Supporting Information

Contents

Table S1 Shape measures of {$LnCu_4$} relative to ideal 8-vertex polyhedra shown of complexes $[LnCu_4(H_4L)_4](Cl)_2(ClO_4)\cdot 6CH_3OH$ (Gd **1**, Tb **2**, Dy **3** and La **4**). The lowest CShMs value, and thus most coincident geometry is highlighted in pink.[1]

	1	2	3	4	Symmetry	Ideal shape
OP-8	33.263	33.124	32.973	33.997	D_{8h}	Octagon
HPY-8	22.159	22.271	22.220	21.998	C_{7v}	Heptagonal pyramid
HBPY-8	15.297	15.268	15.410	14.966	D_{6h}	Hexagonal bipyramid
CU-8	7.811	7.740	7.914	7.482	*Oh*	Cube
SAPR-8	**1.125**	**1.081**	**1.060**	**1.371**	$\boldsymbol{D_{4d}}$	**Square antiprism**
TDD-8	1.973	1.878	1.909	2.019	D_{2d}	Triangular dodecahedron
JGBF-8	16.888	16.872	16.928	16.861	D_{2d}	Johnson gyrobifastigium J26
JETBPY-	28.557	28.696	28.476	28.315	D_{3h}	Johnson elongated triangular bipyramid J14
JBTPR-8	3.563	3.535	3.506	3.874	C_{2v}	Biaugmented trigonal prism J50
BTPR-8	3.020	2.952	2.930	3.259	C_{2v}	Biaugmented trigonal prism
JSD-8	5.371	5.348	5.324	5.696	D_{2d}	Snub diphenoid J84
TT-8	8.364	8.362	8.518	8.090	*Td*	Triakis tetrahedron
ETBPY-8	23.386	23.509	23.453	23.095	D_{3h}	Elongated trigonal bipyramid

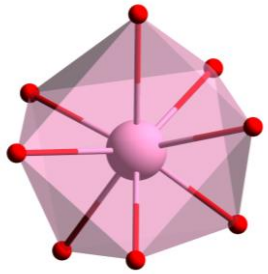


Table S2 Summary of the average intramolecular distances between metal ions for complexes **1**–**4**.

Complex	$d^{Avg}_{(Cu1\cdots Cu2)}$/Å	$d^{Avg}_{(Cu\cdots Cu')}$/Å	$d_{(Cu1\cdots Ln1)}$/Å	$d_{(Cu2\cdots Ln1)}$/Å
1 (Gd)	4.777(6)	6.332(1)	3.250(2)	3.311(5)
2 (Tb)	4.766(7)	6.318(7)	3.242(8)	3.304(7)
3 (Dy)	4.761(5)	6.309(6)	3.242(3)	3.295(4)
4 (La)	4.874(6)	6.471(6)	3.313(9)	3.383(9)

Table S3 Summary of structural parameters of **1**−**4**: geometry around the Cu(II) centres (Cu1, Cu2), Cu−O−Ln angles, Cu−O···O−Ln torsion angles, and dihedral angles (*α*). Note Sbp means square−based pyramidal geometry, and Sp means square−planar geometry.

Complex	Atom	Coord. environment	Cu−O−Ln (°)	Cu−O···O−Ln (°)	*α* (°)
1 (Gd)	Cu1	Sbp	94.3(9)	135.83(20)	44.17
	Cu2	Sp	101.07(10)	160.61(21)	19.39
2 (Tb)	Cu1	Sbp	94.5(6)	136.18(13)	43.81
	Cu2	Sp	101.16(6)	160.74(14)	18.97
3 (Dy)	Cu1	Sbp	94.75(7)	136.68(1)	43.28
	Cu2	Sp	101.45(7)	161.06(1)	18.53
4 (La)	Cu1	Sbp	93.95(6)	134.87(3)	45.13
	Cu2	Sp	100.75(6)	160.08(3)	19.92

Table S4 Summary of the calculated ($\chi_M T_{cal}$) and experimental ($\chi_M T_{exp}$) susceptibility values for **1**–**4** (at room temperature). *L*, *S*, g_J and ground state (GS) term symbol are related to each lanthanide ion.

Complex	***L***	***S***	g_J	**GS term symbol**	$\chi_M T_{cal}$ **{LnCu$_4$}** (cm^3·mol^{-1}·K)	$\chi_M T_{exp}$ **{LnCu$_4$}** (cm^3·mol^{-1}·K)
1 (Gd)	0	7/2	2	$^8S_{7/2}$	9.54	9.64
2 (Tb)	3	3	3/2	$^7F_6$	13.5	13.5
3 (Dy)	5	5/2	4/3	$^6H_{15/2}$	15.8	15.9
4 (La)*	−	−	−	−	1.67	1.73

*****Lanthanum does not have any 4*f* electrons. Therefore $\chi_M T_{cal}$ {LaCu$_4$} was calculated considering four isolated Cu(II) ions, S_{Cu} = 1/2 and g_{Cu} = 2.11.

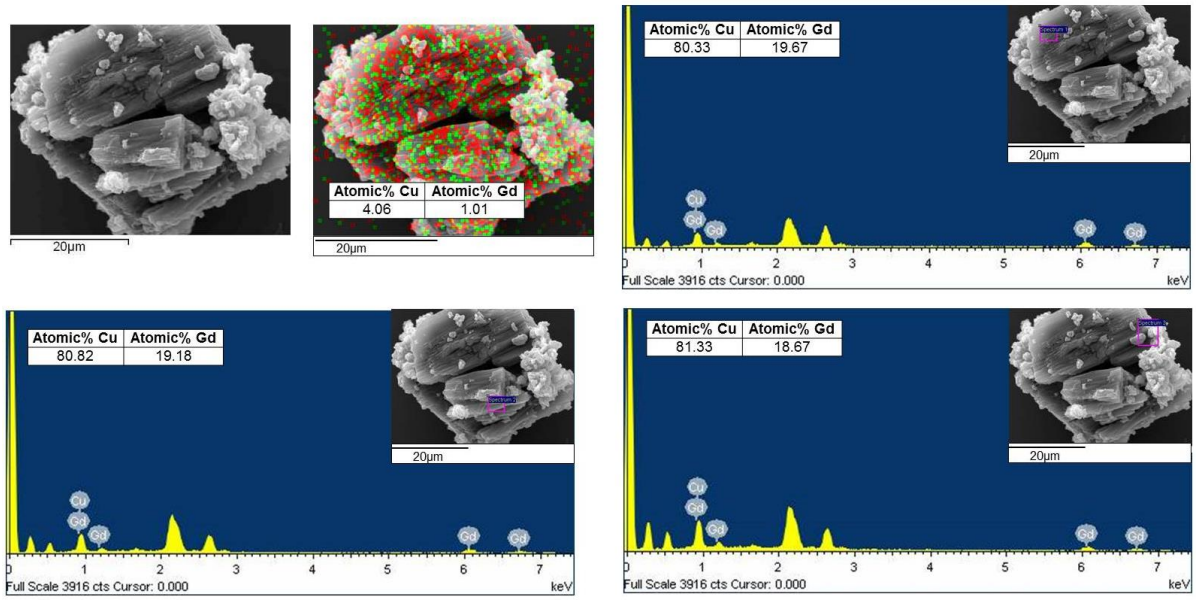


Figure S1 EDX spectra and elemental map (Cu, red; Gd, green) showing the distribution of Gd and Cu in a bulk sample of **1**. The inset displays the area of the sample used for the analysis; the Atomic% is shown for each area.

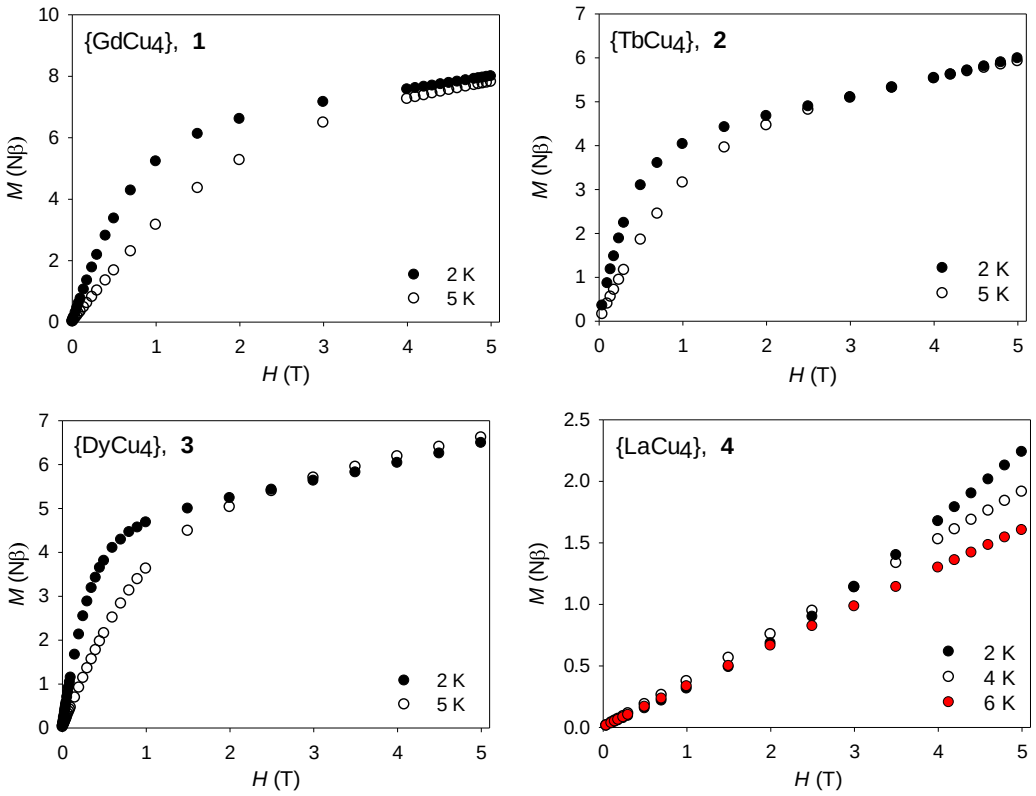


Figure S2 Magnetisation vs field at different temperatures for complexes **1**, **2**, **3** (2 K, 5 K) and **4** (2 K, 4 K, 6 K).

