Electronic Supplementary Material (ESI) for CrystEngComm.

Electronic Supplementary Information

Mesoxalate as Cu(II)-Ln(III) linker in the construction of MOFs in DMSO/water medium

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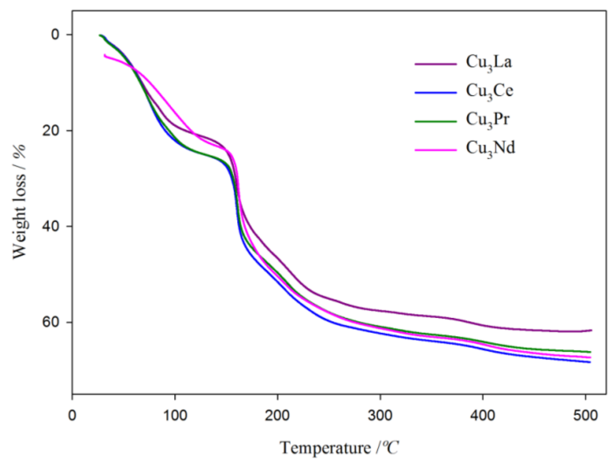

Fig. S1 TG plots of compounds **$LaCu_3$**, **$CeCu_3$**, **$PrCu_3$** and **$NdCu_3$**.
IR most intense bands correspond to asymmetric and symmetric carboxylate absorptions υ_{as} and υ_s: 1638 (s,b) and 1377 (s) cm^{-1}, respectively (average values).

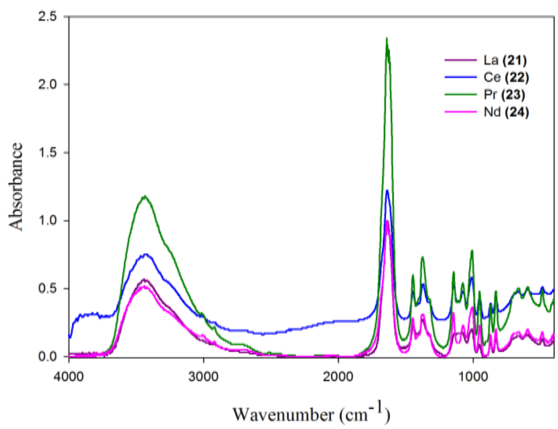

Fig. S2 IR spectra **$LaCu_3$**, **$CeCu_3$**, **$PrCu_3$** and **$NdCu_3$**.

The C-O stretching bands are observed around 1144 (vs) cm^{-1} and O-H bands in the range of 3400-3500 cm^{-1}. [1, 2] The values observed are within the expected ranges and Figure S2 shows that all the compounds are IR-isostructural

Powder X-Ray Diffraction Patterns

The Powder Diffraction Patterns matched very well the simulated ones for compounds **$LaCu_3$, $CeCu_3$, $PrCu_3$** and **$NdCu_3$** (see Figure S3). So the polycrystalline samples correspond to the single crystals and they constitute pure phases. The testing tubes containing the solutions to get the compounds involving the other Ln(III) cations (Gd, Tb, Dy, Er and Yb) afforded low-crystallinity materials which did not allow us neither the determination of the structure nor the magnetic properties.

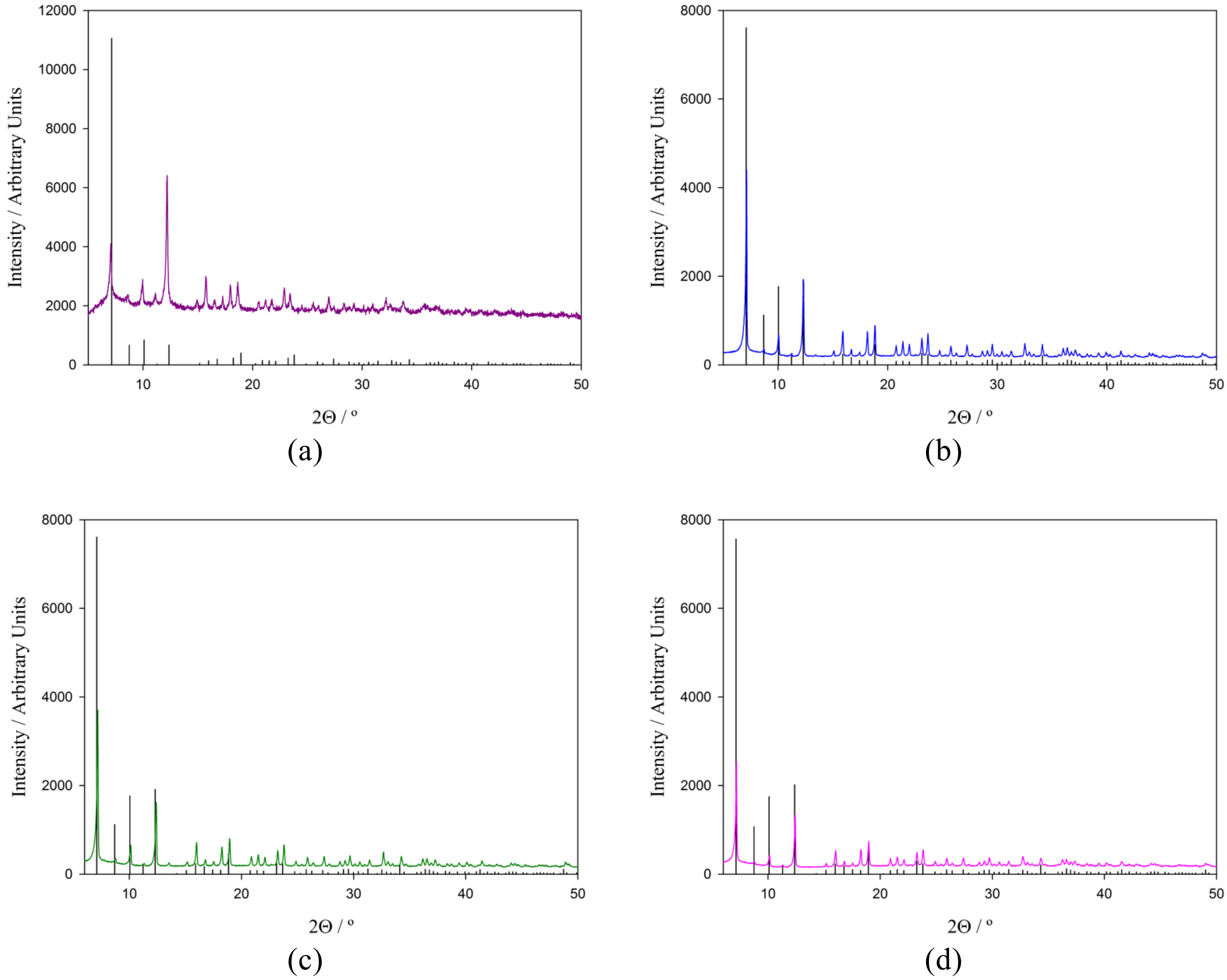

Fig. S3 Simulated (vertical bar plot) and experimental XRPD spectra (colored) for compounds **$LaCu_3$**,(a); **$CeCu_3$**, (b); **$PrCu_3$**, (c); and **$NdCu_3$**, (d).

