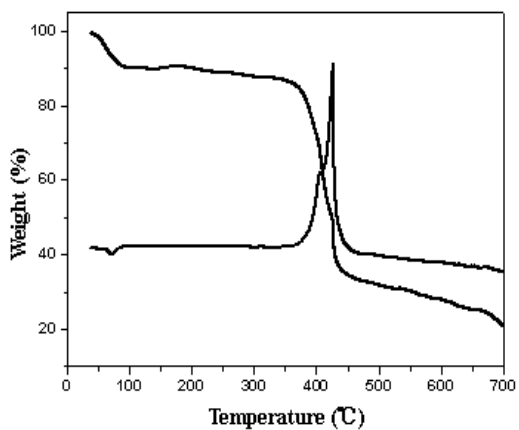
Fig. S8. XRD patterns for **1a** recorded at 25 °C and after being heated at 80 °C.



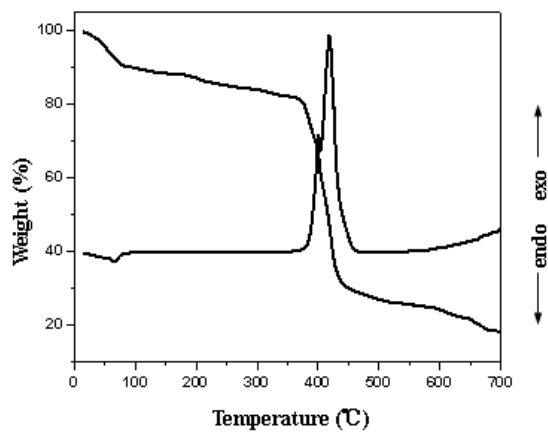
(a)



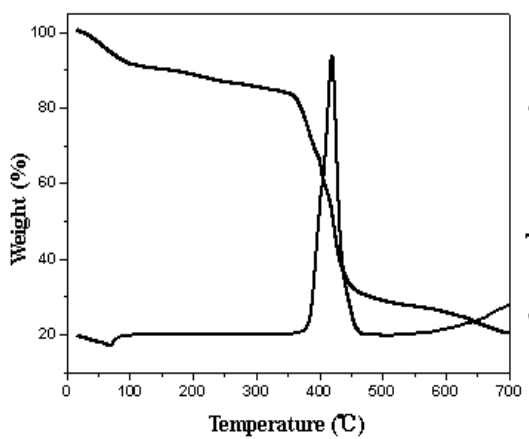
(b)



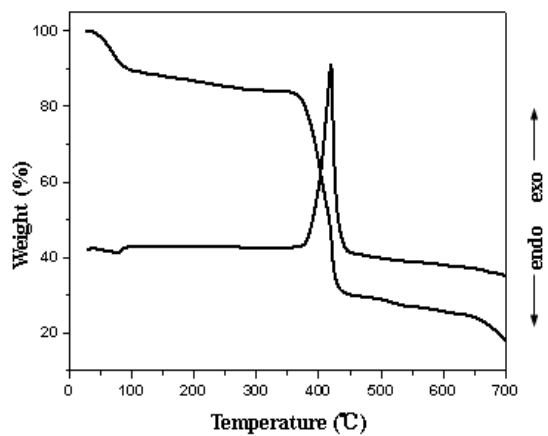
(c)



(d)



(e)



(f)

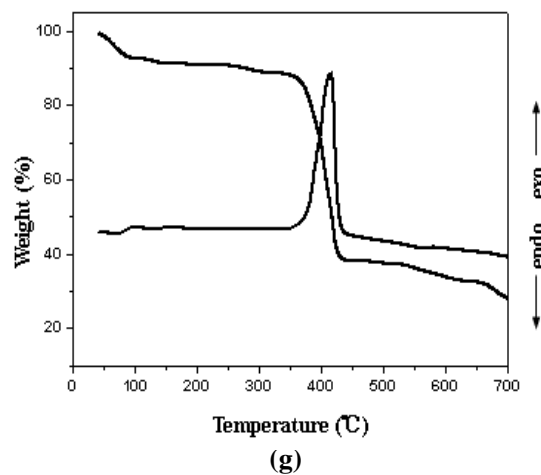


Fig. S9. TG-DTA curves for **2a** (a), **3a** (b), **4a** (c), **5a** (d), **6a** (e), **7a** (f) and **8a** (g).

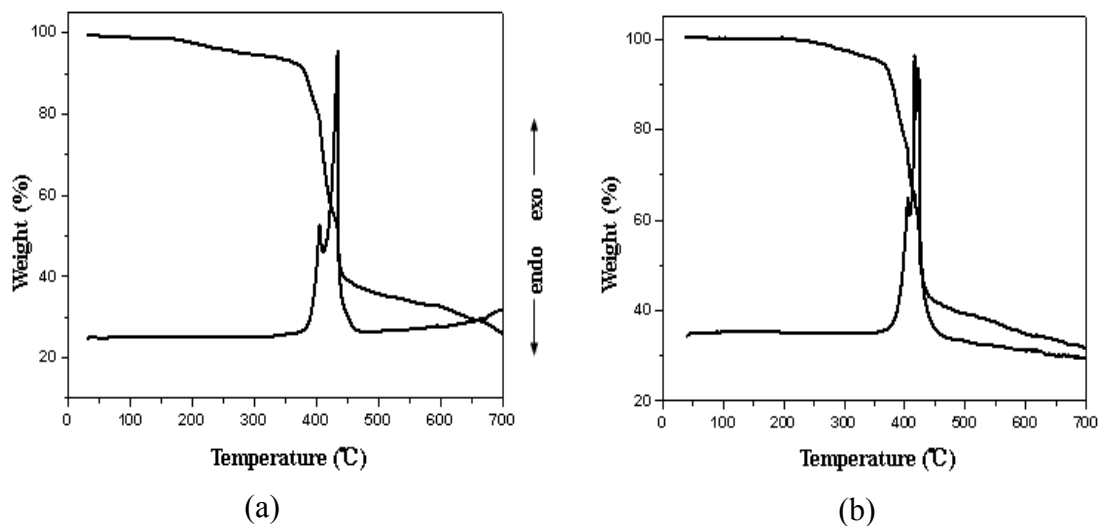


Fig. S10. TGA-DTA curves for **3b** (a), **4b** (b) in air.

Table S1. Crystallographic Data and Structure Refinements for **1(a,b)-8(a,b)**.

	1a	1b	2a	2b
Empirical formula	C ₃₂ H ₃₂ N ₄ O ₃₄ CuGd ₂	C ₃₂ H ₁₆ N ₄ O ₂₆ CuGd ₂	C ₃₂ H ₃₂ N ₄ O ₃₄ CuNd ₂	C ₃₂ H ₁₆ N ₄ O ₂₆ CuNd ₂
Formula weight	1394.66	1250.54	1368.64	1224.52
Crystal system	Triclinic	Triclinic	Triclinic	Triclinic
Space group	<i>P-1</i>	<i>P-1</i>	<i>P-1</i>	<i>P-1</i>
a (Å)	10.464(2)	9.815(2)	10.546(2)	9.849(2)
b (Å)	10.607(2)	10.285(2)	10.653(2)	10.440(2)
c (Å)	11.353(2)	10.957(2)	11.422(2)	11.057(2)
α (°)	83.08(3)	70.75(3)	82.68(3)	70.65(3)
β (°)	74.54(3)	85.05(3)	74.10(3)	84.44(3)
γ (°)	69.67(3)	71.09(3)	69.42(3)	70.73(3)
Volume (Å ³)	1138.4(4)	987.6(3)	1154.8(4)	1012.5(3)
Z	1	1	1	1
D _{Calc} (mg/m ⁻³)	2.034	2.103	1.968	2.008
μ (mm ⁻¹)	3.457	3.957	2.784	3.149
F ₍₀₀₀₎	681	601	673	593
Data /restraints /parameters	5178 / 0 / 331	4410 / 6 / 295	5237 / 0 / 331	3648 / 0 / 295
GoF	1.026	1.071	1.095	0.0987
R ₁ [I>2σ(I)] ^a	0.0265	0.0704	0.0365	0.0861
wR ₂ [I>2σ(I)] ^a	0.0957	0.1866	0.0950	0.01988
R ₁ (all data) ^a	0.0277	0.0832	0.0393	0.0949
wR ₂ (all data) ^a	0.0992	0.2011	0.0963	0.2053
	3a	3b	4a	4b
Empirical formula	C ₃₂ H ₃₂ N ₄ O ₃₄ CuSm ₂	C ₃₂ H ₁₆ N ₄ O ₂₆ CuSm ₂	C ₃₂ H ₃₂ N ₄ O ₃₄ CuEu ₂	C ₃₂ H ₁₆ N ₄ O ₂₆ CuEu ₂
Formula weight	1380.86	1236.76	1384.08	1239.96
Crystal system	Triclinic	Triclinic	Triclinic	Triclinic
Space group	<i>P-1</i>	<i>P-1</i>	<i>P-1</i>	<i>P-1</i>
a (Å)	10.528(2)	9.849(2)	10.500(2)	9.833(2)
b (Å)	10.671(2)	10.341(2)	10.635(2)	10.222(2)
c (Å)	11.378(2)	10.999(2)	11.373(2)	11.026(2)
α (°)	83.14(3)	70.72(3)	82.98(3)	71.83(3)
β (°)	74.61(3)	84.80(3)	74.42(3)	84.19(3)
γ (°)	69.34(3)	70.78(3)	69.60(3)	71.53(3)
Volume (Å ³)	1152.7(4)	998.3(3)	1146.2(4)	999.3(3)
Z	1	1	1	1
D _{Calc} (mg/m ⁻³)	1.989	2.057	2.005	2.061
μ (mm ⁻¹)	3.084	3.534	3.276	3.731
F ₍₀₀₀₎	677	597	679	599
Data /restraints /parameters	5187 / 0 / 331	3725 / 0 / 295	5193 / 0 / 331	3779 / 0 / 295