Ac susceptibility measurements of 2 and 3

Studies were performed as a function of the frequency in the absence of dc field and under different applied fields, at 2 K (for **2** and **3**) and over the temperature range of 1.8–5 K (**3**). Compound **2** displays the onset of an out−of−phase χ'' signal in zero dc field, however, the signal is very weak, and no enhancement was observed despite the application of an external field (see dc field sweep experiments in Figure S3, left). On the other hand, compound **3** shows a promising stronger χ'' signal in zero dc field, which is improved under the influence of an external dc field (see Figure S3, right). The different dynamic properties between **2** and **3** arise due to the nature of the central Ln(III) ion. Dy(III) is a Kramers ion, therefore its ground state is well described as a doublet. In contrast Tb(III) is a non−Kramers ion, and thus its ground state depends on the axiality generated by crystal field effects. The effect of the dc field on **3** effectively improves the magnitude of the χ'' signal, but it was not possible to move the out−of−phase signal enough to see the maxima. The dynamics of **3** have been studied by the application of three different fields strengths, H_{dc} = 1000, 1500 and 2000 Oe (see Figure S4). All the experiments show slow relaxation of the magnetisation. Given the lack of local χ'' maxima in the ac plots, the relaxation rate (τ_0) and the energy barrier ($\Delta E/k_B$) parameters were calculated by using the Kramers−Kronig−derivate equation of the Arrhenius law $\ln(\chi''/\chi') = \ln(\omega\tau_0) + \Delta E/k_B T$. The fit of the experimental ac susceptibility gives the relaxation rates τ_0 = 7.2·10^{-7} s, 7.4·10^{-7} s and 8.8·10^{-7} s, and the energy barriers $\Delta E/k_B$ = 9.7 ± 0.2 K, 9.9 ±0.3 K and 9.8 ± 0.3 K for fields of 1000, 1500, and 2000 Oe, respectively (see Table S5). The calculated τ_0 and $\Delta E/k_B$ values are reasonable compared to those reported for similar {LnCu} SMMs.

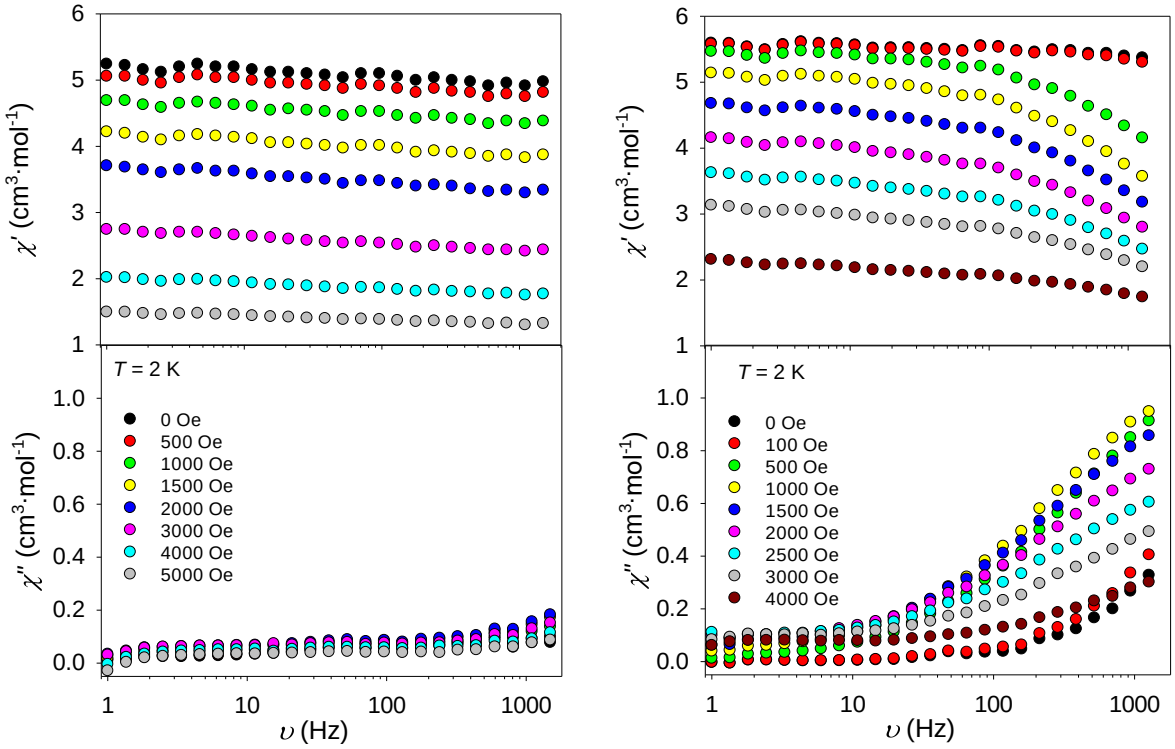


Figure S3 Field–sweep ac susceptibility measurements for **2** (left) and **3** (right) at T = 2 K.

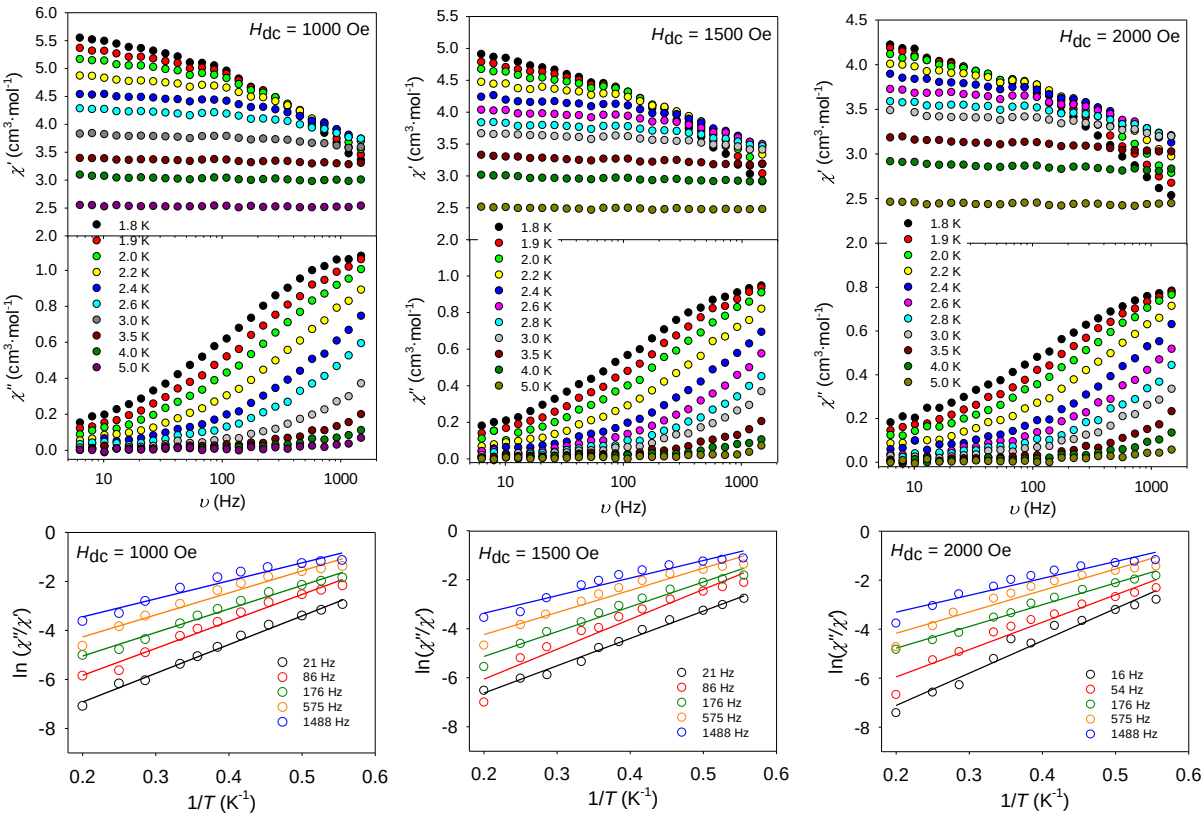
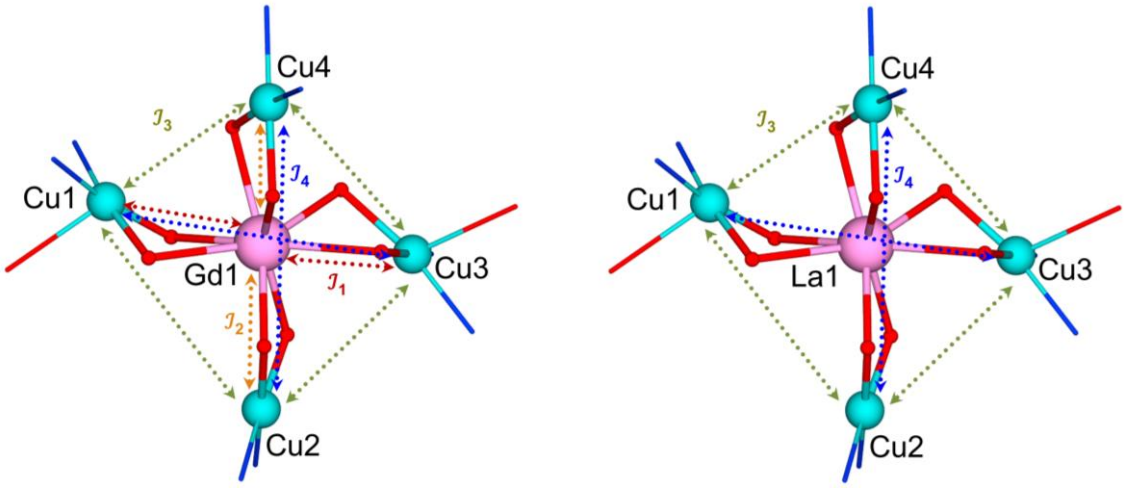