Table S1. Selected distances and angles for **$LaCu_3$**.

La—O1W	2.409(13)	C1—C2	1.532(10)
La—O6^{i}	2.556(5)	C2—O3	1.376(8)
La—O6	2.556(5)	C2—O4	1.404(8)
La—O6^{ii}	2.556(5)	C2—C3	1.544(9)
La—O4^{i}	2.623(5)	O3—Cu^{iv}	1.946(5)
La—O4^{ii}	2.623(5)	C3—O6	1.241(9)
La—O4	2.623(5)	C3—O5	1.281(9)
La—O2^{i}	2.623(6)	O5—Cu^{iv}	1.938(5)
La—O2	2.623(6)	S1S—O1S	1.506(13)
La—O2^{ii}	2.623(6)	S1S—C2S	1.768(10)
Cu—O3	1.929(5)	S1S—C1S	1.77(1)
Cu—O5^{iii}	1.938(5)	S2S—O2S	1.47(2)
Cu—O1	1.944(6)	S2S—C3S	1.772(10)
Cu—O3^{iii}	1.946(5)	S2S—C4S	1.779(10)
Cu—O1S	2.471(8)	S3S—O3S	1.50(2)
C1—O1	1.245(10)	S3S—C5S	1.759(10)
C1—O2	1.249(10)	S3S—C6S	1.771(10)
O1W—La—O6^{i}	138.01(13)	O2^{i}—La—O2^{ii}	109.24(14)
O1W—La—O6	138.01(13)	O2—La—O2^{ii}	109.24(14)
O6^{i}—La—O6	70.8(2)	O3—Cu—O5^{iii}	175.0(2)
O1W—La—O6^{ii}	138.01(13)	O3—Cu—O1	85.6(2)
O6^{i}—La—O6^{ii}	70.8(2)	O5^{iii}—Cu—O1	92.2(2)
O6—La—O6^{ii}	70.8(2)	O3—Cu—O3^{iii}	95.9(3)
O1W—La—O4^{i}	93.19(11)	O5^{iii}—Cu—O3^{iii}	85.6(2)
O6^{i}—La—O4^{i}	62.73(16)	O1—Cu—O3^{iii}	170.4(3)
O6—La—O4^{i}	73.44(16)	O3—Cu—O1S	81.1(2)
O6^{ii}—La—O4^{i}	128.25(17)	O5^{iii}—Cu—O1S	103.9(2)
O1W—La—O4^{ii}	93.19(11)	O1—Cu—O1S	108.8(2)
O6^{i}—La—O4^{ii}	73.44(16)	O3^{iii}—Cu—O1S	80.8(2)
O6—La—O4^{ii}	128.25(17)	O1—C1—O2	125.3(8)
O6^{ii}—La—O4^{ii}	62.73(16)	O1—C1—C2	118.5(7)
O4^{i}—La—O4^{ii}	119.69(2)	O2—C1—C2	116.1(7)
O1W—La—O4	93.19(11)	C1—O1—Cu	111.1(5)
O6^{i}—La—O4	128.25(17)	C1—O2—La	118.9(5)
O6—La—O4	62.73(16)	O3—C2—O4	113.7(6)
O6^{ii}—La—O4	73.44(16)	O3—C2—C1	110.8(6)
O4^{i}—La—O4	119.69(2)	O4—C2—C1	108.8(6)
O4^{ii}—La—O4	119.69(2)	O3—C2—C3	111.4(6)
O1W—La—O2^{i}	70.30(14)	O4—C2—C3	104.1(6)
O6^{i}—La—O2^{i}	68.00(19)	C1—C2—C3	107.7(6)
O6—La—O2^{i}	129.02(17)	C2—O3—Cu	111.7(4)
O6^{ii}—La—O2^{i}	119.78(19)	C2—O3—Cu^{iv}	111.3(4)
O4^{i}—La—O2^{i}	61.71(16)	Cu—O3—Cu^{iv}	114.5(3)
O4^{ii}—La—O2^{i}	64.65(18)	C2—O4—La	107.4(4)
O4—La—O2^{i}	163.41(19)	O6—C3—O5	124.9(7)
O1W—La—O2	70.30(14)	O6—C3—C2	118.0(7)
O6^{i}—La—O2	119.78(19)	O5—C3—C2	117.2(6)
O6—La—O2	68.00(19)	C3—O5—Cu^{iv}	111.2(4)
O6^{ii}—La—O2	129.02(17)	C3—O6—La	118.2(5)
O4^{i}—La—O2	64.65(18)	O1S—S1S—C2S	107.6(14)
O4^{ii}—La—O2	163.41(19)	O1S—S1S—C1S	106.8(12)
O4—La—O2	61.71(16)	C2S—S1S—C1S	99.6(11)
O2^{i}—La—O2	109.24(14)	S1S—O1S—Cu	138.1(14)
O1W—La—O2^{ii}	70.30(14)	O2S—S2S—C3S	108.9(12)
O6^{i}—La—O2^{ii}	129.02(17)	O2S—S2S—C4S	108.4(13)
O6—La—O2^{ii}	119.78(19)	C3S—S2S—C4S	98.(1)
O6^{ii}—La—O2^{ii}	68.00(19)	O3S—S3S—C5S	108.9(13)
O4^{i}—La—O2^{ii}	163.41(19)	O3S—S3S—C6S	107.7(13)
O4^{ii}—La—O2^{ii}	61.71(16)	C5S—S3S—C6S	100.3(11)
O4—La—O2^{ii}	64.65(18)		

(i) y, z, x; (ii) z, x, y; (iii) -0.5+y, 0.5-z, -x; (iv) -z, 0.5+x, 0.5-y.