GoF	1.052	1.028	1.150	1.072
$R_1 [I > 2\sigma(I)]^a$	0.0331	0.0661	0.0299	0.0777
$wR_2 [I > 2\sigma(I)]^a$	0.1209	0.1739	0.0908	0.2070
R_1 (all data) ^a	0.0347	0.0703	0.0322	0.0845
wR_2 (all data) ^a	0.1218	0.1780	0.0975	0.2130
	5a	5b	6a	6b
Empirical formula	C ₃₂ H ₃₂ N ₄ O ₃₄ CuTb ₂	C ₃₂ H ₁₆ N ₄ O ₂₆ CuTb ₂	C ₃₂ H ₃₂ N ₄ O ₃₄ CuDy ₂	C ₃₂ H ₁₆ N ₄ O ₂₆ CuDy ₂
Formula weight	1398.00	1253.90	1405.16	1261.04
Crystal system	Triclinic	Triclinic	Triclinic	Triclinic
Space group	<i>P-1</i>	<i>P-1</i>	<i>P-1</i>	<i>P-1</i>
a (Å)	10.445(2)	9.829(2)	10.425(2)	9.805(2)
b (Å)	10.636(2)	10.242(2)	10.620(2)	10.235(2)
c (Å)	11.326(2)	10.948(2)	11.323(2)	10.981(2)
α (°)	83.28(3)	70.76(3)	83.41(3)	70.29(3)
β (°)	74.83(3)	84.94(3)	74.96(3)	86.24(3)
γ (°)	69.60(3)	71.26(3)	69.67(3)	71.16(3)
Volume (Å ³)	1137.8(4)	985.2(3)	1134.7(4)	980.7(3)
Z	1	1	1	1
D _{calc} (mg/m ⁻³)	2.040	2.113	2.056	2.135
μ (mm ⁻¹)	3.652	4.190	3.838	4.413
F ₍₀₀₀₎	683	603	685	605
Data /restraints /parameters	5171 / 0 / 331	4418 / 0 / 295	5163 / 0 / 331	4438 / 6 / 295
GoF	1.026	1.056	1.076	1.077
$R_1 [I > 2\sigma(I)]^a$	0.0273	0.0579	0.0257	0.0341
$wR_2 [I > 2\sigma(I)]^a$	0.0800	0.1525	0.0752	0.1049
R_1 (all data) ^a	0.0288	0.0631	0.0273	0.0370
wR_2 (all data) ^a	0.0843	0.1561	0.0809	0.1062
	7a	7b	8a	8b
Empirical formula	C ₃₂ H ₃₂ N ₄ O ₃₄ CuHo ₂	C ₃₂ H ₁₆ N ₄ O ₂₆ CuHo ₂	C ₃₂ H ₃₂ N ₄ O ₃₄ CuEr ₂	C ₃₂ H ₁₆ N ₄ O ₂₆ CuEr ₂
Formula weight	1410.02	1265.90	1414.69	1270.56
Crystal system	Triclinic	Triclinic	Triclinic	Triclinic
Space group	<i>P-1</i>	<i>P-1</i>	<i>P-1</i>	<i>P-1</i>
a (Å)	10.414(2)	9.795(2)	10.399(2)	9.779(2)
b (Å)	10.615(2)	10.221(2)	10.606(2)	10.195(2)
c (Å)	11.317(2)	10.940(2)	11.300(2)	10.951(2)
α (°)	83.45(3)	70.80(3)	83.50(3)	70.27(3)
β (°)	75.04(3)	84.87(3)	75.15(3)	86.24(3)
γ (°)	69.61(3)	71.50(3)	69.62(3)	71.41(3)
Volume (Å ³)	1132.5(4)	980.7(3)	1128.9(4)	973.0(3)
Z	1	1	1	1
D _{calc} (mg/m ⁻³)	2.067	2.143	2.081	2.168
μ (mm ⁻¹)	4.040	4.637	4.265	4.921

$F_{(000)}$	687	607	689	609
Data /restraints /parameters	5144 / 0 / 331	4386 / 0 / 285	5131 / 0 / 331	4373 / 12 / 295
GoF	1.042	1.061	1.028	0.994
$R_1 [I > 2\sigma(I)]^a$	0.0293	0.0574	0.0310	0.0428
$wR_2 [I > 2\sigma(I)]^a$	0.0861	0.1676	0.0981	0.1294
R_1 (all data) ^a	0.0312	0.0619	0.0319	0.0468
wR_2 (all data) ^a	0.0941	0.1717	0.1005	0.1383

$$^a R_1 = \sum ||F_o| - |F_c|| / \sum |F_o| ; wR_2 = \{ \sum [w(F_o^2 - F_c^2)^2] / \sum [w(F_o^2)]^2 \}^{1/2}$$

Table S2. Crystallographic Data and Structure Refinements for **La-1**, **La-2**, **Ce-1** and **Pr-a**.

	La-1	La-2	Ce-1	Pr-a
Empirical formula	C ₂₄ H ₁₈ N ₃ O ₂₂ CuLa	C ₃₂ H ₁₆ N ₄ O ₂₆ CuLa ₂	C ₃₂ H ₂₄ N ₄ O ₃₀ CuCe ₂	C ₃₂ H ₃₂ N ₄ O ₃₄ CuPr ₂
Formula weight	902.86	1213.85	1288.33	1361.98
Crystal system	Triclinic	Triclinic	Triclinic	Triclinic
Space group	<i>P-1</i>	<i>P-1</i>	<i>P-1</i>	<i>P-1</i>
a (Å)	10.845(2)	9.835(2)	10.236(2)	10.599(2)
b (Å)	12.041(2)	10.322(2)	10.476(2)	10.681(2)
c (Å)	13.634(3)	10.979(2)	11.089(2)	11.424(2)
α (°)	108.07(3)	70.75(3)	75.71(3)	82.67(3)
β (°)	108.82(3)	84.63(3)	63.72(3)	74.14(3)
γ (°)	103.88(3)	70.97(3)	67.03(3)	69.32(3)
Volume (Å ³)	1483.5(5)	994.7(3)	977.8(3)	1163.2(4)
Z	2	1	1	1
D _{Calc} (mg/m ⁻³)	2.021	2.026	2.188	1.944
μ (mm ⁻¹)	2.243	2.743	2.947	2.626
$F_{(000)}$	890	587	629	671
Data /restraints /parameters	6724 / 0 / 463	3570 / 0 / 295	4453 / 0 / 313	5240 / 0 / 331
GoF	1.053	1.075	1.023	1.084
$R_1 [I > 2\sigma(I)]^a$	0.0220	0.0773	0.0179	0.0289
$wR_2 [I > 2\sigma(I)]^a$	0.0726	0.1889	0.0662	0.0963
R_1 (all data) ^a	0.0247	0.0863	0.0201	0.0306
wR_2 (all data) ^a	0.0777	0.1957	0.0800	0.1022

$$^a R_1 = \sum ||F_o| - |F_c|| / \sum |F_o| ; wR_2 = \{ \sum [w(F_o^2 - F_c^2)^2] / \sum [w(F_o^2)]^2 \}^{1/2}$$

Table S3 Selected bond lengths [Å] and angles [°] for **1(a,b)**-**8(a,b)**.

1a			
Gd(1)-O(8)	2.312(3)	Gd(1)-O(10)#3	2.458(3)
Gd(1)-O(2)	2.329(3)	Gd(1)-O(9)#3	2.522(3)
Gd(1)-O(1)#1	2.328(3)	Cu(1)-O(7)#2	1.955(3)
Gd(1)-O(13)	2.386(4)	Cu(1)-O(4)#4	1.904(3)
Gd(1)-O(14)	2.417(3)	Cu(1)-O(4)	1.904(3)
Gd(1)-O(3)#2	2.427(3)	Cu(1)-O(7)#5	1.955(3)
O(8)-Gd(1)-O(2)	155.05(12)	O(1)#1-Gd(1)-O(3)#2	137.93(11)
O(8)-Gd(1)-O(1)#1	85.17(12)	O(13)-Gd(1)-O(3)#2	72.27(14)
O(2)-Gd(1)-O(1)#1	108.23(11)	O(14)-Gd(1)-O(3)#2	71.37(11)
O(8)-Gd(1)-O(13)	90.70(17)	O(8)-Gd(1)-O(10)#3	129.74(11)
O(2)-Gd(1)-O(13)	88.48(16)	O(2)-Gd(1)-O(10)#3	74.50(11)
O(1)#1-Gd(1)-O(13)	147.63(14)	O(1)#1-Gd(1)-O(10)#3	79.03(11)
O(8)-Gd(1)-O(14)	88.25(11)	O(13)-Gd(1)-O(10)#3	79.15(14)
O(2)-Gd(1)-O(14)	77.77(12)	O(14)-Gd(1)-O(10)#3	127.63(10)
O(1)#1-Gd(1)-O(14)	68.78(11)	O(3)#2-Gd(1)-O(10)#3	138.55(11)
O(13)-Gd(1)-O(14)	143.30(14)	O(8)-Gd(1)-O(9)#3	77.87(11)
O(8)-Gd(1)-O(3)#2	80.66(12)	O(2)-Gd(1)-O(9)#3	124.89(11)
O(2)-Gd(1)-O(3)#2	75.35(11)	O(1)#1-Gd(1)-O(9)#3	77.38(12)
O(14)-Gd(1)-O(9)#3	144.36(11)	O(13)-Gd(1)-O(9)#3	70.38(15)
O(3)#2-Gd(1)-O(9)#3	136.25(11)	O(10)#3-Gd(1)-O(9)#3	52.24(10)
O(4)#4-Cu(1)-O(4)	180.000(1)	O(4)-Cu(1)-O(7)#2	89.12(13)
O(4)#4-Cu(1)-O(7)#5	89.12(13)	O(7)#5-Cu(1)-O(7)#2	180.000(1)
O(4)-Cu(1)-O(7)#5	90.88(13)	O(4)#4-Cu(1)-O(7)#2	90.88(13)
1b			
Gd(1)-O(8)#1	2.351(7)	Gd(1)-O(3)#4	2.572(7)
Gd(1)-O(7)	2.378(8)	Gd(1)-O(1)	2.560(8)
Gd(1)-O(9)#2	2.389(8)	Cu(1)-O(4)#9	2.545(8)
Gd(1)-O(3)#3	2.395(8)	Cu(1)-O(10)#5	1.886(8)
Gd(1)-O(13)	2.411(8)	Cu(1)-O(10)	1.886(8)
Gd(1)-O(2)	2.503(8)	Cu(1)-O(1)#6	1.991(8)
Gd(1)-O(4)#4	2.516(8)	Cu(1)-O(1)#7	1.991(8)
Cu(1)-O(4)#8	2.545(8)	O(9)#2-Gd(1)-O(4)#4	77.9(3)
O(8)#1-Gd(1)-O(7)	136.8(3)	O(3)#3-Gd(1)-O(4)#4	122.1(2)
O(8)#1-Gd(1)-O(9)#2	76.6(3)	O(13)-Gd(1)-O(4)#4	155.7(3)
O(7)-Gd(1)-O(9)#2	140.3(3)	O(2)-Gd(1)-O(4)#4	117.6(3)
O(8)#1-Gd(1)-O(3)#3	77.0(3)	O(8)#1-Gd(1)-O(1)	147.1(3)
O(7)-Gd(1)-O(3)#3	70.5(3)	O(7)-Gd(1)-O(1)	71.6(3)
O(9)#2-Gd(1)-O(3)#3	149.1(3)	O(9)#2-Gd(1)-O(1)	71.2(3)
O(8)#1-Gd(1)-O(13)	71.9(3)	O(3)#3-Gd(1)-O(1)	135.7(3)

O(7)-Gd(1)-O(13)	126.1(3)	O(13)-Gd(1)-O(1)	106.8(3)
O(9)#2-Gd(1)-O(13)	78.1(3)	O(2)-Gd(1)-O(1)	51.4(3)
O(3)#3-Gd(1)-O(13)	78.7(3)	O(4)#4-Gd(1)-O(1)	68.4(3)
O(8)#1-Gd(1)-O(2)	140.2(3)	O(8)#1-Gd(1)-O(3)#4	72.5(3)
O(7)-Gd(1)-O(2)	71.4(3)	O(7)-Gd(1)-O(3)#4	71.9(3)
O(9)#2-Gd(1)-O(2)	95.3(3)	O(9)#2-Gd(1)-O(3)#4	112.2(3)
O(3)#3-Gd(1)-O(2)	94.7(3)	O(3)#3-Gd(1)-O(3)#4	74.2(3)
O(13)-Gd(1)-O(2)	68.3(3)	O(13)-Gd(1)-O(3)#4	139.0(3)
O(8)#1-Gd(1)-O(4)#4	99.0(3)	O(2)-Gd(1)-O(3)#4	143.2(3)
O(7)-Gd(1)-O(4)#4	76.1(3)	O(10)#5-Cu(1)-O(10)	180.000(2)
O(4)#4-Gd(1)-O(3)#4	50.7(2)	O(10)#5-Cu(1)-O(1)#6	89.7(4)
O(1)-Gd(1)-O(3)#4	114.1(3)	O(10)-Cu(1)-O(1)#6	90.3(4)
O(1)#6-Cu(1)-O(1)#7	180.0(5)	O(10)#5-Cu(1)-O(1)#7	90.3(4)
O(10)#5-Cu(1)-O(4)#8	87.4(3)	O(10)-Cu(1)-O(1)#7	89.7(4)
O(10)-Cu(1)-O(4)#8	92.6(3)	O(10)#5-Cu(1)-O(4)#9	92.6(3)
O(1)#6-Cu(1)-O(4)#8	76.9(3)	O(10)-Cu(1)-O(4)#9	87.4(3)
O(1)#7-Cu(1)-O(4)#8	103.1(3)	O(1)#6-Cu(1)-O(4)#9	103.1(3)
O(4)#8-Cu(1)-O(4)#9	180.000(1)	O(1)#7-Cu(1)-O(4)#9	76.9(3)