Figure S4 Top: Ac dynamic measurements for **3** under dc fields of 1000 Oe (left), 1500 Oe (centre) and 2000 Oe (right) at various temperatures in the range 1.8 – 5.0 K. Bottom: fit of the experimental ac susceptibility by the Kramers–Kronig–derivate equation of the Arrhenius law (see main article for more info).[2]

Table S5 Table with the relaxation rate (τ_0) and the energy barrier ($\Delta E_a/k_B$) parameters extracted from the fit of the ac experiments at different dc fields.

Applied H_{dc}	$\Delta E/k_B$ (K)	τ_0 (s)
1000 Oe	9.7 ± 0.2	7.2×10^{-7}
1500 Oe	9.9 ± 0.3	7.4×10^{-7}
2000 Oe	9.8 ± 0.3	8.8×10^{-7}



{GdCu$_4$} (**1**): $\hat{\mathcal{H}} = -2\mathcal{J}_1(\hat{S}_{Gd1}\cdot\hat{S}_{Cu1} + \hat{S}_{Gd1}\cdot\hat{S}_{Cu3}) - 2\mathcal{J}_2(\hat{S}_{Gd1}\cdot\hat{S}_{Cu2} + \hat{S}_{Gd1}\cdot\hat{S}_{Cu4}) -$
$2\mathcal{J}_3(\hat{S}_{Cu1}\cdot\hat{S}_{Cu4} + \hat{S}_{Cu3}\cdot\hat{S}_{Cu4} + \hat{S}_{Cu2}\cdot\hat{S}_{Cu3} + \hat{S}_{Cu1}\cdot\hat{S}_{Cu2}) -$
$2\mathcal{J}_4(\hat{S}_{Cu1}\cdot\hat{S}_{Cu3} + \hat{S}_{Cu2}\cdot\hat{S}_{Cu4}) + g_{Gd}\mu_B\vec{B}\vec{s}_{Gd} + g_{Cu}\mu_B\vec{B}\sum_{i=1}^{4}\vec{s}_i$

{LaCu$_4$} (**4**): $\hat{\mathcal{H}} = -2\mathcal{J}_3(\hat{S}_{Cu1}\cdot\hat{S}_{Cu4} + \hat{S}_{Cu3}\cdot\hat{S}_{Cu4} + \hat{S}_{Cu2}\cdot\hat{S}_{Cu3} + \hat{S}_{Cu1}\cdot\hat{S}_{Cu2}) -$
$2\mathcal{J}_4(\hat{S}_{Cu1}\cdot\hat{S}_{Cu3} + \hat{S}_{Cu2}\cdot\hat{S}_{Cu4}) + g_{Cu}\mu_B\vec{B}\sum_{i=1}^{4}\vec{s}_i$

Figure S5 Magnetic model used for the DFT calculations and spin Hamiltonians used for the fit of the magnetic data for [GdCu$_4$(H$_4$L)$_4$](Cl)$_2$(ClO$_4$)·6CH$_3$OH (**1**) and [LaCu$_4$(H$_4$L)$_4$](Cl)$_2$(ClO$_4$)·6CH$_3$OH (**4**).

Table S6 Experimental values for Cu···Gd distance, Cu−O−Gd angle, Cu−O−Gd−O torsion and magnetic exchange interaction ($\mathcal{J}_{exp}$) based on previously reported {GdCu} systems. Refcodes from the CSD are also displayed. All distances in Å, angles in degrees and exchange interactions in cm^{-1}.

	Refcode	Cu···Gd	Cu-O-Gd	Cu-O-Gd	Cu-O-Gd-O	$\mathcal{J}_{exp}$	Ref.
$GdCu(OTf)_3(bdmap)_2(H_2O)\cdot THF$	NEBLUB	3.310	105.46	104.67	0.51	−0.08	[3]
$[LCu(OH_2)Gd(NO_3)_3]$	YEBNAV	3.547	108.76	109.89	0.98	0.00	[4]
$[CuGd\{pyCO(OEt)py(COH(OEt)py\}_3](ClO_4)_2EtOH$	KAJKAJ	3.031	87.88	86.95	36.14	0.32	[5]
$[CuGd\{pyCO(OEt)py(COH(OEt)py\}_3](ClO_4)_2EtOH$	KAJKAJ	3.031	87.88	82.34	44.94	0.32	[5]
$[CuGd\{pyCO(OEt)py(COH(OEt)py\}_3](ClO_4)_2EtOH$	KAJKAJ	3.031	86.95	82.34	41.73	0.32	[5]
$Gd(hfa)_3Cu(salen)$	RINQAG	3.230	94.28	95.79	33.52	0.40	[6]
$Gd(hfa)_3Cu(salen)$	RINQAG	3.199	93.84	93.60	34.43	0.40	[6]
$Cu(salabza)Gd(hfac)_3$	JOGQAX	3.248	98.54	93.14	34.28	0.80	[7]
$Cu(salen)Gd(pta)_3$	OFELAM	3.288	99.81	95.15	23.72	1.21	[8]
$Cu(acacen)Gd(hfa)_3$	OFELIU	3.288	96.62	98.08	27.88	1.25	[9]
$Cu(acacen)Gd(hfa)_3$	OFELIU	3.313	96.69	99.76	25.60	1.25	[9]
$[TTF\text{-}salphen)CuGd(hfac)_3]$	UCIDER	3.260	97.23	96.45	27.18	1.29	[10]
$LCuGd(NO_3)_3\cdot Me2CO$	OBEMAK	3.444	105.15	106.80	4.05	1.30	[11]
$Gd(hfa)_3Cu(salen)(Meim)$	RINQIO	3.252	98.28	95.05	29.40	1.42	[12]
$Cu(acacen)Gd(pta)_3$	OFELEQ	3.274	94.63	97.98	29.18	1.47	[13]
$Cu(ehphi)Gd(hfac)_3$	MIDHIQ	3.252	94.50	99.66	30.01	1.91	[14]

$[GdCu(L^1\text{-}3H)(NO_3)](NO_3)H_2O$	AHICID	3.246	91.42	97.19	24.20	2.20	[15]
$[GdCu(L^1\text{-}3H)(NO_3)](NO_3)H_2O$	AHICID	3.246	91.42	89.21	44.49	2.20	[15]
$[GdCu(L^1\text{-}3H)(NO_3)](NO_3)H_2O$	AHICID	3.246	97.19	89.21	44.35	2.20	[15]
$[Cu(3\text{-}MeOsaltn)(ac)Gd(hfac)_2]$	WISREX	3.437	105.24	103.74	19.24	2.60	[16]
$CuGd(hmp)_2(NO_3)_3(H_2O)_2$	XAYTIB	3.346	102.05	102.83	15.32	3.36	[17]
$L_1Cu(O_2COMe)Gd(thd)_2$	JOQTEO	3.473	103.98	103.78	14.60	3.50	[18]
$[CuGd(ems)(NO_3)\ 3H_2O]Cu(ems)$	XOZZUH	3.306	100.15	98.90	17.79	3.76	[19]
$LCuGd(NO_3)_3{\cdot}CH_3OH$	WIXYIL	3.224	97.13	96.99	23.44	4.33	[20]
$[L_1CuGd(O_2CCF_3)_3(C_2H_5OH)_2]$	AXIGUJ	3.391	103.21	103.33	10.25	4.42	[21]
$LCu(C_3H_6O)Gd(NO_3)_3$	NEVHIF	3.523	108.12	108.03	13.52	4.80	[22]
$[Cu(valaepy)_2Gd(O_2NO)_3]CH_3CN$	VIBKOI	3.506	106.55	110.78	2.00	4.94	[23]
$LCuGd(NO_3)_3$	AWUQUE	3.443	103.42	103.72	14.14	4.98	[24]
$LCu(H_2O)Gd(NCS)_3{\cdot}Me_2CO$	BERPAQ	3.454	106.28	106.57	15.41	5.50	[25]
$LCuGd(NO_3)_3.Me_2CO$	QEMYAI	3.425	109.84	108.97	9.68	5.60	[26]
$[(HL_3)_2CuGd(NO_3)_3]$	BUXZAW	3.473	108.11	108.53	0.25	6.50	[27]
$LCu(MeOH)Gd(NO_3)_3$	NEVHEB	3.484	109.03	106.49	10.13	6.80	[28]
$LCuGd(NO_3)_3{\cdot}Me_2CO$	ZUVTIT	3.428	105.86	107.38	10.21	7.00	[29]
$[(HL_1)_2Cu(CH_3CN)_2Gd(NO_3)_3]$	BUXYUP	3.459	105.84	106.98	0.30	7.20	[30]
$[[\{CuL\}Gd(H_2O)_3\{Co(CN)_6\}]{\cdot}4H_2O$	UMATEH	3.510	106.68	107.50	7.46	7.24	[31]
$LCuGd(NO_3)_3{\cdot}Me_2CO$	NAMDIP	3.475	107.36	106.88	10.09	7.30	[32]