Table S2. Selected distances and angles for compound **$CeCu_3$**

C1—O1	1.249(6)	O5—Ce1	2.557(3)
C1—O2	1.258(6)	O4—Ce1	2.642(3)
C1—C2	1.539(7)	O2—Ce1	2.582(4)
C2—O3	1.389(6)	O1—Cu1^{i}	1.943(4)
C2—O4	1.402(6)	O1S—S1	1.395(8)
C2—C3	1.542(7)	Cu1—O1^{ii}	1.943(4)
C3—O6	1.234(6)	Cu1—O3^{ii}	1.956(3)
C3—O5	1.235(6)	Ce1—O5^{iii}	2.557(3)
C1S—S1	1.772(10)	Ce1—O5^{iv}	2.557(3)
C2S—S1	1.776(10)	Ce1—O2^{iii}	2.582(4)
O6—Cu1	1.940(3)	Ce1—O2^{iv}	2.582(4)
O3—Cu1	1.937(3)	Ce1—O4^{iii}	2.642(3)
O3—Cu1^{i}	1.956(3)	Ce1—O4^{iv}	2.642(3)
O1W—Ce1	2.487(8)		
O1—C1—O2	125.8(5)	O5—Ce1—O2	68.33(12)
O1—C1—C2	118.4(4)	O5^{iv}—Ce1—O2	120.48(12)
O2—C1—C2	115.8(5)	O1W—Ce1—O2^{iii}	69.88(9)
O3—C2—O4	112.3(4)	O5^{iii}—Ce1—O2^{iii}	68.33(12)
O3—C2—C1	110.7(4)	O5—Ce1—O2^{iii}	120.48(12)
O4—C2—C1	105.9(4)	O5^{iv}—Ce1—O2^{iii}	128.94(11)
O3—C2—C3	111.8(4)	O2—Ce1—O2^{iii}	108.81(9)
O4—C2—C3	106.0(4)	O1W—Ce1—O2^{iv}	69.88(9)
C1—C2—C3	109.9(4)	O5^{iii}—Ce1—O2^{iv}	120.48(12)
O6—C3—O5	126.1(5)	O5—Ce1—O2^{iv}	128.94(11)
O6—C3—C2	117.5(4)	O5^{iv}—Ce1—O2^{iv}	68.33(12)
O5—C3—C2	116.5(4)	O2—Ce1—O2^{iv}	108.81(9)
C3—O6—Cu1	112.1(3)	O2^{iii}—Ce1—O2^{iv}	108.81(9)
C2—O3—Cu1	110.1(3)	O1W—Ce1—O4^{iii}	92.95(8)
C2—O3—Cu1^{i}	111.2(3)	O5^{iii}—Ce1—O4^{iii}	62.9(1)
Cu1—O3—Cu1^{i}	114.64(17)	O5—Ce1—O4^{iii}	128.53(11)
C3—O5—Ce1	119.3(3)	O5^{iv}—Ce1—O4^{iii}	73.63(11)
C2—O4—Ce1	106.5(3)	O2—Ce1—O4^{iii}	162.69(12)
C1—O2—Ce1	119.8(3)	O2^{iii}—Ce1—O4^{iii}	61.15(11)
C1—O1—Cu1^{i}	111.4(3)	O2^{iv}—Ce1—O4^{iii}	65.22(12)
O1S—S1—C1S	110.1(13)	O1W—Ce1—O4^{iv}	92.95(8)
O1S—S1—C2S	109.5(11)	O5^{iii}—Ce1—O4^{iv}	128.53(11)
C1S—S1—C2S	98.7(11)	O5—Ce1—O4^{iv}	73.63(11)
O3—Cu1—O6	85.72(14)	O5^{iv}—Ce1—O4^{iv}	62.9(1)
O3—Cu1—O1^{ii}	170.71(18)	O2—Ce1—O4^{iv}	65.22(12)
O6—Cu1—O1^{ii}	92.18(16)	O2^{iii}—Ce1—O4^{iv}	162.69(12)
O3—Cu1—O3^{ii}	95.93(18)	O2^{iv}—Ce1—O4^{iv}	61.15(11)
O6—Cu1—O3^{ii}	175.39(16)	O4^{iii}—Ce1—O4^{iv}	119.738(14)
O1^{ii}—Cu1—O3^{ii}	85.51(14)	O1W—Ce1—O4	92.95(8)
O1W—Ce1—O5^{iii}	137.96(8)	O5^{iii}—Ce1—O4	73.63(11)
O1W—Ce1—O5	137.96(8)	O5—Ce1—O4	62.9(1)
O5^{iii}—Ce1—O5	70.88(13)	O5^{iv}—Ce1—O4	128.53(11)
O1W—Ce1—O5^{iv}	137.96(8)	O2—Ce1—O4	61.15(11)
O5^{iii}—Ce1—O5^{iv}	70.88(13)	O2^{iii}—Ce1—O4	65.22(12)
O5—Ce1—O5^{iv}	70.88(13)	O2^{iv}—Ce1—O4	162.69(12)
O1W—Ce1—O2	69.88(9)	O4^{iii}—Ce1—O4	119.738(14)
O5^{iii}—Ce1—O2	128.94(11)	O4^{iv}—Ce1—O4	119.738(14)

(i) 0.5+y, 0.5-z, 1-x; (ii) 1-z, -0.5+x, 0.5-y; (iii) z, x, y; (iv) y, z, x.

Table S3. Selected distances and angles for compound **$PrCu_3$**

Cu1—O3	1.912(9)	C2—O4	1.349(18)
Cu1—O3^{i}	1.949(9)	C2—O3	1.397(17)
Cu1—O1^{i}	1.957(11)	C2—C3	1.53(2)
Cu1—O6	1.98(1)	C2—C1	1.63(2)
Pr1—O1W	2.46(3)	C3—O6	1.221(17)
Pr1—O5^{ii}	2.532(10)	C3—O5	1.280(16)
Pr1—O5	2.532(10)	C1—O1	1.20(2)
Pr1—O5^{iii}	2.532(10)	C1—O2	1.32(2)
Pr1—O2^{ii}	2.570(12)	O3—Cu1^{iv}	1.949(9)
Pr1—O2	2.570(12)	O1—Cu1^{iv}	1.957(11)
Pr1—O2^{iii}	2.570(12)	S1—O1S	1.467(15)
Pr1—O4^{iii}	2.624(11)	S1—C1S	1.76(2)
Pr1—O4	2.624(11)	S1—C2S	1.779(14)
Pr1—O4^{ii}	2.624(11)		
O3—Cu1—O3^{i}	95.5(5)	O5^{iii}—Pr1—O4	73.3(3)
O3—Cu1—O1^{i}	172.6(5)	O2^{ii}—Pr1—O4	161.1(3)
O3^{i}—Cu1—O1^{i}	86.2(4)	O2—Pr1—O4	61.6(3)
O3—Cu1—O6	86.3(4)	O2^{iii}—Pr1—O4	65.4(4)
O3^{i}—Cu1—O6	176.8(4)	O4^{iii}—Pr1—O4	119.76(3)
O1^{i}—Cu1—O6	91.7(5)	O1W—Pr1—O4^{ii}	92.8(2)
O1W—Pr1—O5^{ii}	138.4(2)	O5^{ii}—Pr1—O4^{ii}	63.7(3)
O1W—Pr1—O5	138.4(2)	O5—Pr1—O4^{ii}	73.3(3)
O5^{ii}—Pr1—O5	70.3(4)	O5^{iii}—Pr1—O4^{ii}	128.4(3)
O1W—Pr1—O5^{iii}	138.4(2)	O2^{ii}—Pr1—O4^{ii}	61.6(3)
O5^{ii}—Pr1—O5^{iii}	70.3(4)	O2—Pr1—O4^{ii}	65.4(4)
O5—Pr1—O5^{iii}	70.3(4)	O2^{iii}—Pr1—O4^{ii}	161.1(3)
O1W—Pr1—O2^{ii}	68.4(3)	O4^{iii}—Pr1—O4^{ii}	119.76(4)
O5^{ii}—Pr1—O2^{ii}	70.1(4)	O4—Pr1—O4^{ii}	119.76(3)
O5—Pr1—O2^{ii}	129.5(3)	O4—C2—O3	116.4(13)
O5^{iii}—Pr1—O2^{ii}	122.0(4)	O4—C2—C3	108.0(13)
O1W—Pr1—O2	68.4(3)	O3—C2—C3	110.8(13)
O5^{ii}—Pr1—O2	122.0(4)	O4—C2—C1	106.4(13)
O5—Pr1—O2	70.1(4)	O3—C2—C1	107.8(12)
O5^{iii}—Pr1—O2	129.5(3)	C3—C2—C1	107.0(13)
O2^{ii}—Pr1—O2	107.2(3)	O6—C3—O5	123.0(14)
O1W—Pr1—O2^{iii}	68.4(3)	O6—C3—C2	120.6(13)
O5^{ii}—Pr1—O2^{iii}	129.5(3)	O5—C3—C2	116.3(13)
O5—Pr1—O2^{iii}	122.0(4)	O1—C1—O2	127.6(16)
O5^{iii}—Pr1—O2^{iii}	70.1(4)	O1—C1—C2	119.3(14)
O2^{ii}—Pr1—O2^{iii}	107.2(3)	O2—C1—C2	112.7(15)
O2—Pr1—O2^{iii}	107.2(3)	C2—O3—Cu1	110.0(9)
O1W—Pr1—O4^{iii}	92.8(2)	C2—O3—Cu1^{iv}	112.3(9)
O5^{ii}—Pr1—O4^{iii}	73.3(3)	Cu1—O3—Cu1^{iv}	116.0(4)
O5—Pr1—O4^{iii}	128.4(3)	C2—O4—Pr1	108.2(9)
O5^{iii}—Pr1—O4^{iii}	63.7(3)	C1—O2—Pr1	119.7(10)
O2^{ii}—Pr1—O4^{iii}	65.4(4)	C3—O5—Pr1	118.1(9)
O2—Pr1—O4^{iii}	161.1(3)	C3—O6—Cu1	108.5(10)
O2^{iii}—Pr1—O4^{iii}	61.6(3)	C1—O1—Cu1^{iv}	111.8(11)
O1W—Pr1—O4	92.8(2)	O1S—S1—C1S	110.0(18)
O5^{ii}—Pr1—O4	128.4(3)	O1S—S1—C2S	108.0(13)
O5—Pr1—O4	63.7(3)	C1S—S1—C2S	99.6(13)