2a

Nd(1)-O(8)	2.363(3)	Nd(1)-O(3)#2	2.473(3)
Nd(1)-O(2)	2.377(3)	Nd(1)-O(10)#3	2.492(3)
Nd(1)-O(1)#1	2.388(3)	Nd(1)-O(9)#3	2.575(3)
Nd(1)-O(13)	2.454(4)	Nd(1)-O(14)	2.463(3)
Cu(1)-O(4)#4	1.909(3)	Cu(1)-O(7)#2	1.956(3)
Cu(1)-O(4)	1.909(3)	Cu(1)-O(7)#5	1.956(3)
O(8)-Nd(1)-O(2)	155.05(12)	O(1)#1-Nd(1)-O(10)#3	78.92(11)
O(8)-Nd(1)-O(1)#1	85.06(12)	O(13)-Nd(1)-O(10)#3	79.14(15)
O(2)-Nd(1)-O(1)#1	108.43(11)	O(14)-Nd(1)-O(10)#3	127.10(10)
O(8)-Nd(1)-O(13)	90.61(17)	O(3)#2-Nd(1)-O(10)#3	139.98(10)
O(2)-Nd(1)-O(13)	88.49(16)	O(8)-Nd(1)-O(9)#3	78.30(11)
O(1)#1-Nd(1)-O(13)	147.53(14)	O(2)-Nd(1)-O(9)#3	124.37(11)
O(8)-Nd(1)-O(14)	89.11(12)	O(1)#1-Nd(1)-O(9)#3	77.68(12)
O(2)-Nd(1)-O(14)	77.10(12)	O(13)-Nd(1)-O(9)#3	69.94(15)
O(1)#1-Nd(1)-O(14)	68.71(11)	O(14)-Nd(1)-O(9)#3	145.00(11)
O(13)-Nd(1)-O(14)	143.52(14)	O(3)#2-Nd(1)-O(9)#3	136.02(11)
O(8)-Nd(1)-O(3)#2	79.58(11)	O(10)#3-Nd(1)-O(9)#3	51.40(10)
O(2)-Nd(1)-O(3)#2	76.34(11)	O(4)#4-Cu(1)-O(4)	180.000(1)
O(1)#1-Nd(1)-O(3)#2	137.16(11)	O(4)#4-Cu(1)-O(7)#2	91.05(13)
O(13)-Nd(1)-O(3)#2	72.81(14)	O(4)-Cu(1)-O(7)#2	88.95(13)
O(14)-Nd(1)-O(3)#2	71.28(11)	O(4)#4-Cu(1)-O(7)#5	88.95(13)
O(8)-Nd(1)-O(10)#3	129.28(10)	O(4)-Cu(1)-O(7)#5	91.05(13)
O(2)-Nd(1)-O(10)#3	74.94(11)	O(7)#2-Cu(1)-O(7)#5	180.000(1)

2b

Nd(1)-O(8)#1	2.405(8)	Nd(1)-O(3)#4	2.601(9)
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Nd(1)-O(9)#2	2.445(8)	Nd(1)-O(1)	2.622(8)
Nd(1)-O(7)	2.446(9)	Cu(1)-O(10)	1.887(8)
Nd(1)-O(3)#3	2.457(8)	Cu(1)-O(10)#5	1.887(8)
Nd(1)-O(13)	2.475(10)	Cu(1)-O(1)#6	2.001(8)
Nd(1)-O(2)	2.502(9)	Cu(1)-O(1)#7	2.001(8)
Nd(1)-O(4)#4	2.574(9)	Cu(1)-O(4)#8	2.562(9)
Cu(1)-O(4)#9	2.562(9)	O(3)#3-Nd(1)-O(1)	135.4(3)
O(8)#1-Nd(1)-O(9)#2	77.5(3)	O(13)-Nd(1)-O(1)	107.7(3)
O(8)#1-Nd(1)-O(7)	136.0(3)	O(2)-Nd(1)-O(1)	50.4(3)
O(9)#2-Nd(1)-O(7)	140.6(3)	O(4)#4-Nd(1)-O(1)	67.2(3)
O(8)#1-Nd(1)-O(3)#3	76.2(3)	O(3)#4-Nd(1)-O(1)	113.0(2)
O(9)#2-Nd(1)-O(3)#3	149.7(3)	O(10)-Cu(1)-O(10)#5	180.000(2)
O(7)-Nd(1)-O(3)#3	69.6(3)	O(10)-Cu(1)-O(1)#6	91.1(4)
O(8)#1-Nd(1)-O(13)	71.7(3)	O(10)#5-Cu(1)-O(1)#6	88.9(4)
O(9)#2-Nd(1)-O(13)	79.3(3)	O(10)-Cu(1)-O(1)#7	88.9(4)
O(7)-Nd(1)-O(13)	124.8(3)	O(10)#5-Cu(1)-O(1)#7	91.1(4)
O(3)#3-Nd(1)-O(13)	78.5(3)	O(1)#6-Cu(1)-O(1)#7	180.000(2)
O(8)#1-Nd(1)-O(2)	140.8(3)	O(10)-Cu(1)-O(4)#8	95.1(4)
O(9)#2-Nd(1)-O(2)	94.9(3)	O(10)#5-Cu(1)-O(4)#8	84.9(4)
O(7)-Nd(1)-O(2)	71.0(3)	O(1)#6-Cu(1)-O(4)#8	77.0(3)
O(3)#3-Nd(1)-O(2)	96.1(3)	O(1)#7-Cu(1)-O(4)#8	103.0(3)
O(13)-Nd(1)-O(2)	69.1(3)	O(10)-Cu(1)-O(4)#9	84.9(4)
O(8)#1-Nd(1)-O(4)#4	100.7(3)	O(10)#5-Cu(1)-O(4)#9	95.1(4)
O(9)#2-Nd(1)-O(4)#4	78.1(3)	O(1)#6-Cu(1)-O(4)#9	103.0(3)
O(7)-Nd(1)-O(4)#4	75.7(3)	O(1)#7-Cu(1)-O(4)#9	77.0(3)
O(3)#3-Nd(1)-O(4)#4	121.4(3)	O(4)#8-Cu(1)-O(4)#9	180.000(1)
O(13)-Nd(1)-O(4)#4	157.3(3)	O(2)-Nd(1)-O(3)#4	142.7(3)
O(2)-Nd(1)-O(4)#4	115.4(3)	O(4)#4-Nd(1)-O(3)#4	50.4(3)
O(8)#1-Nd(1)-O(3)#4	72.8(3)	O(8)#1-Nd(1)-O(1)	148.3(3)
O(9)#2-Nd(1)-O(3)#4	111.7(3)	O(9)#2-Nd(1)-O(1)	71.5(3)
O(7)-Nd(1)-O(3)#4	71.9(3)	O(7)-Nd(1)-O(1)	71.5(3)
O(3)#3-Nd(1)-O(3)#4	74.1(3)	O(13)-Nd(1)-O(3)#4	139.3(3)
3a			
Sm(1)-O(8)	2.323(4)	Sm(1)-O(10)#3	2.479(4)
Sm(1)-O(2)	2.350(4)	Sm(1)-O(9)#3	2.560(4)
Sm(1)-O(1)#1	2.353(4)	Cu(1)-O(4)	1.906(3)
Sm(1)-O(13)	2.417(5)	Cu(1)-O(4)#4	1.906(3)
Sm(1)-O(14)	2.435(4)	Cu(1)-O(7)#5	1.954(3)
Sm(1)-O(3)#2	2.456(4)	Cu(1)-O(7)#2	1.954(3)
O(8)-Sm(1)-O(2)	154.85(15)	O(2)-Sm(1)-O(10)#3	74.42(13)
O(8)-Sm(1)-O(1)#1	84.94(15)	O(1)#1-Sm(1)-O(10)#3	79.36(13)
O(2)-Sm(1)-O(1)#1	108.44(14)	O(13)-Sm(1)-O(10)#3	79.37(18)
O(8)-Sm(1)-O(13)	89.2(2)	O(14)-Sm(1)-O(10)#3	127.77(13)
O(2)-Sm(1)-O(13)	90.3(2)	O(3)#2-Sm(1)-O(10)#3	138.61(13)

O(1)#1-Sm(1)-O(13)	146.48(18)	O(8)-Sm(1)-O(9)#3	78.49(13)
O(8)-Sm(1)-O(14)	88.12(14)	O(2)-Sm(1)-O(9)#3	124.50(13)
O(2)-Sm(1)-O(14)	77.61(14)	O(1)#1-Sm(1)-O(9)#3	77.44(14)
O(1)#1-Sm(1)-O(14)	68.97(14)	O(13)-Sm(1)-O(9)#3	69.05(18)
O(13)-Sm(1)-O(14)	143.90(17)	O(14)-Sm(1)-O(9)#3	144.79(14)
O(8)-Sm(1)-O(3)#2	80.33(14)	O(3)#2-Sm(1)-O(9)#3	136.39(14)
O(2)-Sm(1)-O(3)#2	75.51(14)	O(10)#3-Sm(1)-O(9)#3	51.91(12)
O(1)#1-Sm(1)-O(3)#2	137.66(14)	O(4)-Cu(1)-O(4)#4	180.000(1)
O(13)-Sm(1)-O(3)#2	73.01(17)	O(4)-Cu(1)-O(7)#5	90.81(16)
O(14)-Sm(1)-O(3)#2	71.06(14)	O(8)-Sm(1)-O(10)#3	130.03(13)
O(4)#4-Cu(1)-O(7)#5	89.19(16)	O(4)#4-Cu(1)-O(7)#2	90.81(16)
O(4)-Cu(1)-O(7)#2	89.19(16)	O(7)#5-Cu(1)-O(7)#2	180.00(6)