$LCuGd(NO_3)_3 \cdot Me_2CO$	EZAPAW	3.473	107.57	107.27	9.29	7.40	[33]
$LCuGd(NO_3)_3 \cdot Me_2CO$	EZAPAW	3.477	107.68	107.68	11.06	7.40	[33]
$[(3\text{-MeOsalamo})CuGd(Oac)_3]$	GANFEH	3.433	104.56	102.91	15.81	7.60	[34]
$LCuGd(NO_3)_3$	GANFIL	3.498	108.94	107.42	7.52	7.60	[35]
$LCuGd(NO_3)_3$	GANFIL	3.499	108.66	106.70	10.99	7.60	[35]
$[CuGd(L)(NO_3)_2(H_2O)_3MeOH]NO_3 \cdot MeOH$	YABZOS	3.539	108.81	107.06	2.05	7.89	[36]
$LCuGd(NO_3)_3$	LOYTOI	3.400	106.62	103.72	3.36	8.08	[37]
$[Cu(L^1)(m\text{-}OH)Gd(NO_3)_3(H_2O)]$	DOFMUH	3.417	105.86	106.46	0.22	8.40	[38]
$[L^2CuGd(trif)_2(H_2O)_2] \cdot trif \cdot H_2O \cdot acetone$	LOKNIJ	3.369	106.24	105.42	3.13	8.60	[39]
$LCuGd(NO_3)(CH_3)_2CO]$	FAKLOT	3.454	107.25	106.71	8.96	8.63	[40]
$[CuGd(mmi)_2(NO_3)_3(H_2O)_2]$	YIWNIC	3.366	103.62	104.71	3.80	8.70	[41]
$[(CN)_5(bipy)W(CN)Cu(3\text{-MeOsalpn})Gd(O_2NO_2)(H_2O)] \cdot 3MeCN$	GAWPOL	3.466	106.61	107.50	10.36	8.79	[42]
$[LCuCl_2Gd(H_2O)_4]Cl \cdot 2H_2O$	KEQRED	3.512	108.65	108.81	1.38	10.10	[43]
$LCuGd(NO_3)_3$	LAMBOR	3.449	107.85	105.27	5.63	10.80	[44]
$[(GdCuL^1Cl_3(CH_3OH)_2]$	LEWZUK	3.409	104.81	105.56	11.92	11.20	[45]
$LCuGd(NO_3)_3$	LAMBUX	3.401	104.18	105.77	1.61	12.60	[46]

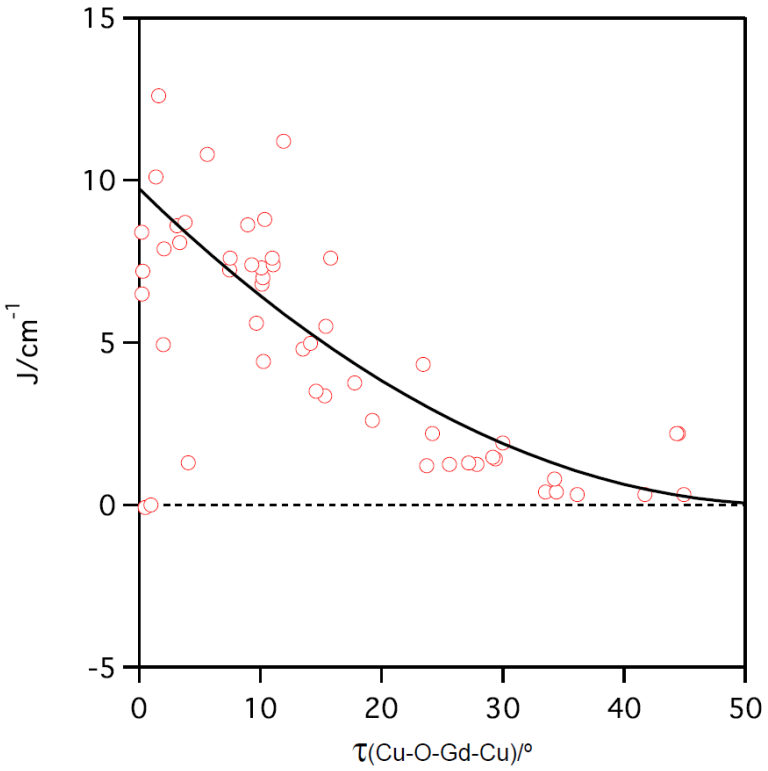


Figure S6 Experimental dependence of the $\mathcal{J}$ values for {GdCu} systems[4-46] with the torsion angle defined as τ(Cu−O−Gd−Cu).

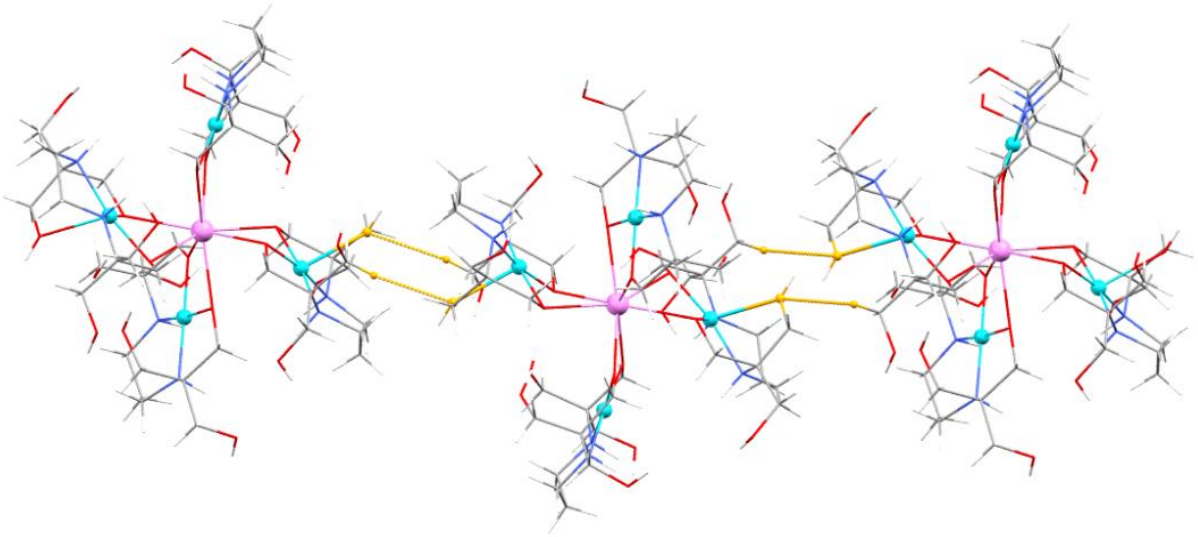


Figure S7 Van der Waals interactions (highlighted in orange) for $[LnCu_4(H_4L)_4](Cl)_2(ClO_4)\cdot 6CH_3OH$. The shortest intermolecular Cu···Cu' interaction is 7.561(1) Å in **1** and 7.436(1) Å in **4** and is between the Cu(Sbp) centres. C, grey; Cu, turquoise; H, white; Ln, pink; N, blue; O, red.