(i) 1.5-z, 1-x, 0.5+y; (ii) 0.5-y, 1-z, 0.5+x; (iii) -0.5+z, 0.5-x, 1-y; (iv) 1-y, -0.5+z, 1.5-x.

Table S4. Selected distances and angles for compound **$NdCu_3$**

C1—O1	1.239(9)	O4—Nd	2.606(5)
C1—O2	1.261(8)	O2—Nd	2.548(6)
C1—C2	1.527(10)	O1—Cu1^{i}	1.936(6)
C2—O3	1.373(7)	O1W—Nd	2.489(17)
C2—O4	1.403(7)	O1S—S1	1.503(12)
C2—C3	1.569(9)	Nd—O5^{ii}	2.503(5)
C3—O5	1.245(8)	Nd—O5^{iii}	2.503(5)
C3—O6	1.242(8)	Nd—O2^{ii}	2.548(6)
C1S—S1	1.772(10)	Nd—O2^{iii}	2.548(6)
C2S—S1	2.66(5)	Nd—O4^{iii}	2.606(5)
O6—Cu1	1.937(5)	Nd—O4^{ii}	2.606(5)
O5—Nd	2.503(5)	Cu1—O1^{iv}	1.936(6)
O3—Cu1	1.940(4)	Cu1—O3^{iv}	1.949(4)
O3—Cu1^{i}	1.949(4)		
O1—C1—O2	125.6(7)	O2—Nd—O2^{ii}	108.36(15)
O1—C1—C2	119.3(6)	O1W—Nd—O2^{iii}	69.44(14)
O2—C1—C2	114.9(6)	O5—Nd—O2^{iii}	128.83(16)
O3—C2—O4	113.5(5)	O5^{ii}—Nd—O2^{iii}	121.18(18)
O3—C2—C1	111.2(5)	O5^{iii}—Nd—O2^{iii}	68.90(18)
O4—C2—C1	107.1(6)	O2—Nd—O2^{iii}	108.36(15)
O3—C2—C3	111.5(5)	O2^{ii}—Nd—O2^{iii}	108.36(15)
O4—C2—C3	105.2(5)	O1W—Nd—O4^{iii}	92.42(11)
C1—C2—C3	107.9(6)	O5—Nd—O4^{iii}	73.50(15)
O5—C3—O6	127.3(6)	O5^{ii}—Nd—O4^{iii}	128.98(16)
O5—C3—C2	115.6(5)	O5^{iii}—Nd—O4^{iii}	63.93(15)
O6—C3—C2	117.1(6)	O2—Nd—O4^{iii}	64.84(16)
C3—O6—Cu1	111.6(4)	O2^{ii}—Nd—O4^{iii}	161.76(19)
C3—O5—Nd	119.9(4)	O2^{iii}—Nd—O4^{iii}	61.31(15)
C2—O3—Cu1	110.5(4)	O1W—Nd—O4	92.42(11)
C2—O3—Cu1^{i}	110.9(3)	O5—Nd—O4	63.93(15)
Cu1—O3—Cu1^{i}	114.6(2)	O5^{ii}—Nd—O4	73.50(15)
C2—O4—Nd	106.9(3)	O5^{iii}—Nd—O4	128.98(16)
C1—O2—Nd	120.5(5)	O2—Nd—O4	61.31(15)
C1—O1—Cu1^{i}	111.2(5)	O2^{ii}—Nd—O4	64.84(16)
O1S—S1—C1S	106.9(12)	O2^{iii}—Nd—O4	161.76(19)
O1S—S1—C2S	73.4(16)	O4^{iii}—Nd—O4	119.823(16)
C1S—S1—C2S	71.6(14)	O1W—Nd—O4^{ii}	92.42(11)
O1W—Nd—O5	138.15(12)	O5—Nd—O4^{ii}	128.98(16)
O1W—Nd—O5^{ii}	138.15(12)	O5^{ii}—Nd—O4^{ii}	63.93(15)
O5—Nd—O5^{ii}	70.60(18)	O5^{iii}—Nd—O4^{ii}	73.50(15)
O1W—Nd—O5^{iii}	138.15(12)	O2—Nd—O4^{ii}	161.76(19)
O5—Nd—O5^{iii}	70.60(18)	O2^{ii}—Nd—O4^{ii}	61.31(15)
O5^{ii}—Nd—O5^{iii}	70.60(18)	O2^{iii}—Nd—O4^{ii}	64.84(16)
O1W—Nd—O2	69.44(14)	O4^{iii}—Nd—O4^{ii}	119.823(16)
O5—Nd—O2	68.90(18)	O4—Nd—O4^{ii}	119.823(16)
O5^{ii}—Nd—O2	128.83(16)	O6—Cu1—O3	86.1(2)
O5^{iii}—Nd—O2	121.18(18)	O6—Cu1—O1^{iv}	91.8(2)
O1W—Nd—O2^{ii}	69.44(14)	O3—Cu1—O1^{iv}	170.3(3)
O5—Nd—O2^{ii}	121.18(18)	O6—Cu1—O3^{iv}	175.9(2)
O5^{ii}—Nd—O2^{ii}	68.90(18)	O3—Cu1—O3^{iv}	95.7(2)
O5^{iii}—Nd—O2^{ii}	128.83(16)	O1^{iv}—Cu1—O3^{iv}	85.7(2)

(i) y, 1+z, -1+x; (ii) 0.5+z, 1.5-x, 1-y; (iii) 1.5-y, 1-z, -0.5+x; (iv) 1+z, x, -1+y.