3b

Sm(1)-O(8)#1	2.388(6)	Sm(1)-O(3)#4	2.592(6)
Sm(1)-O(7)	2.399(6)	Cu(1)-O(10)#5	1.888(7)
Sm(1)-O(3)#2	2.411(6)	Cu(1)-O(10)	1.888(7)
Sm(1)-O(9)#3	2.426(7)	Cu(1)-O(1)#6	2.000(6)
Sm(1)-O(13)	2.447(7)	Cu(1)-O(1)#7	2.000(6)
Sm(1)-O(2)	2.485(6)	Cu(1)-O(4)#8	2.537(6)
Sm(1)-O(4)#4	2.538(6)	Cu(1)-O(4)#9	2.537(6)
Sm(1)-O(1)	2.580(6)	O(8)#1-Sm(1)-O(7)	136.6(2)
O(8)#1-Sm(1)-O(3)#2	76.3(2)	O(3)#2-Sm(1)-O(4)#4	122.1(2)
O(7)-Sm(1)-O(3)#2	70.4(2)	O(9)#3-Sm(1)-O(4)#4	77.9(2)
O(8)#1-Sm(1)-O(9)#3	77.1(2)	O(13)-Sm(1)-O(4)#4	156.2(3)
O(7)-Sm(1)-O(9)#3	140.4(2)	O(2)-Sm(1)-O(4)#4	116.3(2)
O(3)#2-Sm(1)-O(9)#3	149.2(2)	O(8)#1-Sm(1)-O(1)	147.8(2)
O(8)#1-Sm(1)-O(13)	71.8(2)	O(7)-Sm(1)-O(1)	71.5(2)
O(7)-Sm(1)-O(13)	125.6(3)	O(3)#2-Sm(1)-O(1)	135.7(2)
O(3)#2-Sm(1)-O(13)	78.6(2)	O(9)#3-Sm(1)-O(1)	71.3(2)
O(9)#3-Sm(1)-O(13)	78.5(2)	O(13)-Sm(1)-O(1)	106.8(2)
O(8)#1-Sm(1)-O(2)	140.3(2)	O(2)-Sm(1)-O(1)	50.64(19)
O(7)-Sm(1)-O(2)	71.3(2)	O(4)#4-Sm(1)-O(1)	67.80(19)
O(3)#2-Sm(1)-O(2)	95.6(2)	O(8)#1-Sm(1)-O(3)#4	72.9(2)
O(9)#3-Sm(1)-O(2)	95.0(3)	O(7)-Sm(1)-O(3)#4	71.6(2)
O(13)-Sm(1)-O(2)	68.5(2)	O(3)#2-Sm(1)-O(3)#4	74.0(2)
O(8)#1-Sm(1)-O(4)#4	100.1(2)	O(9)#3-Sm(1)-O(3)#4	112.2(2)
O(7)-Sm(1)-O(4)#4	75.9(2)	O(13)-Sm(1)-O(3)#4	139.4(2)
O(10)#5-Cu(1)-O(4)#8	93.8(3)	O(2)-Sm(1)-O(3)#4	142.9(2)
O(10)-Cu(1)-O(4)#8	86.2(3)	O(4)#4-Sm(1)-O(3)#4	50.92(19)
O(1)#6-Cu(1)-O(4)#8	103.0(2)	O(1)-Sm(1)-O(3)#4	113.77(19)
O(1)#7-Cu(1)-O(4)#8	77.0(2)	O(10)#5-Cu(1)-O(10)	180.000(2)
O(10)#5-Cu(1)-O(4)#9	86.2(3)	O(10)#5-Cu(1)-O(1)#6	89.6(3)
O(10)-Cu(1)-O(4)#9	93.8(3)	O(10)-Cu(1)-O(1)#6	90.4(3)
O(1)#6-Cu(1)-O(4)#9	77.0(2)	O(10)#5-Cu(1)-O(1)#7	90.4(3)

O(1)#7-Cu(1)-O(4)#9	103.0(2)	O(10)-Cu(1)-O(1)#7	89.6(3)
O(4)#8-Cu(1)-O(4)#9	180.000(1)	O(1)#6-Cu(1)-O(1)#7	180.000(2)

4a

Eu(1)-O(8)	2.321(3)	Eu(1)-O(10)#3	2.462(3)
Eu(1)-O(2)	2.336(3)	Eu(1)-O(9)#3	2.535(4)
Eu(1)-O(1)#1	2.350(3)	Cu(1)-O(4)#4	1.912(3)
Eu(1)-O(13)	2.399(4)	Cu(1)-O(4)	1.912(3)
Eu(1)-O(14)	2.429(3)	Cu(1)-O(7)#5	1.954(3)
Eu(1)-O(3)#2	2.441(3)	Cu(1)-O(7)#2	1.954(3)
O(8)-Eu(1)-O(2)	155.04(12)	O(3)#2-Eu(1)-O(10)#3	138.97(12)
O(8)-Eu(1)-O(1)#1	85.32(13)	O(8)-Eu(1)-O(9)#3	78.00(11)
O(2)-Eu(1)-O(1)#1	108.02(12)	O(2)-Eu(1)-O(9)#3	124.78(12)
O(8)-Eu(1)-O(13)	90.60(19)	O(1)#1-Eu(1)-O(9)#3	77.56(13)
O(2)-Eu(1)-O(13)	88.65(18)	O(13)-Eu(1)-O(9)#3	70.22(17)
O(1)#1-Eu(1)-O(13)	147.67(16)	O(14)-Eu(1)-O(9)#3	144.62(13)
O(8)-Eu(1)-O(14)	88.52(13)	O(3)#2-Eu(1)-O(9)#3	136.28(13)
O(2)-Eu(1)-O(14)	77.45(13)	O(10)#3-Eu(1)-O(9)#3	52.01(11)
O(1)#1-Eu(1)-O(14)	68.76(12)	O(4)#4-Cu(1)-O(4)	180.000(1)
O(13)-Eu(1)-O(14)	143.31(16)	O(4)#4-Cu(1)-O(7)#5	89.03(14)
O(8)-Eu(1)-O(3)#2	80.36(12)	O(4)-Cu(1)-O(7)#5	90.97(14)
O(2)-Eu(1)-O(3)#2	75.63(12)	O(4)#4-Cu(1)-O(7)#2	90.97(14)
O(1)#1-Eu(1)-O(3)#2	137.63(12)	O(4)-Cu(1)-O(7)#2	89.03(14)
O(13)-Eu(1)-O(3)#2	72.51(16)	O(7)#5-Cu(1)-O(7)#2	180.000(1)
O(14)-Eu(1)-O(3)#2	71.19(12)	O(13)-Eu(1)-O(10)#3	79.17(16)
O(8)-Eu(1)-O(10)#3	129.63(11)	O(14)-Eu(1)-O(10)#3	127.51(11)
O(2)-Eu(1)-O(10)#3	74.63(12)	O(1)#1-Eu(1)-O(10)#3	78.96(12)

4b

Eu(1)-O(3)#1	2.374(8)	Eu(1)-O(3)#4	2.601(8)
Eu(1)-O(8)#2	2.379(7)	Cu(1)-O(10)#5	1.910(9)
Eu(1)-O(9)#3	2.386(8)	Cu(1)-O(10)	1.910(9)
Eu(1)-O(7)	2.407(7)	Cu(1)-O(1)#6	2.002(7)
Eu(1)-O(2)	2.476(8)	Cu(1)-O(1)#7	2.002(7)
Eu(1)-O(13)	2.488(9)	Cu(1)-O(4)#8	2.514(8)
Eu(1)-O(1)	2.556(7)	Cu(1)-O(4)#9	2.514(8)
Eu(1)-O(4)#4	2.560(8)	O(3)#1-Eu(1)-O(8)#2	77.1(3)
O(3)#1-Eu(1)-O(9)#3	148.6(3)	O(4)#4-Eu(1)-O(3)#4	49.9(2)
O(8)#2-Eu(1)-O(9)#3	75.8(3)	O(10)#5-Cu(1)-O(10)	180.000(1)
O(3)#1-Eu(1)-O(7)	70.9(3)	O(10)#5-Cu(1)-O(1)#6	88.5(4)
O(8)#2-Eu(1)-O(7)	137.2(3)	O(10)-Cu(1)-O(1)#6	91.5(4)
O(9)#3-Eu(1)-O(7)	140.5(3)	O(10)#5-Cu(1)-O(1)#7	91.5(4)
O(3)#1-Eu(1)-O(2)	94.6(3)	O(10)-Cu(1)-O(1)#7	88.5(4)
O(8)#2-Eu(1)-O(2)	139.7(3)	O(1)#6-Cu(1)-O(1)#7	180.000(1)
O(9)#3-Eu(1)-O(2)	95.8(3)	O(10)#5-Cu(1)-O(4)#8	87.0(3)
O(7)-Eu(1)-O(2)	71.7(3)	O(10)-Cu(1)-O(4)#8	93.0(3)

O(3)#1-Eu(1)-O(13)	79.2(3)	O(1)#6-Cu(1)-O(4)#8	102.6(3)
O(8)#2-Eu(1)-O(13)	71.1(3)	O(1)#7-Cu(1)-O(4)#8	77.4(3)
O(9)#3-Eu(1)-O(13)	77.3(3)	O(10)#5-Cu(1)-O(4)#9	93.0(3)
O(7)-Eu(1)-O(13)	127.3(3)	O(10)-Cu(1)-O(4)#9	87.0(3)
O(2)-Eu(1)-O(13)	68.6(3)	O(1)#6-Cu(1)-O(4)#9	77.4(3)
O(3)#1-Eu(1)-O(1)	135.2(3)	O(1)#7-Cu(1)-O(4)#9	102.6(3)
O(8)#2-Eu(1)-O(1)	147.5(3)	O(4)#8-Cu(1)-O(4)#9	180.000(1)
O(9)#3-Eu(1)-O(1)	72.3(3)	O(3)#1-Eu(1)-O(3)#4	74.8(3)
O(7)-Eu(1)-O(1)	70.9(3)	O(8)#2-Eu(1)-O(3)#4	73.8(3)
O(2)-Eu(1)-O(1)	51.4(2)	O(9)#3-Eu(1)-O(3)#4	112.0(3)
O(13)-Eu(1)-O(1)	107.0(3)	O(7)-Eu(1)-O(3)#4	71.0(3)
O(3)#1-Eu(1)-O(4)#4	121.6(3)	O(2)-Eu(1)-O(3)#4	142.6(3)
O(8)#2-Eu(1)-O(4)#4	100.5(3)	O(2)-Eu(1)-O(4)#4	116.8(3)
O(9)#3-Eu(1)-O(4)#4	79.1(3)	O(13)-Eu(1)-O(4)#4	156.2(3)
O(7)-Eu(1)-O(4)#4	74.3(3)	O(1)-Eu(1)-O(3)#4	113.0(2)
O(13)-Eu(1)-O(3)#4	139.9(3)	O(1)-Eu(1)-O(4)#4	67.8(2)

5a

Tb(1)-O(8)	2.280(3)	Tb(1)-O(9)#3	2.523(3)
Tb(1)-O(2)	2.313(3)	Cu(1)-O(4)	1.908(3)
Tb(1)-O(1)#1	2.318(3)	Cu(1)-O(4)#4	1.908(3)
Tb(1)-O(13)	2.371(4)	Cu(1)-O(7)#2	1.953(3)
Tb(1)-O(14)	2.394(3)	Cu(1)-O(7)#5	1.953(3)
Tb(1)-O(3)#2	2.420(3)	Tb(1)-O(10)#3	2.441(3)
O(8)-Tb(1)-O(2)	154.75(12)	O(1)#1-Tb(1)-O(10)#3	79.00(11)
O(8)-Tb(1)-O(1)#1	85.54(12)	O(13)-Tb(1)-O(10)#3	79.36(15)
O(2)-Tb(1)-O(1)#1	108.13(11)	O(14)-Tb(1)-O(10)#3	127.96(11)
O(8)-Tb(1)-O(13)	89.20(17)	O(3)#2-Tb(1)-O(10)#3	137.96(11)
O(2)-Tb(1)-O(13)	90.13(17)	O(8)-Tb(1)-O(9)#3	77.98(11)
O(1)#1-Tb(1)-O(13)	146.51(15)	O(2)-Tb(1)-O(9)#3	125.07(11)
O(8)-Tb(1)-O(14)	87.88(12)	O(1)#1-Tb(1)-O(9)#3	77.06(12)
O(2)-Tb(1)-O(14)	77.94(12)	O(13)-Tb(1)-O(9)#3	69.50(15)
O(1)#1-Tb(1)-O(14)	69.06(11)	O(14)-Tb(1)-O(9)#3	144.16(11)
O(13)-Tb(1)-O(14)	143.84(14)	O(3)#2-Tb(1)-O(9)#3	136.49(12)
O(8)-Tb(1)-O(3)#2	80.77(12)	O(10)#3-Tb(1)-O(9)#3	52.48(10)
O(2)-Tb(1)-O(3)#2	74.95(11)	O(4)-Cu(1)-O(4)#4	180.000(1)
O(1)#1-Tb(1)-O(3)#2	138.33(12)	O(4)-Cu(1)-O(7)#2	89.26(14)
O(13)-Tb(1)-O(3)#2	72.70(15)	O(4)#4-Cu(1)-O(7)#2	90.74(14)
O(14)-Tb(1)-O(3)#2	71.26(12)	O(4)-Cu(1)-O(7)#5	90.74(14)
O(8)-Tb(1)-O(10)#3	130.15(11)	O(4)#4-Cu(1)-O(7)#5	89.26(14)
O(2)-Tb(1)-O(10)#3	74.34(11)	O(7)#2-Cu(1)-O(7)#5	180.000(1)