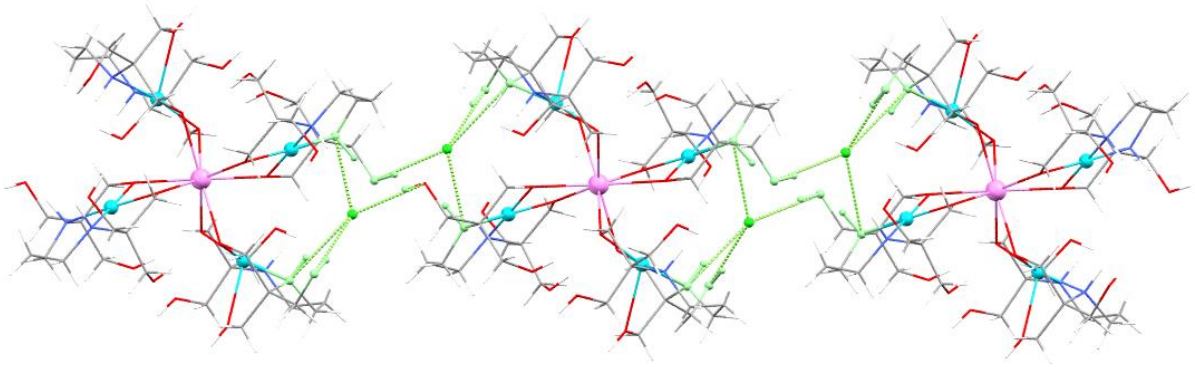


Figure S8 Intermolecular hydrogen bonding interactions via Cl^- anions (highlighted in green) for $[LnCu_4(H_4L)_4](Cl)_2(ClO_4)\cdot 6CH_3OH$. Cu(Sp)···Cu(Sp)' is 7.821(1) Å in **1** and 7.710(1) Å in **4**. C, grey; Cl, green; Cu, turquoise; Ln, pink; H, white; N, blue; O, red.

Table S7: Computed spin densities and energies for each of the calculated spin distributions in systems **1** ({$GdCu_4$}) and **4** ({$LaCu_4$}). All energies in atomic units.

	La_1^{III}	Cu_2^{II}	Cu_3^{II}	Cu_4^{II}	Cu_5^{II}	Energy/au
HS	-0.0057	0.5929	0.6156	0.5929	0.6159	-18783.2622632
SD1	-0.0102	-0.5942	0.6145	-0.5943	0.6147	-18783.2622579
SD2	0.0102	0.5942	-0.6145	0.5943	-0.6147	-18783.2622579
SD3	-0.0080	0.5927	0.6160	-0.5941	0.6143	-18783.2622597

	Gd_1^{III}	Cu_2^{II}	Cu_3^{II}	Cu_4^{II}	Cu_5^{II}	Energy/au
HS	6.9276	0.6074	0.5863	0.6075	0.5863	-21704.3580600
SD1	6.9478	-0.6042	0.5872	-0.6042	0.5872	-21704.3580370
SD2	6.9291	0.6081	-0.5839	0.6082	-0.5838	-21704.3578087
SD3	6.9385	-0.6040	-0.5829	0.6079	0.5862	-21704.3579818
SD4	6.9384	-0.6039	0.5872	0.6078	-0.5839	-21704.3578905
SD5	6.9377	-0.6043	0.5872	0.6075	0.5863	-21704.3580496
SD6	6.9377	0.6075	0.5863	-0.6043	0.5872	-21704.3580495

Table S8: Bond lengths for **1** (Gd).

Atom 1	Atom 2	Length/Å		Atom 1	Atom 2	Length/Å
Gd1	Cu1[1]	3.2495(7)		N101	C102	1.490(7)
Gd1	Cu1	3.2495(7)		N101	C103	1.511(7)
Gd1	Cu2	3.3105(8)		N102	C107	1.487(7)
Gd1	Cu2[1]	3.3104(8)		N102	C108	1.513(7)
Gd1	O105[1]	2.428(4)		N201	C202	1.474(7)
Gd1	O105	2.428(4)		N201	C203	1.496(7)
Gd1	O109	2.519(4)		N202	C207	1.488(7)
Gd1	O109[1]	2.519(4)		N202	C208	1.490(7)
Gd1	O204	2.379(4)		C101	C102	1.509(8)
Gd1	O204[1]	2.379(4)		C101	C107	1.515(8)
Gd1	O209	2.341(4)		C103	C104	1.543(9)
Gd1	O209[1]	2.341(4)		C103	C105	1.546(8)
Cu1	O104	2.408(4)		C103	C106	1.513(9)
Cu1	O105	1.917(4)		C108	C109	1.535(8)
Cu1	O109	1.947(4)		C108	C110	1.524(8)
Cu1	N101	2.015(5)		C108	C111	1.536(8)
Cu1	N102	1.972(5)		C201	C202	1.523(8)
Cu2	O204	1.929(4)		C201	C207	1.520(9)
Cu2	O209	1.898(4)		C203	C204	1.547(8)
Cu2	N201	1.983(5)		C203	C205	1.523(8)
Cu2	N202	1.991(5)		C203	C206	1.517(8)
O104	C104	1.442(8)		C208	C209	1.543(8)
O105	C105	1.421(7)		C208	C210	1.527(8)
O106	C106	1.415(8)		C208	C211	1.531(8)
O109	C109	1.417(7)		Cl2	O1	1.395(10)
O110	C110	1.435(7)		Cl2	O2	1.421(12)
O111	C111	1.425(8)		Cl2	O3	1.388(9)
O204	C204	1.400(7)		Cl2	O4	1.296(6)
O205	C205	1.419(7)		O7	C7	1.391(9)
O206	C206	1.423(7)		O6	C6	1.40(2)
O209	C209	1.399(7)		O5	C5	1.506(14)
O210	C210	1.412(7)		O8	C8	1.400(8)
O211	C211	1.425(7)				

[1]1-X,+Y,3/2-Z

Table S9: Bond lengths for **2** (Tb).

Atom 1	Atom 2	Length/Å		Atom 1	Atom 2	Length/Å
Tb1	Cu1	3.2417(4)		N101	C102	1.485(5)
Tb1	Cu1[1]	3.2416(4)		N101	C103	1.504(5)
Tb1	Cu2	3.3036(4)		N102	C107	1.486(5)
Tb1	Cu2[1]	3.3035(4)		N102	C108	1.502(5)
Tb1	O105[1]	2.418(2)		N201	C202	1.487(5)
Tb1	O105	2.418(2)		N201	C203	1.493(5)
Tb1	O109[1]	2.501(2)		N202	C207	1.496(5)
Tb1	O109	2.501(2)		N202	C208	1.500(5)
Tb1	O204[1]	2.368(2)		C101	C102	1.522(5)
Tb1	O204	2.368(2)		C101	C107	1.523(5)
Tb1	O209[1]	2.323(2)		C103	C104	1.541(5)
Tb1	O209	2.323(2)		C103	C105	1.530(5)
Cu1	O104	2.411(3)		C103	C106	1.529(5)
Cu1	O105	1.918(2)		C108	C109	1.544(5)
Cu1	O109	1.939(2)		C108	C110	1.527(5)
Cu1	N101	2.016(3)		C108	C111	1.539(5)
Cu1	N102	1.978(3)		C201	C202	1.518(5)
Cu2	O204	1.925(2)		C201	C207	1.521(5)
Cu2	O209	1.906(2)		C203	C204	1.539(5)
Cu2	N201	1.985(3)		C203	C205	1.533(5)
Cu2	N202	1.989(3)		C203	C206	1.529(5)
O104	C104	1.442(5)		C208	C209	1.551(5)
O105	C105	1.422(4)		C208	C210	1.534(5)
O106	C106	1.411(5)		C208	C211	1.523(5)
O109	C109	1.428(4)		O7	C7	1.405(6)
O110	C110	1.440(5)		O8	C8	1.415(5)
O111	C111	1.430(5)		Cl2	O1	1.408(7)
O204	C204	1.410(4)		Cl2	O2	1.407(9)
O205	C205	1.424(5)		Cl2	O3	1.406(6)
O206	C206	1.424(5)		Cl2	O4	1.292(4)
O209	C209	1.398(4)		O5	C5	1.508(10)
O210	C210	1.428(5)		O6	C6	1.416(15)
O211	C211	1.423(5)				

[1] 1-X,+Y,3/2-Z

Table S10: Bond lengths for **3** (Dy).

Atom 1	Atom 2	Length/Å		Atom 1	Atom 2	Length/Å
Dy1	Cu1[1]	3.2347(6)		N101	C103	1.502(5)
Dy1	Cu1	3.2347(6)		N102	C107	1.483(5)
Dy1	Cu2	3.2941(6)		N102	C108	1.492(5)
Dy1	Cu2[1]	3.2941(6)		N201	C202	1.482(5)
Dy1	O105[1]	2.409(3)		N201	C203	1.490(5)
Dy1	O105	2.409(3)		N202	C207	1.498(5)
Dy1	O109[1]	2.487(3)		N202	C208	1.491(5)
Dy1	O109	2.487(3)		C101	C102	1.509(6)
Dy1	O204	2.351(2)		C101	C107	1.523(6)
Dy1	O204[1]	2.351(2)		C103	C104	1.549(6)
Dy1	O209[1]	2.311(3)		C103	C105	1.541(5)
Dy1	O209	2.311(3)		C103	C106	1.530(6)
Cu1	O104	2.424(3)		C108	C109	1.537(5)
Cu1	O105	1.914(3)		C108	C110	1.518(5)
Cu1	O109	1.938(3)		C108	C111	1.545(6)
Cu1	N101	2.009(3)		C201	C202	1.517(6)
Cu1	N102	1.979(3)		C201	C207	1.515(6)
Cu2	O204	1.920(3)		C203	C204	1.536(5)
Cu2	O209	1.903(3)		C203	C205	1.537(5)
Cu2	N201	1.979(3)		C203	C206	1.529(5)
Cu2	N202	1.986(3)		C208	C209	1.534(5)
O11B	C110	1.498(13)		C208	C210	1.536(6)
O104	C104	1.456(6)		C208	C211	1.533(6)
O105	C105	1.437(5)		Cl2	O1	1.371(12)
O106	C106	1.391(7)		Cl2	O2	1.397(14)
O109	C109	1.419(5)		Cl2	O3	1.388(7)
O110	C110	1.457(5)		Cl2	O4	1.248(5)
O111	C111	1.429(6)		O5	C5	1.573(15)
O204	C204	1.409(4)		O1AA	O8	1.791(18)
O205	C205	1.416(5)		O1AA	C8	1.275(18)
O206	C206	1.421(5)		O2AA	C8	1.45(3)
O209	C209	1.402(5)		O8	C8	1.418(8)
O210	C210	1.417(5)		O6	C6	1.56(4)
O211	C211	1.419(5)		O7	C7	1.349(10)
N101	C102	1.481(5)				

[1] 1-X,+Y,3/2-Z

Table S11: Bond lengths for **4** (La).