Table S5. Selected distances and angles for compound **$EuCu_3$**

C1A—O2A	1.264(12)	C3E—O6E	1.264(14)
C1A—O1A	1.270(13)	C3E—Eu3	3.172(11)
C1A—C2A	1.521(11)	C3F—O6F	1.239(14)
C1A—Eu1	3.165(10)	C3F—O5F	1.251(13)
C1B—O1B	1.249(13)	C3F—O4FX	1.466(19)
C1B—O2B	1.251(13)	Cu1—O6C	1.937(8)
C1B—C2B	1.528(14)	Cu1—O3A	1.944(6)
C1B—Eu2	3.263(10)	Cu1—O1A	1.944(7)
C1C—O2C	1.214(13)	Cu1—O3C	1.945(6)
C1C—O1C	1.283(14)	Cu1—O1S	2.355(7)
C1C—O4CX	1.529(19)	Cu2—O1B	1.907(7)
C1C—C2C	1.556(13)	Cu2—O3A	1.940(6)
C1D—O2D	1.247(14)	Cu2—O6A	1.943(7)
C1D—O1D	1.260(14)	Cu2—O3B	1.955(6)
C1D—C2D	1.531(12)	Cu3—O1C	1.926(8)
C1D—Eu2	3.193(11)	Cu3—O6B	1.944(8)
C1E—O1E	1.253(12)	Cu3—O3C	1.947(6)
C1E—O2E	1.253(13)	Cu3—O3B	1.983(6)
C1E—C2E	1.539(13)	Cu4—O6F	1.922(7)
C1E—Eu3	3.238(10)	Cu4—O1D	1.937(8)
C1F—O1F	1.231(13)	Cu4—O3F	1.962(6)
C1F—O2F	1.260(13)	Cu4—O3D	1.963(6)
C1F—O4FX	1.539(17)	Cu4—O2S	2.313(7)
C1F—C2F	1.555(12)	Cu5—O1E	1.917(7)
C1S1—S1	1.769(9)	Cu5—O6D	1.919(7)
C1S2—S1	1.779(9)	Cu5—O3D	1.941(6)
C2A—O3A	1.39(1)	Cu5—O3E	1.951(6)
C2A—O4A	1.409(10)	Cu6—O3F	1.930(6)
C2A—C3A	1.577(12)	Cu6—O6E	1.935(7)
C2A—Eu1	3.149(9)	Cu6—O1F	1.946(8)
C2B—O3B	1.37(1)	Cu6—O3E	1.978(6)
C2B—O4B	1.419(11)	Eu1—O1W	2.327(10)
C2B—C3B	1.527(13)	Eu1—O1W^{i}	2.327(10)
C2C—O3C	1.370(11)	Eu1—O2A	2.388(8)
C2C—O4C	1.408(13)	Eu1—O2A^{i}	2.388(8)
C2C—C3C	1.567(13)	Eu1—O4A^{i}	2.469(6)
C2C—O4CX	1.780(17)	Eu1—O4A	2.469(6)
C2D—O3D	1.386(10)	Eu1—O5A	2.583(8)
C2D—O4D	1.405(11)	Eu1—O5A^{i}	2.583(8)
C2D—C3D	1.562(14)	Eu1—C2A^{i}	3.149(9)
C2D—Eu2	3.181(9)	Eu1—C1A^{i}	3.165(10)
C2E—O3E	1.359(10)	Eu2—O3W	2.293(10)
C2E—O4E	1.400(12)	Eu2—O2W	2.31(1)
C2E—C3E	1.555(12)	Eu2—O5B	2.375(9)
C2F—O3F	1.389(9)	Eu2—O2D	2.436(9)
C2F—O4F	1.393(13)	Eu2—O4D	2.483(7)
C2F—C3F	1.571(12)	Eu2—O2B	2.495(8)
C2F—O4FX	1.720(16)	Eu2—O5D	2.608(9)
C2S1—S2	1.771(8)	Eu2—O4B	2.692(7)
C2S2—S2	1.780(9)	Eu3—O5E	2.333(9)
C3A—O5A	1.229(11)	Eu3—O5E^{ii}	2.333(9)
C3A—O6A	1.264(12)	Eu3—O4W^{ii}	2.352(12)
C3B—O5B	1.227(14)	Eu3—O4W	2.352(12)
C3B—O6B	1.259(15)	Eu3—O2E	2.445(8)
C3B—Eu2	3.175(12)	Eu3—O2E^{ii}	2.445(8)
C3C—O5C	1.235(13)	Eu3—O4E^{ii}	2.753(8)
C3C—O6C	1.256(14)	Eu3—O4E	2.753(8)
C3C—O4CX	1.547(18)	Eu3—C3E^{ii}	3.172(11)
C3D—O5D	1.218(13)	Eu3—C1E^{ii}	3.238(10)
C3D—O6D	1.265(13)	O1S—S1	1.536(7)
C3E—O5E	1.255(13)	O2S—S2	1.539(7)
O2A—C1A—O1A	124.1(9)	O1W^{i}—Eu1—C1A	103.7(3)