5b

Tb(1)-O(8)#1	2.342(5)	Tb(1)-O(1)	2.542(5)
Tb(1)-O(7)	2.358(5)	Tb(1)-O(3)#4	2.550(5)
Tb(1)-O(9)#2	2.373(5)	Cu(1)-O(10)#5	1.882(5)

Tb(1)-O(3)#3	2.377(5)	Cu(1)-O(10)	1.882(5)
Tb(1)-O(13)	2.393(6)	Cu(1)-O(1)#6	2.003(5)
Tb(1)-O(2)	2.454(6)	Cu(1)-O(1)#7	2.003(5)
Tb(1)-O(4)#4	2.500(6)	Cu(1)-O(4)#8	2.534(5)
Cu(1)-O(4)#9	2.534(5)	O(8)#1-Tb(1)-O(7)	136.90(18)
O(8)#1-Tb(1)-O(9)#2	75.94(19)	O(13)-Tb(1)-O(4)#4	155.3(2)
O(7)-Tb(1)-O(9)#2	140.43(19)	O(2)-Tb(1)-O(4)#4	117.61(18)
O(8)#1-Tb(1)-O(3)#3	77.41(18)	O(8)#1-Tb(1)-O(1)	147.03(18)
O(7)-Tb(1)-O(3)#3	70.44(18)	O(7)-Tb(1)-O(1)	71.56(18)
O(9)#2-Tb(1)-O(3)#3	149.10(18)	O(9)#2-Tb(1)-O(1)	71.65(18)
O(8)#1-Tb(1)-O(13)	72.2(2)	O(3)#3-Tb(1)-O(1)	135.39(17)
O(7)-Tb(1)-O(13)	126.9(2)	O(13)-Tb(1)-O(1)	105.8(2)
O(9)#2-Tb(1)-O(13)	77.4(2)	O(2)-Tb(1)-O(1)	51.37(17)
O(3)#3-Tb(1)-O(13)	79.8(2)	O(4)#4-Tb(1)-O(1)	68.87(17)
O(8)#1-Tb(1)-O(2)	140.8(2)	O(8)#1-Tb(1)-O(3)#4	71.90(18)
O(7)-Tb(1)-O(2)	70.7(2)	O(7)-Tb(1)-O(3)#4	72.01(18)
O(9)#2-Tb(1)-O(2)	96.8(2)	O(9)#2-Tb(1)-O(3)#4	111.93(19)
O(3)#3-Tb(1)-O(2)	93.99(18)	O(3)#3-Tb(1)-O(3)#4	73.62(19)
O(13)-Tb(1)-O(2)	68.6(2)	O(13)-Tb(1)-O(3)#4	138.99(18)
O(8)#1-Tb(1)-O(4)#4	98.8(2)	O(2)-Tb(1)-O(3)#4	142.72(19)
O(7)-Tb(1)-O(4)#4	75.6(2)	O(4)#4-Tb(1)-O(3)#4	51.00(17)
O(9)#2-Tb(1)-O(4)#4	78.1(2)	O(1)-Tb(1)-O(3)#4	115.06(17)
O(3)#3-Tb(1)-O(4)#4	121.55(17)	O(10)#5-Cu(1)-O(10)	180.000(2)
O(10)-Cu(1)-O(1)#6	89.7(2)	O(10)#5-Cu(1)-O(1)#6	90.3(2)
O(10)#5-Cu(1)-O(1)#7	89.7(2)	O(10)-Cu(1)-O(4)#9	92.2(2)
O(10)-Cu(1)-O(1)#7	90.3(2)	O(1)#6-Cu(1)-O(4)#9	103.1(2)
O(1)#6-Cu(1)-O(1)#7	180.000(1)	O(1)#7-Cu(1)-O(4)#9	76.9(2)
O(10)#5-Cu(1)-O(4)#8	92.2(2)	O(4)#8-Cu(1)-O(4)#9	180.000(1)
O(10)-Cu(1)-O(4)#8	87.8(2)	O(10)#5-Cu(1)-O(4)#9	87.8(2)
O(1)#6-Cu(1)-O(4)#8	76.9(2)	O(1)#7-Cu(1)-O(4)#8	103.1(2)
6a			
Dy(1)-O(8)	2.266(3)	Dy(1)-O(10)#3	2.437(3)
Dy(1)-O(1)#1	2.298(3)	Dy(1)-O(9)#3	2.506(3)
Dy(1)-O(2)	2.298(3)	Cu(1)-O(4)	1.905(3)
Dy(1)-O(13)	2.359(4)	Cu(1)-O(4)#4	1.905(3)
Dy(1)-O(14)	2.393(3)	Cu(1)-O(7)#2	1.954(3)
Dy(1)-O(3)#2	2.413(3)	Cu(1)-O(7)#5	1.954(3)
O(8)-Dy(1)-O(1)#1	85.57(12)	O(3)#2-Dy(1)-O(10)#3	137.73(12)
O(8)-Dy(1)-O(2)	154.94(12)	O(8)-Dy(1)-O(9)#3	77.56(11)
O(1)#1-Dy(1)-O(2)	107.90(11)	O(1)#1-Dy(1)-O(9)#3	76.86(12)
O(8)-Dy(1)-O(13)	89.50(17)	O(2)-Dy(1)-O(9)#3	125.40(11)
O(1)#1-Dy(1)-O(13)	146.81(15)	O(13)-Dy(1)-O(9)#3	70.04(15)
O(2)-Dy(1)-O(13)	89.87(16)	O(14)-Dy(1)-O(9)#3	144.04(12)
O(8)-Dy(1)-O(14)	87.80(12)	O(3)#2-Dy(1)-O(9)#3	136.31(12)

O(1)#1-Dy(1)-O(14)	69.33(12)	O(10)#3-Dy(1)-O(9)#3	52.74(10)
O(2)-Dy(1)-O(14)	77.92(12)	O(4)-Cu(1)-O(4)#4	180.000(1)
O(13)-Dy(1)-O(14)	143.33(14)	O(4)-Cu(1)-O(7)#2	89.52(14)
O(8)-Dy(1)-O(3)#2	80.97(12)	O(4)#4-Cu(1)-O(7)#2	90.48(14)
O(1)#1-Dy(1)-O(3)#2	138.66(12)	O(4)-Cu(1)-O(7)#5	90.48(14)
O(2)-Dy(1)-O(3)#2	75.01(12)	O(4)#4-Cu(1)-O(7)#5	89.52(14)
O(13)-Dy(1)-O(3)#2	72.21(15)	O(7)#2-Cu(1)-O(7)#5	180.000(1)
O(14)-Dy(1)-O(3)#2	71.25(12)	O(13)-Dy(1)-O(10)#3	79.34(15)
O(8)-Dy(1)-O(10)#3	130.01(11)	O(14)-Dy(1)-O(10)#3	128.27(11)
O(2)-Dy(1)-O(10)#3	74.32(11)	O(1)#1-Dy(1)-O(10)#3	78.93(11)

6b

Dy(1)-O(8)#1	2.331(2)	Dy(1)-O(3)#4	2.564(2)
Dy(1)-O(7)	2.3381(19)	Cu(1)-O(10)#5	1.8920(19)
Dy(1)-O(3)#2	2.352(2)	Cu(1)-O(10)	1.8920(19)
Dy(1)-O(9)#3	2.369(2)	Cu(1)-O(1)#6	1.9838(18)
Dy(1)-O(13)	2.424(2)	Cu(1)-O(1)#7	1.9838(18)
Dy(1)-O(2)	2.441(2)	Cu(1)-O(4)#8	2.537(2)
Dy(1)-O(4)#4	2.4779(19)	Cu(1)-O(4)#9	2.537(2)
Dy(1)-O(1)	2.522(2)	O(8)#1-Dy(1)-O(3)#2	77.56(7)
O(8)#1-Dy(1)-O(7)	137.10(8)	O(7)-Dy(1)-O(3)#2	70.94(7)
O(7)-Dy(1)-O(3)#4	71.69(7)	O(8)#1-Dy(1)-O(9)#3	75.65(7)
O(3)#2-Dy(1)-O(3)#4	73.34(6)	O(7)-Dy(1)-O(9)#3	141.32(7)
O(9)#3-Dy(1)-O(3)#4	114.44(7)	O(3)#2-Dy(1)-O(9)#3	147.53(6)
O(13)-Dy(1)-O(3)#4	138.69(7)	O(8)#1-Dy(1)-O(13)	72.72(7)
O(2)-Dy(1)-O(3)#4	144.63(7)	O(7)-Dy(1)-O(13)	126.36(8)
O(4)#4-Dy(1)-O(3)#4	51.43(7)	O(3)#2-Dy(1)-O(13)	78.87(8)
O(1)-Dy(1)-O(3)#4	114.02(6)	O(9)#3-Dy(1)-O(13)	75.92(8)
O(10)#5-Cu(1)-O(10)	180.000(1)	O(8)#1-Dy(1)-O(2)	139.83(7)
O(10)#5-Cu(1)-O(1)#6	89.66(9)	O(7)-Dy(1)-O(2)	72.95(8)
O(10)-Cu(1)-O(1)#6	90.34(9)	O(3)#2-Dy(1)-O(2)	95.76(7)
O(10)#5-Cu(1)-O(1)#7	90.34(9)	O(9)#3-Dy(1)-O(2)	93.00(8)
O(10)-Cu(1)-O(1)#7	89.66(9)	O(13)-Dy(1)-O(2)	67.13(7)
O(1)#6-Cu(1)-O(1)#7	180.000(1)	O(8)#1-Dy(1)-O(4)#4	96.70(7)
O(10)#5-Cu(1)-O(4)#8	89.05(9)	O(7)-Dy(1)-O(4)#4	77.44(7)
O(10)-Cu(1)-O(4)#8	90.95(9)	O(3)#2-Dy(1)-O(4)#4	122.58(7)
O(1)#6-Cu(1)-O(4)#8	75.92(7)	O(9)#3-Dy(1)-O(4)#4	78.77(7)
O(1)#7-Cu(1)-O(4)#8	104.08(7)	O(13)-Dy(1)-O(4)#4	154.28(8)
O(10)#5-Cu(1)-O(4)#9	90.95(9)	O(2)-Dy(1)-O(4)#4	119.09(6)
O(10)-Cu(1)-O(4)#9	89.05(9)	O(8)#1-Dy(1)-O(1)	146.35(7)
O(1)#6-Cu(1)-O(4)#9	104.08(7)	O(7)-Dy(1)-O(1)	71.13(8)
O(1)#7-Cu(1)-O(4)#9	75.92(7)	O(3)#2-Dy(1)-O(1)	136.04(6)
O(4)#8-Cu(1)-O(4)#9	180.000(1)	O(9)#3-Dy(1)-O(1)	71.94(7)
O(8)#1-Dy(1)-O(3)#4	71.88(7)	O(13)-Dy(1)-O(1)	107.23(8)