Atom 1	Atom 2	Length/Å		Atom 1	Atom 2	Length/Å
La1	Cu1	3.3831(6)		N31	C202	1.485(5)
La1	Cu1[1]	3.3830(6)		N31	C203	1.499(5)
La1	Cu2	3.3134(5)		N35	C207	1.487(5)
La1	Cu2[1]	3.3134(6)		N35	C208	1.503(5)
La1	O104[1]	2.466(2)		N101	C102	1.490(5)
La1	O104	2.466(2)		N101	C103	1.487(5)
La1	O109[1]	2.420(2)		N102	C107	1.498(5)
La1	O109	2.420(2)		N102	C108	1.503(5)
La1	O205	2.532(3)		C18	C108	1.531(5)
La1	O205[1]	2.532(3)		C101	C102	1.523(5)
La1	O209[1]	2.581(2)		C101	C107	1.518(5)
La1	O209	2.581(2)		C103	C104	1.540(5)
Cu1	O104	1.940(3)		C103	C105	1.533(5)
Cu1	O109	1.917(2)		C103	C106	1.530(5)
Cu1	N101	1.995(3)		C108	C109	1.539(5)
Cu1	N102	1.996(3)		C108	C110	1.530(5)
Cu2	O204	2.393(3)		C201	C202	1.524(6)
Cu2	O205	1.934(3)		C201	C207	1.516(5)
Cu2	O209	1.946(3)		C203	C204	1.551(5)
Cu2	N31	2.016(3)		C203	C205	1.531(5)
Cu2	N35	1.991(3)		C203	C206	1.532(6)
O104	C104	1.405(4)		C208	C209	1.533(5)
O105	C105	1.407(5)		C208	C210	1.531(5)
O106	C106	1.422(5)		C208	C211	1.536(5)
O109	C109	1.389(4)		Cl2	O1	1.287(5)
O110	C110	1.413(5)		Cl2	O2	1.401(7)
O111	C18	1.417(5)		Cl2	O3	1.452(12)
O204	C204	1.436(5)		Cl2	O4	1.401(9)
O205	C205	1.416(5)		O1	C7S	1.602(17)
O206	C206	1.406(6)		O5S	C6S	1.43(2)
O209	C209	1.419(5)		O1S	C2S	1.414(6)
O210	C210	1.424(5)		O1SA	C2S	1.38(3)
O211	C211	1.438(6)		O3S	C4S	1.384(8)

[1]1-X,+Y,3/2-Z

Table S12: Bond angles for **1** (Gd).

Atom 1	Atom 2	Atom 3	Angle/˚		Atom 1	Atom 2	Atom 3	Angle/˚
Cu1	Gd1	Cu1[1]	146.74(3)		O204	Cu2	N201	87.57(18)
Cu1[1]	Gd1	Cu2[1]	84.357(19)		O204	Cu2	N202	172.18(18)
Cu1[1]	Gd1	Cu2	103.440(18)		O209	Cu2	Gd1	43.72(11)
Cu1	Gd1	Cu2	84.357(18)		O209	Cu2	O204	86.42(16)
Cu1	Gd1	Cu2[1]	103.440(18)		O209	Cu2	N201	173.10(18)
Cu2[1]	Gd1	Cu2	152.90(3)		O209	Cu2	N202	86.67(18)
O105	Gd1	Cu1[1]	168.67(10)		N201	Cu2	Gd1	129.54(14)
O105[1]	Gd1	Cu1[1]	35.91(9)		N201	Cu2	N202	99.5(2)
O105	Gd1	Cu1	35.91(9)		N202	Cu2	Gd1	129.10(14)
O105[1]	Gd1	Cu1	168.67(10)		C104	O104	Cu1	102.4(3)
O105	Gd1	Cu2[1]	84.51(10)		Cu1	O105	Gd1	96.12(15)
O105[1]	Gd1	Cu2[1]	87.48(10)		C105	O105	Gd1	129.9(3)
O105	Gd1	Cu2	87.48(10)		C105	O105	Cu1	108.6(3)
O105[1]	Gd1	Cu2	84.51(10)		Cu1	O109	Gd1	92.47(14)
O105	Gd1	O105[1]	145.32(18)		C109	O109	Gd1	132.1(3)
O105	Gd1	O109	64.67(12)		C109	O109	Cu1	110.1(3)
O105	Gd1	O109[1]	148.86(12)		Cu2	O204	Gd1	99.90(15)
O105[1]	Gd1	O109[1]	64.67(12)		C204	O204	Gd1	146.3(3)
O105[1]	Gd1	O109	148.86(13)		C204	O204	Cu2	109.9(3)
O109[1]	Gd1	Cu1[1]	36.76(8)		Cu2	O209	Gd1	102.20(16)
O109	Gd1	Cu1[1]	112.95(9)		C209	O209	Gd1	145.0(4)
O109	Gd1	Cu1	36.77(9)		C209	O209	Cu2	112.3(3)
O109[1]	Gd1	Cu1	112.95(8)		C102	N101	Cu1	119.0(4)
O109[1]	Gd1	Cu2[1]	111.11(9)		C102	N101	C103	115.6(4)
O109	Gd1	Cu2	111.11(9)		C103	N101	Cu1	100.6(3)
O109[1]	Gd1	Cu2	88.65(9)		C107	N102	Cu1	115.7(4)
O109	Gd1	Cu2[1]	88.65(9)		C107	N102	C108	117.6(4)
O109[1]	Gd1	O109	88.17(17)		C108	N102	Cu1	107.4(3)
O204	Gd1	Cu11	107.60(9)		C202	N201	Cu2	115.4(4)
O204[1]	Gd1	Cu11	61.30(9)		C202	N201	C203	117.0(4)
O204	Gd1	Cu1	61.30(9)		C203	N201	Cu2	106.8(4)
O204[1]	Gd1	Cu1	107.60(9)		C207	N202	Cu2	118.1(4)
O204	Gd1	Cu2[1]	164.67(9)		C207	N202	C208	115.5(5)
O204	Gd1	Cu2	35.04(9)		C208	N202	Cu2	107.8(4)
O204[1]	Gd1	Cu2[1]	35.04(9)		C102	C101	C107	115.4(5)
O204[1]	Gd1	Cu2	164.67(9)		N101	C102	C101	112.0(5)
O204[1]	Gd1	O105	107.83(13)		N101	C103	C104	108.3(5)
O204[1]	Gd1	O105[1]	83.05(13)		N101	C103	C105	103.0(4)
O204	Gd1	O105[1]	107.84(13)		N101	C103	C106	116.0(5)
O204	Gd1	O105	83.05(13)		C104	C103	C105	111.4(5)
O204[1]	Gd1	O109	76.24(13)		C106	C103	C104	106.5(5)
O204	Gd1	O109	77.95(13)		C106	C103	C105	111.7(5)
O204[1]	Gd1	O109[1]	77.95(13)		O104	C104	C103	111.7(5)
O204	Gd1	O109[1]	76.24(13)		O105	C105	C103	110.7(5)
O204[1]	Gd1	O204	143.78(18)		O106	C106	C103	116.1(5)
O209[1]	Gd1	Cu1[1]	96.65(9)		N102	C107	C101	109.6(5)
O209	Gd1	Cu1[1]	107.87(9)		N102	C108	C109	104.5(4)