O2A—C1A—C2A	117.6(9)	O2A—Eu1—C1A	20.9(2)
O1A—C1A—C2A	118.3(8)	O2A^{i}—Eu1—C1A	101.9(3)
O2A—C1A—Eu1	42.3(5)	O4A^{i}—Eu1—C1A	90.4(2)
O1A—C1A—Eu1	164.5(7)	O4A—Eu1—C1A	47.1(2)
C2A—C1A—Eu1	75.5(5)	O5A—Eu1—C1A	60.6(3)
O1B—C1B—O2B	124.(1)	O5A^{i}—Eu1—C1A	156.6(2)
O1B—C1B—C2B	116.4(9)	C2A^{i}—Eu1—C1A	110.5(2)
O2B—C1B—C2B	119.6(9)	C2A—Eu1—C1A	27.9(2)
O1B—C1B—Eu2	166.8(8)	O1W—Eu1—C1A^{i}	103.7(3)
O2B—C1B—Eu2	42.8(5)	O1W^{i}—Eu1—C1A^{i}	126.8(3)
C2B—C1B—Eu2	76.8(5)	O2A—Eu1—C1A^{i}	101.9(3)
O2C—C1C—O1C	123.6(10)	O2A^{i}—Eu1—C1A^{i}	20.9(2)
O2C—C1C—O4CX	94.3(11)	O4A^{i}—Eu1—C1A^{i}	47.1(2)
O1C—C1C—O4CX	104.5(10)	O4A—Eu1—C1A^{i}	90.4(2)
O2C—C1C—C2C	122.1(10)	O5A—Eu1—C1A^{i}	156.6(2)
O1C—C1C—C2C	114.3(8)	O5A^{i}—Eu1—C1A^{i}	60.6(3)
O4CX—C1C—C2C	70.5(8)	C2A^{i}—Eu1—C1A^{i}	27.9(2)
O2D—C1D—O1D	123.4(9)	C2A—Eu1—C1A^{i}	110.5(2)
O2D—C1D—C2D	118.1(9)	C1A—Eu1—C1A^{i}	105.8(4)
O1D—C1D—C2D	118.4(9)	O3W—Eu2—O2W	91.4(5)
O2D—C1D—Eu2	43.1(6)	O3W—Eu2—O5B	94.1(4)
O1D—C1D—Eu2	165.6(7)	O2W—Eu2—O5B	145.2(3)
C2D—C1D—Eu2	75.7(5)	O3W—Eu2—O2D	144.0(3)
O1E—C1E—O2E	123.3(10)	O2W—Eu2—O2D	109.2(5)
O1E—C1E—C2E	117.1(8)	O5B—Eu2—O2D	85.6(4)
O2E—C1E—C2E	119.7(9)	O3W—Eu2—O4D	92.3(3)
O1E—C1E—Eu3	164.8(7)	O2W—Eu2—O4D	76.3(3)
O2E—C1E—Eu3	41.5(5)	O5B—Eu2—O4D	137.6(3)
C2E—C1E—Eu3	78.2(5)	O2D—Eu2—O4D	65.8(3)
O1F—C1F—O2F	123.8(9)	O3W—Eu2—O2B	143.6(3)
O1F—C1F—O4FX	110.1(10)	O2W—Eu2—O2B	80.0(4)
O2F—C1F—O4FX	88.5(9)	O5B—Eu2—O2B	75.3(3)
O1F—C1F—C2F	117.4(8)	O2D—Eu2—O2B	70.9(3)
O2F—C1F—C2F	118.8(8)	O4D—Eu2—O2B	119.2(2)
O4FX—C1F—C2F	67.5(7)	O3W—Eu2—O5D	75.0(3)
O3A—C2A—O4A	113.1(7)	O2W—Eu2—O5D	138.1(3)
O3A—C2A—C1A	111.8(7)	O5B—Eu2—O5D	76.3(3)
O4A—C2A—C1A	106.1(7)	O2D—Eu2—O5D	70.0(3)
O3A—C2A—C3A	110.5(6)	O4D—Eu2—O5D	65.1(2)
O4A—C2A—C3A	107.8(7)	O2B—Eu2—O5D	132.8(4)
C1A—C2A—C3A	107.3(7)	O3W—Eu2—O4B	80.0(3)
O3A—C2A—Eu1	162.2(6)	O2W—Eu2—O4B	84.6(3)
O4A—C2A—Eu1	49.1(4)	O5B—Eu2—O4B	62.7(3)
C1A—C2A—Eu1	76.7(5)	O2D—Eu2—O4B	129.7(2)
C3A—C2A—Eu1	80.3(5)	O4D—Eu2—O4B	159.2(2)
O3B—C2B—O4B	113.1(8)	O2B—Eu2—O4B	64.1(2)
O3B—C2B—C3B	112.6(8)	O5D—Eu2—O4B	129.7(2)
O4B—C2B—C3B	101.2(7)	O3W—Eu2—C3B	96.3(4)
O3B—C2B—C1B	111.2(7)	O2W—Eu2—C3B	125.7(3)
O4B—C2B—C1B	108.2(8)	O5B—Eu2—C3B	19.5(3)
C3B—C2B—C1B	109.9(9)	O2D—Eu2—C3B	95.1(3)
O3C—C2C—O4C	112.2(8)	O4D—Eu2—C3B	156.0(3)
O3C—C2C—C1C	111.4(8)	O2B—Eu2—C3B	62.8(3)
O4C—C2C—C1C	109.2(8)	O5D—Eu2—C3B	95.5(3)
O3C—C2C—C3C	111.9(8)	O4B—Eu2—C3B	44.8(3)
O4C—C2C—C3C	104.8(8)	O3W—Eu2—C2D	100.7(3)
C1C—C2C—C3C	107.1(9)	O2W—Eu2—C2D	99.7(3)
O3C—C2C—O4CX	117.5(9)	O5B—Eu2—C2D	112.9(3)
O4C—C2C—O4CX	130.3(9)	O2D—Eu2—C2D	48.1(2)
C1C—C2C—O4CX	54.0(7)	O4D—Eu2—C2D	25.1(2)
C3C—C2C—O4CX	54.6(7)	O2B—Eu2—C2D	115.5(3)
O3D—C2D—O4D	112.9(8)	O5D—Eu2—C2D	47.0(2)
O3D—C2D—C1D	110.9(8)	O4B—Eu2—C2D	175.7(2)
O4D—C2D—C1D	104.4(8)	C3B—Eu2—C2D	131.0(3)
O3D—C2D—C3D	111.6(7)	O3W—Eu2—C1D	127.3(3)