7a

Ho(1)-O(8)	2.254(4)	Ho(1)-O(1)#1	2.284(4)
Ho(1)-O(2)	2.285(4)	Ho(1)-O(9)#3	2.512(4)
Ho(1)-O(13)	2.348(5)	Cu(1)-O(4)	1.902(4)
Ho(1)-O(14)	2.383(4)	Cu(1)-O(4)#4	1.902(4)
Ho(1)-O(3)#2	2.410(4)	Cu(1)-O(7)#2	1.960(4)
Ho(1)-O(10)#3	2.436(4)	Cu(1)-O(7)#5	1.960(4)
O(8)-Ho(1)-O(1)#1	85.71(16)	O(13)-Ho(1)-O(3)#2	72.50(18)
O(8)-Ho(1)-O(2)	154.87(15)	O(14)-Ho(1)-O(3)#2	70.97(15)
O(1)#1-Ho(1)-O(2)	107.90(15)	O(8)-Ho(1)-O(10)#3	130.07(14)
O(8)-Ho(1)-O(13)	89.2(2)	O(1)#1-Ho(1)-O(10)#3	78.93(14)
O(1)#1-Ho(1)-O(13)	146.67(18)	O(2)-Ho(1)-O(10)#3	74.30(14)
O(2)-Ho(1)-O(13)	90.1(2)	O(13)-Ho(1)-O(10)#3	79.39(18)
O(8)-Ho(1)-O(14)	87.84(15)	O(14)-Ho(1)-O(10)#3	128.30(13)
O(1)#1-Ho(1)-O(14)	69.39(14)	O(3)#2-Ho(1)-O(10)#3	137.73(14)
O(2)-Ho(1)-O(14)	77.91(15)	O(8)-Ho(1)-O(9)#3	77.56(14)
O(13)-Ho(1)-O(14)	143.37(18)	O(1)#1-Ho(1)-O(9)#3	76.98(15)
O(8)-Ho(1)-O(3)#2	81.02(15)	O(2)-Ho(1)-O(9)#3	125.41(14)
O(1)#1-Ho(1)-O(3)#2	138.50(15)	O(13)-Ho(1)-O(9)#3	69.76(18)
O(2)-Ho(1)-O(3)#2	74.83(15)	O(14)-Ho(1)-O(9)#3	144.20(15)
O(3)#2-Ho(1)-O(9)#3	136.45(15)	O(4)#4-Cu(1)-O(7)#2	90.49(17)
O(10)#3-Ho(1)-O(9)#3	52.80(13)	O(4)-Cu(1)-O(7)#5	90.49(17)
O(4)-Cu(1)-O(4)#4	180.000(1)	O(4)#4-Cu(1)-O(7)#5	89.51(17)
O(4)-Cu(1)-O(7)#2	89.51(17)	O(7)#2-Cu(1)-O(7)#5	180.000(1)

7b

Ho(1)-O(8)#1	2.321(6)	Ho(1)-O(3)#4	2.551(6)
Ho(1)-O(7)	2.341(6)	Cu(1)-O(10)#5	1.883(6)
Ho(1)-O(3)#2	2.352(6)	Cu(1)-O(10)	1.883(6)
Ho(1)-O(9)#3	2.362(6)	Cu(1)-O(1)#6	1.998(6)
Ho(1)-O(13)	2.372(7)	Cu(1)-O(1)#7	1.998(6)
Ho(1)-O(2)	2.434(6)	Cu(1)-O(4)#8	2.535(6)
Ho(1)-O(4)#4	2.470(6)	Cu(1)-O(4)#9	2.535(6)
Ho(1)-O(1)	2.529(6)	O(8)#1-Ho(1)-O(7)	137.2(2)
O(8)#1-Ho(1)-O(3)#2	78.1(2)	O(8)#1-Ho(1)-O(1)	146.1(2)
O(7)-Ho(1)-O(3)#2	70.9(2)	O(7)-Ho(1)-O(1)	71.8(2)
O(8)#1-Ho(1)-O(9)#3	75.4(2)	O(3)#2-Ho(1)-O(1)	135.6(2)
O(7)-Ho(1)-O(9)#3	140.4(2)	O(9)#3-Ho(1)-O(1)	71.4(2)
O(3)#2-Ho(1)-O(9)#3	148.7(2)	O(13)-Ho(1)-O(1)	105.8(2)
O(8)#1-Ho(1)-O(13)	72.2(2)	O(2)-Ho(1)-O(1)	51.7(2)
O(7)-Ho(1)-O(13)	127.5(3)	O(4)#4-Ho(1)-O(1)	69.1(2)
O(3)#2-Ho(1)-O(13)	79.4(2)	O(8)#1-Ho(1)-O(3)#4	72.0(2)
O(9)#3-Ho(1)-O(13)	76.8(3)	O(7)-Ho(1)-O(3)#4	71.5(2)
O(8)#1-Ho(1)-O(2)	141.0(2)	O(3)#2-Ho(1)-O(3)#4	73.7(2)
O(7)-Ho(1)-O(2)	70.8(2)	O(9)#3-Ho(1)-O(3)#4	112.7(2)
O(3)#2-Ho(1)-O(2)	93.3(2)	O(13)-Ho(1)-O(3)#4	138.7(2)

O(9)#3-Ho(1)-O(2)	96.9(3)	O(2)-Ho(1)-O(3)#4	142.3(2)
O(13)-Ho(1)-O(2)	68.9(2)	O(4)#4-Ho(1)-O(3)#4	51.45(19)
O(8)#1-Ho(1)-O(4)#4	97.9(2)	O(1)-Ho(1)-O(3)#4	115.42(19)
O(7)-Ho(1)-O(4)#4	75.9(2)	O(10)#5-Cu(1)-O(10)	180.000(2)
O(3)#2-Ho(1)-O(4)#4	122.4(2)	O(10)#5-Cu(1)-O(1)#6	90.2(3)
O(9)#3-Ho(1)-O(4)#4	77.9(2)	O(10)-Cu(1)-O(1)#6	89.8(3)
O(13)-Ho(1)-O(4)#4	154.5(3)	O(10)#5-Cu(1)-O(1)#7	89.8(3)
O(10)-Cu(1)-O(4)#9	88.4(3)	O(1)#6-Cu(1)-O(1)#7	180.0(4)
O(1)#6-Cu(1)-O(4)#9	103.6(2)	O(10)#5-Cu(1)-O(4)#8	88.4(3)
O(1)#7-Cu(1)-O(4)#9	76.4(2)	O(10)-Cu(1)-O(4)#8	91.6(3)
O(4)#8-Cu(1)-O(4)#9	180.000(1)	O(1)#6-Cu(1)-O(4)#8	76.4(2)
O(1)#7-Cu(1)-O(4)#8	103.6(2)	O(10)-Cu(1)-O(1)#7	90.2(3)

8a

Er(1)-O(8)	2.238(4)	Er(1)-O(9)#3	2.495(4)
Er(1)-O(2)	2.270(4)	Er(1)-O(10)#3	2.419(4)
Er(1)-O(1)#1	2.270(4)	Cu(1)-O(4)#4	1.903(4)
Er(1)-O(13)	2.338(5)	Cu(1)-O(4)	1.903(4)
Er(1)-O(14)	2.376(4)	Cu(1)-O(7)#5	1.957(4)
Er(1)-O(3)#2	2.401(4)	Cu(1)-O(7)#2	1.957(4)
O(8)-Er(1)-O(2)	154.59(15)	O(2)-Er(1)-O(3)#2	74.61(15)
O(8)-Er(1)-O(1)#1	85.93(16)	O(1)#1-Er(1)-O(3)#2	138.79(16)
O(2)-Er(1)-O(1)#1	107.83(15)	O(13)-Er(1)-O(3)#2	72.04(19)
O(8)-Er(1)-O(13)	89.0(2)	O(14)-Er(1)-O(3)#2	71.12(16)
O(2)-Er(1)-O(13)	90.2(2)	O(8)-Er(1)-O(10)#3	130.30(14)
O(1)#1-Er(1)-O(13)	146.88(19)	O(2)-Er(1)-O(10)#3	74.35(14)
O(8)-Er(1)-O(14)	87.49(15)	O(1)#1-Er(1)-O(10)#3	78.88(15)
O(2)-Er(1)-O(14)	78.06(16)	O(13)-Er(1)-O(10)#3	79.67(18)
O(1)#1-Er(1)-O(14)	69.40(15)	O(14)-Er(1)-O(10)#3	128.48(14)
O(13)-Er(1)-O(14)	143.09(18)	O(3)#2-Er(1)-O(10)#3	137.44(15)
O(8)-Er(1)-O(3)#2	81.00(15)	O(8)-Er(1)-O(9)#3	77.48(14)
O(14)-Er(1)-O(9)#3	144.30(15)	O(2)-Er(1)-O(9)#3	125.69(14)
O(3)#2-Er(1)-O(9)#3	135.96(16)	O(1)#1-Er(1)-O(9)#3	77.30(15)
O(10)#3-Er(1)-O(9)#3	53.13(13)	O(13)-Er(1)-O(9)#3	69.65(19)
O(4)#4-Cu(1)-O(4)	180.000(1)	O(4)#4-Cu(1)-O(7)#2	90.72(18)
O(4)#4-Cu(1)-O(7)#5	89.28(18)	O(4)-Cu(1)-O(7)#2	89.28(18)
O(4)-Cu(1)-O(7)#5	90.72(18)	O(7)#5-Cu(1)-O(7)#2	180.000(1)

8b

Er(1)-O(8)#1	2.298(3)	Er(1)-O(3)#4	2.556(3)
Er(1)-O(7)	2.320(3)	Cu(1)-O(10)#5	1.887(3)
Er(1)-O(3)#2	2.329(3)	Cu(1)-O(10)	1.887(3)
Er(1)-O(9)#3	2.343(3)	Cu(1)-O(1)#6	1.982(2)
Er(1)-O(13)	2.390(3)	Cu(1)-O(1)#7	1.982(2)
Er(1)-O(2)	2.415(3)	Cu(1)-O(4)#8	2.537(3)
Er(1)-O(4)#4	2.448(2)	Cu(1)-O(4)#9	2.537(3)