O209	Gd1	Cu1	96.65(9)		N102	C108	C110	109.5(5)
O209[1]	Gd1	Cu1	107.87(9)		N102	C108	C111	109.8(5)
O209	Gd1	Cu2	34.08(9)		C109	C108	C111	109.7(5)
O209	Gd1	Cu2[1]	118.83(9)		C110	C108	C109	111.7(5)
O209[1]	Gd1	Cu2[1]	34.08(9)		C110	C108	C111	111.5(5)
O209[1]	Gd1	Cu2	118.83(9)		O109	C109	C108	112.4(4)
O209[1]	Gd1	O105	75.08(13)		O110	C110	C108	106.2(5)
O209[1]	Gd1	O105[1]	79.47(13)		O111	C111	C108	111.4(5)
O209	Gd1	O105[1]	75.08(13)		C207	C201	C202	113.8(5)
O209	Gd1	O105	79.47(13)		N201	C202	C201	111.6(5)
O209[1]	Gd1	O109	112.57(13)		N201	C203	C204	105.2(4)
O209[1]	Gd1	O109[1]	132.61(13)		N201	C203	C205	110.5(5)
O209	Gd1	O109	132.61(12)		N201	C203	C206	112.4(5)
O209	Gd1	O109[1]	112.57(13)		C205	C203	C204	110.7(5)
O209[1]	Gd1	O204[1]	67.45(12)		C206	C203	C204	110.1(5)
O209	Gd1	O204	67.45(12)		C206	C203	C205	108.0(5)
O209	Gd1	O204[1]	147.42(13)		O204	C204	C203	113.3(5)
O209[1]	Gd1	O204	147.42(13)		O205	C205	C203	114.5(5)
O209	Gd1	O209[1]	84.80(18)		O206	C206	C203	112.7(5)
O104	Cu1	Gd1	127.86(11)		N202	C207	C201	112.0(5)
O105	Cu1	Gd1	47.97(11)		N202	C208	C209	106.0(5)
O105	Cu1	O104	86.07(16)		N202	C208	C210	110.9(5)
O105	Cu1	O109	86.49(16)		N202	C208	C211	110.6(5)
O105	Cu1	N101	87.88(18)		C210	C208	C209	109.5(5)
O105	Cu1	N102	172.15(18)		C210	C208	C211	109.1(5)
O109	Cu1	Gd1	50.76(11)		C211	C208	C209	110.6(5)
O109	Cu1	O104	115.42(16)		O209	C209	C208	111.7(5)
O109	Cu1	N101	169.48(18)		O210	C210	C208	111.6(5)
O109	Cu1	N102	86.77(18)		O211	C211	C208	114.8(5)
N101	Cu1	Gd1	119.42(14)		O1	Cl2	O2	107.2(10)
N101	Cu1	O104	73.00(18)		O3	Cl2	O1	112.4(7)
N102	Cu1	Gd1	124.22(14)		O3	Cl2	O2	112.5(9)
N102	Cu1	O104	100.47(18)		O4	Cl2	O1	108.7(7)
N102	Cu1	N101	98.14(19)		O4	Cl2	O2	107.0(9)
O204	Cu2	Gd1	45.06(11)		O4	Cl2	O3	108.8(6)

[1]1-X,+Y,3/2-Z

Table S13: Bond Angles for **2** (Tb).

Atom 1	Atom 2	Atom 3	Angle/˚		Atom 1	Atom 2	Atom 3	Angle/˚
$Cu1^{1}$	Tb1	Cu1	146.690(18)		O204	Cu2	N201	87.66(11)
Cu1	Tb1	$Cu2^{1}$	103.482(11)		O204	Cu2	N202	172.07(11)
Cu1	Tb1	Cu2	84.299(11)		O209	Cu2	Tb1	43.41(7)
$Cu1^{1}$	Tb1	Cu2	103.482(11)		O209	Cu2	O204	85.98(10)
$Cu1^{1}$	Tb1	$Cu2^{1}$	84.295(11)		O209	Cu2	N201	172.81(12)
$Cu2^{1}$	Tb1	Cu2	153.009(17)		O209	Cu2	N202	87.00(11)
O105	Tb1	Cu1	36.05(6)		N201	Cu2	Tb1	129.53(9)
$O105^{1}$	Tb1	Cu1	168.56(6)		N201	Cu2	N202	99.55(12)
O105	Tb1	$Cu1^{1}$	168.56(6)		N202	Cu2	Tb1	129.15(9)
$O105^{1}$	Tb1	$Cu1^{1}$	36.05(6)		C104	O104	Cu1	102.4(2)
O105	Tb1	$Cu2^{1}$	84.45(6)		Cu1	O105	Tb1	96.06(10)
$O105^{1}$	Tb1	$Cu2^{1}$	87.53(6)		C105	O105	Tb1	130.2(2)
O105	Tb1	Cu2	87.53(6)		C105	O105	Cu1	108.1(2)
$O105^{1}$	Tb1	Cu2	84.45(6)		Cu1	O109	Tb1	92.91(9)
O105	Tb1	$O105^{1}$	145.16(12)		C109	O109	Tb1	132.4(2)
O105	Tb1	$O109^{1}$	148.98(8)		C109	O109	Cu1	110.18(19)
O105	Tb1	O109	64.77(8)		Cu2	O204	Tb1	100.10(10)
$O105^{1}$	Tb1	O109	148.98(8)		C204	O204	Tb1	146.8(2)
$O105^{1}$	Tb1	$O109^{1}$	64.76(8)		C204	O204	Cu2	109.5(2)
O109	Tb1	Cu1	36.68(5)		Cu2	O209	Tb1	102.27(10)
$O109^{1}$	Tb1	Cu1	112.93(6)		C209	O209	Tb1	145.2(2)
$O109^{1}$	Tb1	$Cu1^{1}$	36.68(5)		C209	O209	Cu2	112.0(2)
O109	Tb1	$Cu1^{1}$	112.93(6)		C102	N101	Cu1	119.1(2)
O109	Tb1	$Cu2^{1}$	88.82(5)		C102	N101	C103	115.9(3)
$O109^{1}$	Tb1	Cu2	88.82(5)		C103	N101	Cu1	100.3(2)
O109	Tb1	Cu2	110.87(5)		C107	N102	Cu1	115.2(2)
$O109^{1}$	Tb1	$Cu2^{1}$	110.87(5)		C107	N102	C108	117.8(3)
O109	Tb1	$O109^{1}$	88.02(11)		C108	N102	Cu1	107.4(2)
$O204^{1}$	Tb1	Cu1	107.52(6)		C202	N201	Cu2	115.5(2)
O204	Tb1	Cu1	61.32(6)		C202	N201	C203	116.9(3)
$O204^{1}$	Tb1	$Cu1^{1}$	61.32(6)		C203	N201	Cu2	106.6(2)
O204	Tb1	$Cu1^{1}$	107.53(6)		C207	N202	Cu2	118.1(2)
$O204^{1}$	Tb1	$Cu2^{1}$	35.01(6)		C207	N202	C208	115.3(3)
$O204^{1}$	Tb1	Cu2	164.72(6)		C208	N202	Cu2	107.5(2)
O204	Tb1	$Cu2^{1}$	164.72(6)		C102	C101	C107	114.8(3)
O204	Tb1	Cu2	35.01(6)		N101	C102	C101	112.7(3)
O204	Tb1	O105	83.24(8)		N101	C103	C104	108.8(3)
O204	Tb1	$O105^{1}$	107.73(8)		N101	C103	C105	103.1(3)
$O204^{1}$	Tb1	$O105^{1}$	83.24(8)		N101	C103	C106	115.3(3)
$O204^{1}$	Tb1	O105	107.73(8)		C105	C103	C104	111.8(3)
O204	Tb1	$O109^{1}$	76.31(8)		C106	C103	C104	106.5(3)
$O204^{1}$	Tb1	$O109^{1}$	77.76(8)		C106	C103	C105	111.3(3)
O204	Tb1	O109	77.76(8)		O104	C104	C103	111.4(3)
$O204^{1}$	Tb1	O109	76.31(8)		O105	C105	C103	110.9(3)
O204	Tb1	$O204^{1}$	143.65(12)		O106	C106	C103	116.4(3)
O209	Tb1	Cu1	96.72(6)		N102	C107	C101	110.2(3)
$O209^{1}$	Tb1	Cu1	107.91(6)		N102	C108	C109	104.5(3)

O209[1]	Tb1	Cu1[1]	96.72(6)		N102	C108	C110	109.9(3)
O209	Tb1	Cu1[1]	107.91(6)		N102	C108	C111	110.0(3)
O209[1]	Tb1	Cu2	118.69(6)		C110	C108	C109	111.4(3)
O209[1]	Tb1	Cu2[1]	34.33(6)		C110	C108	C111	111.8(3)
O209	Tb1	Cu2[1]	118.69(6)		C111	C108	C109	109.0(3)
O209	Tb1	Cu2	34.33(6)		O109	C109	C108	111.8(3)
O209	Tb1	O105	79.43(8)		O110	C110	C108	106.3(3)
O209	Tb1	O105[1]	74.93(8)		O111	C111	C108	111.1(3)
O209[1]	Tb1	O105[1]	79.43(8)		C202	C201	C207	114.2(3)
O209[1]	Tb1	O105	74.93(8)		N201	C202	C201	111.4(3)
O209	Tb1	O109[1]	112.88(8)		N201	C203	C204	105.2(3)
O209	Tb1	O109	132.59(8)		N201	C203	C205	111.1(3)
O209[1]	Tb1	O109[1]	132.59(8)		N201	C203	C206	112.1(3)
O209[1]	Tb1	O109	112.88(8)		C205	C203	C204	111.2(3)
O209	Tb1	O204	67.68(8)		C206	C203	C204	109.9(3)
O209[1]	Tb1	O204[1]	67.69(8)		C206	C203	C205	107.4(3)
O209[1]	Tb1	O204	147.33(8)		O204	C204	C203	113.1(3)
O209	Tb1	O204[1]	147.33(8)		O205	C205	C203	113.5(3)
O209[1]	Tb1	O209	84.42(12)		O206	C206	C203	112.0(3)
O104	Cu1	Tb1	127.69(7)		N202	C207	C201	112.1(3)
O105	Cu1	Tb1	47.89(7)		N202	C208	C209	105.8(3)
O105	Cu1	O104	85.97(10)		N202	C208	C210	110.6(3)
O105	Cu1	O109	86.20(10)		N202	C208	C211	111.3(3)
O105	Cu1	N101	87.76(11)		C210	C208	C209	109.4(3)
O105	Cu1	N102	172.13(11)		C211	C208	C209	110.8(3)
O109	Cu1	Tb1	50.40(7)		C211	C208	C210	108.9(3)
O109	Cu1	O104	115.65(10)		O209	C209	C208	111.8(3)
O109	Cu1	N101	169.09(12)		O210	C210	C208	111.0(3)
O109	Cu1	N102	86.82(11)		O211	C211	C208	114.5(3)
N101	Cu1	Tb1	119.34(9)		O2	Cl2	O1	107.2(7)
N101	Cu1	O104	72.90(11)		O3	Cl2	O1	111.7(5)
N102	Cu1	Tb1	124.33(9)		O3	Cl2	O2	112.5(6)
N102	Cu1	O104	100.34(11)		O4	Cl2	O1	107.9(5)
N102	Cu1	N101	98.55(12)		O4	Cl2	O2	108.5(7)
O204	Cu2	Tb1	44.89(7)		O4	Cl2	O3	108.8(4)