O4D—C2D—C3D	108.4(8)	O2W—Eu2—C1D	104.3(4)
C1D—C2D—C3D	108.4(8)	O5B—Eu2—C1D	99.5(3)
O3D—C2D—Eu2	161.2(6)	O2D—Eu2—C1D	20.5(3)
O4D—C2D—Eu2	48.5(4)	O4D—Eu2—C1D	46.2(3)
C1D—C2D—Eu2	76.5(5)	O2B—Eu2—C1D	89.1(3)
C3D—C2D—Eu2	80.8(5)	O5D—Eu2—C1D	59.7(3)
O3E—C2E—O4E	115.1(8)	O4B—Eu2—C1D	150.1(2)
O3E—C2E—C1E	110.5(7)	C3B—Eu2—C1D	112.6(3)
O4E—C2E—C1E	107.9(7)	C2D—Eu2—C1D	27.8(2)
O3E—C2E—C3E	112.5(7)	O3W—Eu2—C1B	126.0(3)
O4E—C2E—C3E	102.3(7)	O2W—Eu2—C1B	87.7(3)
C1E—C2E—C3E	108.1(8)	O5B—Eu2—C1B	61.5(3)
O3F—C2F—O4F	112.1(7)	O2D—Eu2—C1B	85.2(3)
O3F—C2F—C1F	108.9(7)	O4D—Eu2—C1B	139.1(3)
O4F—C2F—C1F	110.4(7)	O2B—Eu2—C1B	19.9(3)
O3F—C2F—C3F	111.1(7)	O5D—Eu2—C1B	132.5(3)
O4F—C2F—C3F	106.2(8)	O4B—Eu2—C1B	46.1(2)
C1F—C2F—C3F	108.0(8)	C3B—Eu2—C1B	45.7(3)
O3F—C2F—O4FX	119.7(8)	C2D—Eu2—C1B	132.7(2)
O4F—C2F—O4FX	128.1(8)	C1D—Eu2—C1B	105.0(3)
C1F—C2F—O4FX	55.8(7)	O5E—Eu3—O5E^{ii}	92.5(5)
C3F—C2F—O4FX	52.7(7)	O5E—Eu3—O4W^{ii}	86.8(4)
O5A—C3A—O6A	127.3(9)	O5E^{ii}—Eu3—O4W^{ii}	140.6(3)
O5A—C3A—C2A	117.0(9)	O5E—Eu3—O4W	140.6(3)
O6A—C3A—C2A	115.8(7)	O5E^{ii}—Eu3—O4W	86.8(4)
O5B—C3B—O6B	122.5(10)	O4W^{ii}—Eu3—O4W	117.5(8)
O5B—C3B—C2B	119.8(10)	O5E—Eu3—O2E	76.2(3)
O6B—C3B—C2B	117.6(9)	O5E^{ii}—Eu3—O2E	143.6(3)
O5B—C3B—Eu2	40.2(6)	O4W^{ii}—Eu3—O2E	74.1(3)
O6B—C3B—Eu2	161.8(7)	O4W—Eu3—O2E	81.2(4)
C2B—C3B—Eu2	79.8(6)	O5E—Eu3—O2E^{ii}	143.6(3)
O5C—C3C—O6C	126.2(10)	O5E^{ii}—Eu3—O2E^{ii}	76.2(3)
O5C—C3C—O4CX	84.5(10)	O4W^{ii}—Eu3—O2E^{ii}	81.2(4)
O6C—C3C—O4CX	112.5(11)	O4W—Eu3—O2E^{ii}	74.1(3)
O5C—C3C—C2C	117.7(10)	O2E—Eu3—O2E^{ii}	131.6(4)
O6C—C3C—C2C	116.0(8)	O5E—Eu3—O4E^{ii}	79.9(2)
O4CX—C3C—C2C	69.7(8)	O5E^{ii}—Eu3—O4E^{ii}	62.6(3)
O5D—C3D—O6D	128.9(10)	O4W^{ii}—Eu3—O4E^{ii}	78.5(4)
O5D—C3D—C2D	116.3(9)	O4W—Eu3—O4E^{ii}	132.5(3)
O6D—C3D—C2D	114.8(8)	O2E—Eu3—O4E^{ii}	144.4(3)
O5E—C3E—O6E	124.(1)	O2E^{ii}—Eu3—O4E^{ii}	64.1(2)
O5E—C3E—C2E	119.2(9)	O5E—Eu3—O4E	62.6(3)
O6E—C3E—C2E	116.8(8)	O5E^{ii}—Eu3—O4E	79.9(2)
O5E—C3E—Eu3	38.9(5)	O4W^{ii}—Eu3—O4E	132.5(3)
O6E—C3E—Eu3	162.7(7)	O4W—Eu3—O4E	78.5(4)
C2E—C3E—Eu3	80.3(5)	O2E—Eu3—O4E	64.1(2)
O6F—C3F—O5F	126.8(9)	O2E^{ii}—Eu3—O4E	144.4(3)
O6F—C3F—O4FX	114.3(11)	O4E^{ii}—Eu3—O4E	125.4(3)
O5F—C3F—O4FX	85.9(10)	O5E—Eu3—C3E^{ii}	96.2(3)
O6F—C3F—C2F	116.8(8)	O5E^{ii}—Eu3—C3E^{ii}	19.7(3)
O5F—C3F—C2F	116.4(9)	O4W^{ii}—Eu3—C3E^{ii}	121.2(3)
O4FX—C3F—C2F	68.9(8)	O4W—Eu3—C3E^{ii}	96.2(4)
O6C—Cu1—O3A	170.9(3)	O2E—Eu3—C3E^{ii}	162.9(3)
O6C—Cu1—O1A	90.1(3)	O2E^{ii}—Eu3—C3E^{ii}	62.5(3)
O3A—Cu1—O1A	85.9(3)	O4E^{ii}—Eu3—C3E^{ii}	45.0(2)
O6C—Cu1—O3C	85.4(3)	O4E—Eu3—C3E^{ii}	98.8(2)
O3A—Cu1—O3C	96.8(3)	O5E—Eu3—C3E	19.7(3)
O1A—Cu1—O3C	167.7(3)	O5E^{ii}—Eu3—C3E	96.2(3)
O6C—Cu1—O1S	106.1(3)	O4W^{ii}—Eu3—C3E	96.2(4)
O3A—Cu1—O1S	82.9(2)	O4W—Eu3—C3E	121.2(3)
O1A—Cu1—O1S	106.1(3)	O2E—Eu3—C3E	62.5(3)
O3C—Cu1—O1S	86.1(3)	O2E^{ii}—Eu3—C3E	162.9(3)
O1B—Cu2—O3A	172.0(3)	O4E^{ii}—Eu3—C3E	98.8(2)
O1B—Cu2—O6A	91.1(3)	O4E—Eu3—C3E	45.0(2)
O3A—Cu2—O6A	85.0(3)	C3E^{ii}—Eu3—C3E	105.8(4)