Er(1)-O(1)	2.506(3)	O(8)#1-Er(1)-O(7)	137.33(11)
O(8)#1-Er(1)-O(3)#2	77.99(10)	O(8)#1-Er(1)-O(1)	146.08(10)
O(7)-Er(1)-O(3)#2	70.99(9)	O(7)-Er(1)-O(1)	71.05(10)
O(8)#1-Er(1)-O(9)#3	75.58(10)	O(3)#2-Er(1)-O(1)	135.88(9)
O(7)-Er(1)-O(9)#3	141.28(9)	O(9)#3-Er(1)-O(1)	71.84(9)
O(3)#2-Er(1)-O(9)#3	147.43(8)	O(13)-Er(1)-O(1)	107.42(10)
O(8)#1-Er(1)-O(13)	72.59(10)	O(2)-Er(1)-O(1)	52.34(8)
O(7)-Er(1)-O(13)	126.56(10)	O(4)#4-Er(1)-O(1)	68.92(9)
O(3)#2-Er(1)-O(13)	78.68(10)	O(8)#1-Er(1)-O(3)#4	71.48(9)
O(9)#3-Er(1)-O(13)	75.51(10)	O(7)-Er(1)-O(3)#4	71.97(10)
O(8)#1-Er(1)-O(2)	140.20(9)	O(3)#2-Er(1)-O(3)#4	73.20(9)
O(7)-Er(1)-O(2)	72.21(11)	O(9)#3-Er(1)-O(3)#4	115.00(10)
O(3)#2-Er(1)-O(2)	94.77(10)	O(13)-Er(1)-O(3)#4	137.98(10)
O(9)#3-Er(1)-O(2)	93.48(12)	O(2)-Er(1)-O(3)#4	144.18(10)
O(13)-Er(1)-O(2)	67.62(10)	O(4)#4-Er(1)-O(3)#4	51.70(9)
O(8)#1-Er(1)-O(4)#4	95.96(9)	O(1)-Er(1)-O(3)#4	114.54(8)
O(3)#2-Er(1)-O(4)#4	122.77(9)	O(10)#5-Cu(1)-O(1)#6	90.19(12)
O(9)#3-Er(1)-O(4)#4	78.92(10)	O(10)-Cu(1)-O(1)#6	89.81(12)
O(13)-Er(1)-O(4)#4	153.87(11)	O(10)#5-Cu(1)-O(1)#7	89.81(12)
O(2)-Er(1)-O(4)#4	119.74(9)	O(10)-Cu(1)-O(1)#7	90.19(12)
O(10)-Cu(1)-O(4)#9	90.50(13)	O(1)#6-Cu(1)-O(1)#7	180.00(15)
O(1)#6-Cu(1)-O(4)#9	104.43(10)	O(10)#5-Cu(1)-O(4)#8	90.50(13)
O(1)#7-Cu(1)-O(4)#9	75.57(10)	O(10)-Cu(1)-O(4)#8	89.50(13)
O(4)#8-Cu(1)-O(4)#9	180.000(1)	O(1)#6-Cu(1)-O(4)#8	75.57(10)
O(10)#5-Cu(1)-O(10)	180.000(1)	O(1)#7-Cu(1)-O(4)#8	104.43(10)

Symmetry transformations used to generate equivalent atoms: For **1a**: #1 -x+1,-y+1,-z+1; #2 -x+1,-y+2,-z+1; #3 -x+1,-y+1,-z+2; #4 -x,-y+3,-z+1; #5 x-1,y+1,z; #6 x+1,y-1,z; For **1b**: #1 -x+1,-y+1,-z+1; #2 x,y,z-1; #3 -x,-y+1,-z+1; #4 x+1,y,z; #5 -x+1,-y,-z+3; #6 x,y,z+1; #7 -x+1,-y,-z+2; #8 x+1,y,z+1; #9 -x,-y,-z+2; #10 x-1,y,z; #11 x-1,y,z-1. For **2a**: #1 -x+1,-y+1,-z+1; #2 -x+1,-y+2,-z+1; #3 -x+1,-y+1,-z+2; #4 -x,-y+3,-z+1; #5 x-1,y+1,z; #6 x+1,y-1,z. For **2b**: #1 -x+1,-y+1,-z+1; #2 x,y,z-1; #3 -x,-y+1,-z+1; #4 x+1,y,z; #5 -x+1,-y,-z+3; #6 x,y,z+1; #7 -x+1,-y,-z+2; #8 x+1,y,z+1; #9 -x,-y,-z+2; #10 x-1,y,z; #11 x-1,y,z-1. For **3a**: #1 -x+1,-y+1,-z+1; #2 -x+1,-y+2,-z+1; #3 -x+1,-y+1,-z+2; #4 -x,-y+3,-z+1; #5 x-1,y+1,z; #6 x+1,y-1,z. For **3b**: #1 -x+1,-y+1,-z+1; #2 -x,-y+1,-z+1; #3 x,y,z-1; #4 x+1,y,z; #5 -x+1,-y,-z+3; #6 x,y,z+1; #7 -x+1,-y,-z+2; #8 -x,-y,-z+2; #9 x+1,y,z+1; #10 x-1,y,z; #11 x-1,y,z-1. For **4a**: #1 -x+1,-y+1,-z+1; #2 -x+1,-y+2,-z+1; #3 -x+1,-y+1,-z+2; #4 -x,-y+3,-z+1; #5 x-1,y+1,z; #6 x+1,y-1,z. For **4b**: #1 -x,-y+1,-z; #2 -x+1,-y+1,-z; #3 x,y,z-1; #4 x+1,y,z; #5 -x+1,-y,-z+2; #6 -x+1,-y,-z+1; #7 x,y,z+1; #8 x+1,y,z+1; #9 -x,-y,-z+1; #10 x-1,y,z; #11 x-1,y,z-1. For **5a**: #1 -x+1,-y+1,-z+1; #2 -x+1,-y+2,-z+1; #3 -x+1,-y+1,-z+2; #4 -x,-y+3,-z+1; #5 x-1,y+1,z; #6 x+1,y-1,z. For **5b**: #1 -x+1,-y+2,-z+1; #2 x,y,z-1; #3 -x,-y+2,-z+1; #4 x+1,y,z; #5 -x+1,-y+1,-z+3; #6 -x+1,-y+1,-z+2; #7 x,y,z+1; #8 -x,-y+1,-z+2;

#9 x+1,y,z+1; #10 x-1,y,z; #11 x-1,y,z-1. For **6a**: #1 -x+1,-y+1,-z+1; #2 -x+1,-y+2,-z+1; #3 -x+1,-y+1,-z+2; #4 -x,-y+3,-z+1; #5 x-1,y+1,z; #6 x+1,y-1,z. For **6b**: #1 -x+1,-y+1,-z+1; #2 -x,-y+1,-z+1; #3 x,y,z-1; #4 x+1,y,z; #5 -x+1,-y,-z+3; #6 x,y,z+1; #7 -x+1,-y,-z+2; #8 x+1,y,z+1; #9 -x,-y,-z+2; #10 x-1,y,z; #11 x-1,y,z-1. For **7a**: #1 -x+1,-y+1,-z+1; #2 -x+1,-y+2,-z+1; #3 -x+1,-y+1,-z+2; #4 -x,-y+3,-z+1; #5 x-1,y+1,z; #6 x+1,y-1,z. For **7b**: #1 -x+1,-y+1,-z+1; #2 -x,-y+1,-z+1; #3 x,y,z-1; #4 x+1,y,z; #5 -x+1,-y,-z+3; #6 x,y,z+1; #7 -x+1,-y,-z+2; #8 x+1,y,z+1; #9 -x,-y,-z+2; #10 x-1,y,z; #11 x-1,y,z-1. For **8a**: #1 -x+1,-y+1,-z+1; #2 -x+1,-y+2,-z+1; #3 -x+1,-y+1,-z+2; #4 -x,-y+3,-z+1; #5 x-1,y+1,z; #6 x+1,y-1,z. For **8b**: #1 -x+1,-y+1,-z+1; #2 -x,-y+1,-z+1; #3 x,y,z-1; #4 x+1,y,z; #5 -x+1,-y,-z+3; #6 -x+1,-y,-z+2; #7 x,y,z+1; #8 -x,-y,-z+2; #9 x+1,y,z+1; #10 x-1,y,z; #11 x-1,y,z-1.

Table S4 Selected bond lengths [Å] and angles [°] for **La-1**, **La-2**, **Ce-1** and **Pr-a**.

La-1			
La(1)-O(10)#1	2.437(4)	La(1)-O(20)	2.585(4)
La(1)-O(2)	2.454(4)	La(1)-O(3)#2	2.608(4)
La(1)-O(13)	2.509(4)	La(1)-O(4)#2	2.717(4)
La(1)-O(19)	2.513(5)	La(1)-O(16)#3	2.757(4)
La(1)-O(8)	2.524(4)	Cu(1)-O(20)	2.698(4)
Cu(1)-O(7)#4	1.920(4)	Cu(1)-O(20)#4	2.698(4)
Cu(1)-O(7)	1.920(4)	Cu(2)-O(9)#7	1.975(4)
Cu(1)-O(1)	1.967(4)	Cu(2)-O(9)	1.975(4)
Cu(1)-O(1)#4	1.967(4)	Cu(2)-O(14)#6	1.897(4)
Cu(2)-O(14)#5	1.897(4)	O(3)#2-La(1)-C(8)#2	24.32(14)
O(10)#1-La(1)-O(2)	76.73(14)	O(2)-La(1)-O(20)	77.24(15)
O(10)#1-La(1)-O(13)	82.57(14)	O(13)-La(1)-O(20)	70.40(16)
O(2)-La(1)-O(13)	145.58(14)	O(19)-La(1)-O(20)	120.87(18)
O(10)#1-La(1)-O(19)	143.44(15)	O(8)-La(1)-O(20)	67.48(15)
O(2)-La(1)-O(19)	137.07(15)	O(3)#2-La(1)-O(20)	148.46(17)
O(13)-La(1)-O(19)	72.51(15)	O(10)#1-La(1)-O(4)#2	71.68(15)
O(10)#1-La(1)-O(8)	138.24(15)	O(2)-La(1)-O(4)#2	126.00(13)
O(2)-La(1)-O(8)	83.31(14)	O(13)-La(1)-O(4)#2	70.75(13)
O(13)-La(1)-O(8)	94.64(14)	O(19)-La(1)-O(4)#2	75.00(16)
O(19)-La(1)-O(8)	71.56(16)	O(8)-La(1)-O(4)#2	146.25(14)
O(10)#1-La(1)-O(3)#2	79.02(16)	O(3)#2-La(1)-O(4)#2	48.62(13)
O(2)-La(1)-O(3)#2	83.42(15)	O(20)-La(1)-O(4)#2	129.50(14)
O(13)-La(1)-O(3)#2	119.37(14)	O(10)#1-La(1)-O(16)#3	133.18(14)
O(19)-La(1)-O(3)#2	90.17(18)	O(2)-La(1)-O(16)#3	68.44(14)
O(8)-La(1)-O(3)#2	134.82(14)	O(13)-La(1)-O(16)#3	142.00(14)

O(10)#1-La(1)-O(20)	72.47(16)	O(10)#1-La(1)-C(8)#2	73.74(15)
O(19)-La(1)-O(16)#3	69.99(15)	O(2)-La(1)-C(8)#2	104.97(14)
O(8)-La(1)-O(16)#3	67.89(14)	O(13)-La(1)-C(8)#2	95.05(14)
O(3)#2-La(1)-O(16)#3	67.04(14)	O(19)-La(1)-C(8)#2	82.10(17)
O(20)-La(1)-O(16)#3	125.76(15)	O(8)-La(1)-C(8)#2	147.63(14)
O(4)#2-La(1)-O(16)#3	104.71(15)	O(14)#5-Cu(2)-O(14)#6	180.000(1)
O(20)-La(1)-C(8)#2	144.58(15)	O(16)#3-La(1)-C(8)#2	85.84(15)
O(4)#2-La(1)-C(8)#2	24.30(13)	O(7)-Cu(1)-O(7)#4	180.000(1)
O(14)#5-Cu(2)-O(9)	86.49(18)	O(7)-Cu(1)-O(1)	88.59(18)
O(14)#6-Cu(2)-O(9)	93.51(18)	O(7)#4-Cu(1)-O(1)	91.41(18)
O(14)#5-Cu(2)-O(9)#7	93.51(18)	O(7)-Cu(1)-O(1)#4	91.41(18)
O(14)#6-Cu(2)-O(9)#7	86.49(18)	O(7)#4-Cu(1)-O(1)#4	88.59(18)
O(9)-Cu(2)-O(9)#7	180.000(1)	O(1)-Cu(1)-O(1)#4	180.000(1)

La-2

La(1)-O(8)#1	2.379(8)	La(1)-O(2)	2.482(9)
La(1)-O(7)	2.385(8)	La(1)-O(4)#4	2.545(8)
La(1)-O(9)#2	2.400(8)	La(1)-O(3)#4	2.569(8)
La(1)-O(3)#3	2.412(8)	La(1)-O(1)	2.571(8)
La(1)-O(13)	2.430(9)	Cu(1)-O(1)#6	2.001(8)
Cu(1)-O(10)#5	1.886(8)	Cu(1)-O(1)#7	2.001(8)
Cu(1)-O(4)#8	2.550(8)	Cu(1)-O(4)	2.550(8)
Cu(1)-O(10)	1.886(8)		
O(8)#1-La(1)-O(7)	136.0(3)	O(7)-La(1)-O(4)#4	76.2(3)
O(8)#1-La(1)-O(9)#2	76.7(3)	O(9)#2-La(1)-O(4)#4	78.2(3)
O(7)-La(1)-O(9)#2	141.2(3)	O(3)#3-La(1)-O(4)#4	121.6(3)
O(8)#1-La(1)-O(3)#3	76.4(3)	O(13)-La(1)-O(4)#4	155.4(3)
O(7)-La(1)-O(3)#3	70.0(3)	O(2)-La(1)-O(4)#4	116.9(3)
O(9)#2-La(1)-O(3)#3	148.8(3)	O(8)#1-La(1)-O(3)#4	72.4(3)
O(8)#1-La(1)-O(13)	72.2(3)	O(7)-La(1)-O(3)#4	71.6(3)
O(7)-La(1)-O(13)	126.2(3)	O(9)#2-La(1)-O(3)#4	112.2(3)
O(9)#2-La(1)-O(13)	77.3(4)	O(3)#3-La(1)-O(3)#4	73.9(3)
O(3)#3-La(1)-O(13)	79.6(3)	O(13)-La(1)-O(3)#4	139.7(3)
O(8)#1-La(1)-O(2)	140.8(3)	O(2)-La(1)-O(3)#4	142.7(3)
O(7)-La(1)-O(2)	71.1(3)	O(4)#4-La(1)-O(3)#4	50.6(3)
O(9)#2-La(1)-O(2)	95.7(3)	O(8)#1-La(1)-O(1)	147.7(3)
O(3)#3-La(1)-O(2)	95.2(3)	O(7)-La(1)-O(1)	72.0(3)
O(13)-La(1)-O(2)	68.7(3)	O(9)#2-La(1)-O(1)	71.6(3)
O(8)#1-La(1)-O(4)#4	99.3(3)	O(3)#3-La(1)-O(1)	135.8(3)
O(13)-La(1)-O(1)	106.2(3)	O(4)#4-La(1)-O(1)	68.4(3)
O(2)-La(1)-O(1)	50.9(3)	O(3)#4-La(1)-O(1)	114.0(2)
O(10)#5-Cu(1)-O(10)	180.000(2)	O(10)#5-Cu(1)-O(1)#7	90.6(4)
O(10)#5-Cu(1)-O(1)#6	89.4(4)	O(10)-Cu(1)-O(1)#7	89.4(4)
O(10)-Cu(1)-O(1)#6	90.6(4)	O(1)#6-Cu(1)-O(1)#7	180.000(2)

Ce-1

Ce(1)-O(8)	2.405(2)	Ce(1)-O(15)	2.648(3)
Ce(1)-O(7)#1	2.409(2)	Ce(1)-O(10)#3	2.691(2)
Ce(1)-O(3)#2	2.513(2)	Ce(1)-O(1)	2.698(3)
Ce(1)-O(2)	2.562(3)	Ce(1)-O(9)#3	2.773(3)
Ce(1)-O(13)	2.564(3)	Ce(1)-O(14)	2.626(2)
Cu(1)-O(4)	1.928(2)	Cu(1)-O(10)#5	1.942(2)
Cu(1)-O(4)#4	1.928(2)	Cu(1)-O(10)#6	1.942(2)
O(8)-Ce(1)-O(7)#1	91.77(8)	O(7)#1-Ce(1)-O(15)	135.80(10)
O(8)-Ce(1)-O(3)#2	152.34(9)	O(3)#2-Ce(1)-O(15)	72.07(10)
O(7)#1-Ce(1)-O(3)#2	72.13(8)	O(2)-Ce(1)-O(15)	66.08(11)
O(8)-Ce(1)-O(2)	122.86(9)	O(13)-Ce(1)-O(15)	64.97(10)
O(7)#1-Ce(1)-O(2)	81.82(9)	O(14)-Ce(1)-O(15)	132.65(10)
O(3)#2-Ce(1)-O(2)	78.00(9)	O(8)-Ce(1)-O(10)#3	106.35(8)
O(8)-Ce(1)-O(13)	71.07(10)	O(7)#1-Ce(1)-O(10)#3	119.77(8)
O(7)#1-Ce(1)-O(13)	136.48(9)	O(3)#2-Ce(1)-O(10)#3	65.77(8)
O(3)#2-Ce(1)-O(13)	135.78(9)	O(2)-Ce(1)-O(10)#3	126.02(8)
O(2)-Ce(1)-O(13)	75.63(11)	O(13)-Ce(1)-O(10)#3	103.56(9)
O(8)-Ce(1)-O(14)	70.79(9)	O(14)-Ce(1)-O(10)#3	67.93(8)
O(7)#1-Ce(1)-O(14)	65.19(8)	O(15)-Ce(1)-O(10)#3	65.47(10)
O(3)#2-Ce(1)-O(14)	81.93(9)	O(8)-Ce(1)-O(1)	75.13(8)
O(2)-Ce(1)-O(14)	145.36(9)	O(7)#1-Ce(1)-O(1)	68.97(8)
O(13)-Ce(1)-O(14)	136.16(10)	O(3)#2-Ce(1)-O(1)	117.13(8)
O(8)-Ce(1)-O(15)	130.75(10)	O(2)-Ce(1)-O(1)	49.50(8)
O(3)#2-Ce(1)-O(9)#3	112.75(8)	O(13)-Ce(1)-O(1)	68.04(9)
O(2)-Ce(1)-O(9)#3	136.45(10)	O(14)-Ce(1)-O(1)	120.63(9)
O(13)-Ce(1)-O(9)#3	67.94(10)	O(15)-Ce(1)-O(1)	106.45(10)
O(14)-Ce(1)-O(9)#3	77.54(9)	O(10)#3-Ce(1)-O(1)	170.76(7)
O(15)-Ce(1)-O(9)#3	77.17(11)	O(8)-Ce(1)-O(9)#3	66.42(8)
O(10)#3-Ce(1)-O(9)#3	47.09(7)	O(7)#1-Ce(1)-O(9)#3	141.58(9)
O(1)-Ce(1)-O(9)#3	128.52(8)	O(4)-Cu(1)-O(10)#6	90.54(10)
O(4)-Cu(1)-O(4)#4	180.0	O(4)#4-Cu(1)-O(10)#6	89.46(10)
O(4)-Cu(1)-O(10)#5	89.46(10)	O(10)#5-Cu(1)-O(10)#6	180.0
O(4)#4-Cu(1)-O(10)#5	90.54(10)		

Pr-a

Pr(1)-O(13)	2.466(4)	Pr(1)-O(14)	2.472(3)
Pr(1)-O(8)	2.382(3)	Pr(1)-O(3)#2	2.486(3)
Pr(1)-O(2)	2.394(3)	Pr(1)-O(10)#3	2.513(3)
Pr(1)-O(1)#1	2.406(3)	Pr(1)-O(9)#3	2.601(3)
Cu(1)-O(4)	1.906(3)	Cu(1)-O(7)#2	1.958(3)
Cu(1)-O(4)#5	1.906(3)	Cu(1)-O(7)#6	1.958(3)
O(8)-Pr(1)-O(2)	154.77(12)	O(8)-Pr(1)-O(1)#1	84.79(12)
O(2)-Pr(1)-O(1)#1	108.62(12)	O(2)-Pr(1)-O(10)#3	75.06(11)
O(8)-Pr(1)-O(13)	90.3(2)	O(1)#1-Pr(1)-O(10)#3	79.24(11)
O(2)-Pr(1)-O(13)	89.2(2)	O(13)-Pr(1)-O(10)#3	78.88(16)

O(1)#1-Pr(1)-O(13)	146.91(16)	O(14)-Pr(1)-O(10)#3	127.34(11)
O(8)-Pr(1)-O(14)	88.78(12)	O(3)#2-Pr(1)-O(10)#3	139.97(11)
O(2)-Pr(1)-O(14)	77.06(12)	O(8)-Pr(1)-O(9)#3	78.99(11)
O(1)#1-Pr(1)-O(14)	68.73(12)	O(2)-Pr(1)-O(9)#3	124.01(11)
O(13)-Pr(1)-O(14)	144.01(15)	O(1)#1-Pr(1)-O(9)#3	77.79(12)
O(8)-Pr(1)-O(3)#2	79.44(11)	O(13)-Pr(1)-O(9)#3	69.16(16)
O(2)-Pr(1)-O(3)#2	76.26(11)	O(14)-Pr(1)-O(9)#3	145.26(12)
O(1)#1-Pr(1)-O(3)#2	136.92(11)	O(3)#2-Pr(1)-O(9)#3	136.27(11)
O(13)-Pr(1)-O(3)#2	73.39(15)	O(10)#3-Pr(1)-O(9)#3	50.92(10)
O(14)-Pr(1)-O(3)#2	71.08(11)	O(8)-Pr(1)-O(10)#3	129.48(11)
O(4)#4-Cu(1)-O(4)	180.000(1)	O(4)#4-Cu(1)-O(7)#5	88.75(14)
O(4)#4-Cu(1)-O(7)#2	91.25(14)	O(4)-Cu(1)-O(7)#5	91.25(14)
O(4)-Cu(1)-O(7)#2	88.75(14)	O(7)#2-Cu(1)-O(7)#5	180.00(18)

Symmetry transformations used to generate equivalent atoms: For **La-1**: #1 $x+1, y, z$; #2 $-x+1, -y+2, -z$; #3 $x, y+1, z$; #4 $-x+1, -y+2, -z+1$; #5 $-x, -y+1, -z$; #6 $x-1, y, z$; #7 $-x-1, -y+1, -z$. For **La-2**: #1 $-x+1, -y+2, -z+1$; #2 $x, y, z-1$; #3 $-x, -y+2, -z+1$; #4 $x+1, y, z$; #5 $-x+1, -y+1, -z+3$; #6 $x, y, z+1$; #7 $-x+1, -y+1, -z+2$. For **Ce-1**: #1 $-x, -y+1, -z+1$; #2 $-x-1, -y+2, -z+1$; #3 $-x, -y+1, -z+2$; #4 $-x-1, -y+3, -z$; #5 $-x, -y+2, -z+1$; #6 $x-1, y+1, z-1$. For **Pr-a**: #1 $-x+1, -y+1, -z+1$; #2 $-x+1, -y+2, -z+1$; #3 $-x+1, -y+1, -z+2$; #4 $-x, -y+3, -z+1$; #5 $x-1, y+1, z$.