O1B—Cu2—O3B	84.3(3)	O5E—Eu3—C1E	62.8(3)
O3A—Cu2—O3B	98.7(3)	O5E^{ii}—Eu3—C1E	125.7(3)
O6A—Cu2—O3B	172.5(3)	O4W^{ii}—Eu3—C1E	88.7(3)
O1C—Cu3—O6B	90.3(4)	O4W—Eu3—C1E	85.9(3)
O1C—Cu3—O3C	84.3(3)	O2E—Eu3—C1E	19.8(3)
O6B—Cu3—O3C	174.2(3)	O2E^{ii}—Eu3—C1E	150.0(3)
O1C—Cu3—O3B	170.2(3)	O4E^{ii}—Eu3—C1E	141.3(2)
O6B—Cu3—O3B	84.7(3)	O4E—Eu3—C1E	45.9(2)
O3C—Cu3—O3B	100.9(3)	C3E^{ii}—Eu3—C1E	143.6(3)
O6F—Cu4—O1D	90.2(3)	C3E—Eu3—C1E	46.0(3)
O6F—Cu4—O3F	85.6(3)	O5E—Eu3—C1E^{ii}	125.7(3)
O1D—Cu4—O3F	169.0(4)	O5E^{ii}—Eu3—C1E^{ii}	62.8(3)
O6F—Cu4—O3D	169.1(3)	O4W^{ii}—Eu3—C1E^{ii}	85.9(3)
O1D—Cu4—O3D	85.5(3)	O4W—Eu3—C1E^{ii}	88.7(3)
O3F—Cu4—O3D	96.8(3)	O2E—Eu3—C1E^{ii}	150.0(3)
O6F—Cu4—O2S	105.9(3)	O2E^{ii}—Eu3—C1E^{ii}	19.8(3)
O1D—Cu4—O2S	103.7(4)	O4E^{ii}—Eu3—C1E^{ii}	45.9(2)
O3F—Cu4—O2S	87.2(3)	O4E—Eu3—C1E^{ii}	141.3(2)
O3D—Cu4—O2S	84.9(3)	C3E^{ii}—Eu3—C1E^{ii}	46.0(3)
O1E—Cu5—O6D	91.4(3)	C3E—Eu3—C1E^{ii}	143.6(3)
O1E—Cu5—O3D	173.6(3)	C1E—Eu3—C1E^{ii}	169.5(4)
O6D—Cu5—O3D	85.1(3)	C1A—O1A—Cu1	110.9(6)
O1E—Cu5—O3E	84.2(3)	C1B—O1B—Cu2	115.1(7)
O6D—Cu5—O3E	171.3(3)	C1C—O1C—Cu3	114.6(6)
O3D—Cu5—O3E	98.5(3)	C1D—O1D—Cu4	110.4(7)
O3F—Cu6—O6E	173.8(3)	C1E—O1E—Cu5	114.0(7)
O3F—Cu6—O1F	83.9(3)	C1F—O1F—Cu6	113.5(7)
O6E—Cu6—O1F	90.2(3)	S1—O1S—Cu1	133.4(4)
O3F—Cu6—O3E	100.8(3)	C1A—O2A—Eu1	116.8(6)
O6E—Cu6—O3E	85.2(3)	C1B—O2B—Eu2	117.2(7)
O1F—Cu6—O3E	172.8(3)	C1D—O2D—Eu2	116.4(7)
O1W—Eu1—O1W^{i}	92.3(7)	C1E—O2E—Eu3	118.6(7)
O1W—Eu1—O2A	145.3(3)	S2—O2S—Cu4	131.0(4)
O1W^{i}—Eu1—O2A	90.8(4)	C2A—O3A—Cu2	112.6(5)
O1W—Eu1—O2A^{i}	90.8(4)	C2A—O3A—Cu1	110.7(5)
O1W^{i}—Eu1—O2A^{i}	145.3(3)	Cu2—O3A—Cu1	112.9(3)
O2A—Eu1—O2A^{i}	105.7(5)	C2B—O3B—Cu2	112.0(5)
O1W—Eu1—O4A^{i}	140.8(3)	C2B—O3B—Cu3	110.1(6)
O1W^{i}—Eu1—O4A^{i}	89.9(3)	Cu2—O3B—Cu3	112.8(3)
O2A—Eu1—O4A^{i}	73.8(2)	C2C—O3C—Cu1	111.6(5)
O2A^{i}—Eu1—O4A^{i}	66.8(2)	C2C—O3C—Cu3	113.0(6)
O1W—Eu1—O4A	89.9(3)	Cu1—O3C—Cu3	110.7(3)
O1W^{i}—Eu1—O4A	140.8(3)	C2D—O3D—Cu5	112.0(5)
O2A—Eu1—O4A	66.8(2)	C2D—O3D—Cu4	110.6(5)
O2A^{i}—Eu1—O4A	73.8(2)	Cu5—O3D—Cu4	110.3(3)
O4A^{i}—Eu1—O4A	112.2(3)	C2E—O3E—Cu5	113.0(5)
O1W—Eu1—O5A	75.2(3)	C2E—O3E—Cu6	110.1(5)
O1W^{i}—Eu1—O5A	76.4(3)	Cu5—O3E—Cu6	114.6(3)
O2A—Eu1—O5A	71.9(3)	C2F—O3F—Cu6	113.8(5)
O2A^{i}—Eu1—O5A	137.4(2)	C2F—O3F—Cu4	110.7(5)
O4A^{i}—Eu1—O5A	142.7(3)	Cu6—O3F—Cu4	110.1(3)
O4A—Eu1—O5A	66.3(2)	C2A—O4A—Eu1	105.3(5)
O1W—Eu1—O5A^{i}	76.4(3)	C2B—O4B—Eu2	100.8(5)
O1W^{i}—Eu1—O5A^{i}	75.2(3)	C2D—O4D—Eu2	106.5(5)
O2A—Eu1—O5A^{i}	137.4(2)	C2E—O4E—Eu3	99.5(5)
O2A^{i}—Eu1—O5A^{i}	71.9(3)	C3A—O5A—Eu1	113.7(7)
O4A^{i}—Eu1—O5A^{i}	66.3(2)	C3B—O5B—Eu2	120.3(8)
O4A—Eu1—O5A^{i}	142.7(3)	C3D—O5D—Eu2	115.0(7)
O5A—Eu1—O5A^{i}	138.6(4)	C1C—O4CX—C3C	109.6(11)
O1W—Eu1—C2A^{i}	116.3(3)	C1C—O4CX—C2C	55.5(7)
O1W^{i}—Eu1—C2A^{i}	99.9(3)	C3C—O4CX—C2C	55.7(7)
O2A—Eu1—C2A^{i}	97.2(2)	C3E—O5E—Eu3	121.4(7)
O2A^{i}—Eu1—C2A^{i}	48.7(2)	C3F—O4FX—C1F	114.6(11)
O4A^{i}—Eu1—C2A^{i}	25.6(2)	C3F—O4FX—C2F	58.4(7)
O4A—Eu1—C2A^{i}	114.1(2)	C1F—O4FX—C2F	56.7(6)

O5A—Eu1—C2A^{i}	168.3(3)	C3A—O6A—Cu2	113.6(6)
O5A^{i}—Eu1—C2A^{i}	48.2(2)	C3B—O6B—Cu3	112.0(7)
O1W—Eu1—C2A	99.9(3)	C3C—O6C—Cu1	113.6(6)
O1W^{i}—Eu1—C2A	116.3(3)	C3D—O6D—Cu5	115.0(7)
O2A—Eu1—C2A	48.7(2)	C3E—O6E—Cu6	112.1(6)
O2A^{i}—Eu1—C2A	97.2(2)	C3F—O6F—Cu4	114.1(6)
O4A^{i}—Eu1—C2A	114.1(2)	O1S—S1—C1S1	105.5(7)
O4A—Eu1—C2A	25.6(2)	O1S—S1—C1S2	105.1(6)
O5A—Eu1—C2A	48.2(2)	C1S1—S1—C1S2	98.6(9)
O5A^{i}—Eu1—C2A	168.3(3)	O2S—S2—C2S1	106.0(5)
C2A^{i}—Eu1—C2A	127.4(3)	O2S—S2—C2S2	102.7(8)
O1W—Eu1—C1A	126.8(3)	C2S1—S2—C2S2	98.5(9)

(i) 1-x, y, 2.5-z; (ii) -x, y, 0.5-z.

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