[1]1-X,+Y,3/2-Z

Table S14: Bond Angles for **3** (Dy).

Atom 1	Atom 2	Atom 3	Angle/˚		Atom 1	Atom 2	Atom 3	Angle/˚
Cu1	Dy1	Cu1[1]	146.278(19)		O209	Cu2	O204	85.65(11)
Cu1	Dy1	Cu2	84.300(13)		O209	Cu2	N201	172.60(13)
Cu1[1]	Dy1	Cu2[1]	84.301(12)		O209	Cu2	N202	86.98(13)
Cu1[1]	Dy1	Cu2	103.635(12)		N201	Cu2	Dy1	129.47(10)
Cu1	Dy1	Cu2[1]	103.636(12)		N201	Cu2	N202	99.81(14)
Cu2[1]	Dy1	Cu2	152.793(18)		N202	Cu2	Dy1	129.06(10)
O105[1]	Dy1	Cu1	168.74(6)		C104	O104	Cu1	102.4(2)
O105	Dy1	Cu1	36.04(7)		Cu1	O105	Dy1	96.19(11)
O105	Dy1	Cu1[1]	168.74(6)		C105	O105	Dy1	129.9(2)
O105[1]	Dy1	Cu1[1]	36.04(7)		C105	O105	Cu1	109.2(2)
O105[1]	Dy1	Cu2	84.69(6)		Cu1	O109	Dy1	93.09(11)
O105	Dy1	Cu2[1]	84.69(6)		C109	O109	Dy1	133.7(2)
O105	Dy1	Cu2	87.30(6)		C109	O109	Cu1	109.8(2)
O105[1]	Dy1	Cu2[1]	87.30(6)		Cu2	O204	Dy1	100.45(11)
O105	Dy1	O105[1]	145.47(13)		C204	O204	Dy1	146.4(2)
O105[1]	Dy1	O109[1]	64.96(9)		C204	O204	Cu2	109.9(2)
O105	Dy1	O109	64.96(9)		Cu2	O209	Dy1	102.39(11)
O105[1]	Dy1	O109	148.48(9)		C209	O209	Dy1	145.6(2)
O105	Dy1	O109[1]	148.48(9)		C209	O209	Cu2	111.6(2)
O109[1]	Dy1	Cu1	112.44(6)		C102	N101	Cu1	118.8(3)
O109[1]	Dy1	Cu1[1]	36.75(6)		C102	N101	C103	116.1(3)
O109	Dy1	Cu1	36.75(6)		C103	N101	Cu1	100.7(2)
O109	Dy1	Cu1[1]	112.44(6)		C107	N102	Cu1	115.6(3)
O109[1]	Dy1	Cu2[1]	110.89(6)		C107	N102	C108	118.0(3)
O109[1]	Dy1	Cu2	89.06(6)		C108	N102	Cu1	106.8(2)
O109	Dy1	Cu2	110.89(6)		C202	N201	Cu2	115.5(3)
O109	Dy1	Cu2[1]	89.06(6)		C202	N201	C203	117.2(3)
O109[1]	Dy1	O109	87.37(13)		C203	N201	Cu2	106.5(2)
O204	Dy1	Cu1	61.50(7)		C207	N202	Cu2	117.8(3)
O204	Dy1	Cu1[1]	107.23(7)		C208	N202	Cu2	107.3(2)
O204[1]	Dy1	Cu1	107.22(7)		C208	N202	C207	115.8(3)
O204[1]	Dy1	Cu1[1]	61.50(7)		C102	C101	C107	114.9(4)
O204	Dy1	Cu2[1]	165.06(7)		N101	C102	C101	112.8(3)
O204[1]	Dy1	Cu2[1]	34.97(7)		N101	C103	C104	108.8(3)
O204	Dy1	Cu2	34.97(7)		N101	C103	C105	104.2(3)
O204[1]	Dy1	Cu2	165.07(7)		N101	C103	C106	115.4(4)
O204	Dy1	O105	83.25(9)		C105	C103	C104	111.9(3)
O204[1]	Dy1	O105	107.62(9)		C106	C103	C104	106.6(4)
O204	Dy1	O105[1]	107.62(9)		C106	C103	C105	109.9(4)
O204[1]	Dy1	O105[1]	83.25(9)		O104	C104	C103	110.8(3)
O204[1]	Dy1	O109	76.05(9)		O105	C105	C103	109.1(3)
O204[1]	Dy1	O109[1]	77.86(9)		O106	C106	C103	116.6(4)
O204	Dy1	O109	77.86(9)		N102	C107	C101	110.1(3)
O204	Dy1	O109[1]	76.05(9)		N102	C108	C109	105.0(3)
O204[1]	Dy1	O204	143.64(13)		N102	C108	C110	110.3(3)
O209	Dy1	Cu1	96.89(7)		N102	C108	C111	110.0(3)
O209[1]	Dy1	Cu1[1]	96.89(7)		C109	C108	C111	108.9(3)

O209[1]	Dy1	Cu1	108.10(6)		C110	C108	C109	111.3(3)
O209	Dy1	Cu1[1]	108.10(6)		C110	C108	C111	111.1(3)
O209	Dy1	Cu2	34.36(6)		O109	C109	C108	112.3(3)
O209[1]	Dy1	Cu2[1]	34.35(6)		O11B	C110	C108	106.5(10)
O209	Dy1	Cu2[1]	118.45(7)		O110	C110	C108	105.7(3)
O209[1]	Dy1	Cu2	118.45(7)		O111	C111	C108	111.0(4)
O209[1]	Dy1	O105	75.15(9)		C207	C201	C202	114.6(4)
O209	Dy1	O105[1]	75.15(9)		N201	C202	C201	111.3(3)
O209[1]	Dy1	O105[1]	79.38(9)		N201	C203	C204	105.8(3)
O209	Dy1	O105	79.38(9)		N201	C203	C205	110.8(3)
O209[1]	Dy1	O109	113.21(9)		N201	C203	C206	112.2(3)
O209	Dy1	O109	132.80(9)		C204	C203	C205	110.9(3)
O209[1]	Dy1	O109[1]	132.80(9)		C206	C203	C204	110.0(3)
O209	Dy1	O109[1]	113.21(9)		C206	C203	C205	107.1(3)
O209[1]	Dy1	O204[1]	67.76(9)		O204	C204	C203	112.7(3)
O209	Dy1	O204[1]	147.32(9)		O205	C205	C203	113.6(3)
O209	Dy1	O204	67.76(9)		O206	C206	C203	111.8(3)
O209[1]	Dy1	O204	147.32(9)		N202	C207	C201	112.0(4)
O209	Dy1	O209[1]	84.15(13)		N202	C208	C209	106.3(3)
O104	Cu1	Dy1	126.61(9)		N202	C208	C210	110.5(3)
O105	Cu1	Dy1	47.77(8)		N202	C208	C211	110.8(3)
O105	Cu1	O104	85.38(12)		C209	C208	C210	109.3(3)
O105	Cu1	O109	86.11(11)		C211	C208	C209	111.0(3)
O105	Cu1	N101	87.81(13)		C211	C208	C210	108.9(3)
O105	Cu1	N102	172.41(12)		O209	C209	C208	111.7(3)
O109	Cu1	Dy1	50.16(8)		O210	C210	C208	111.2(4)
O109	Cu1	O104	114.96(12)		O211	C211	C208	114.3(3)
O109	Cu1	N101	169.53(13)		O1	Cl2	O2	108.9(11)
O109	Cu1	N102	86.98(12)		O1	Cl2	O3	113.0(9)
N101	Cu1	Dy1	119.92(10)		O3	Cl2	O2	113.3(11)
N101	Cu1	O104	72.96(13)		O4	Cl2	O1	107.4(8)
N102	Cu1	Dy1	124.78(9)		O4	Cl2	O2	103.2(9)
N102	Cu1	O104	100.41(13)		O4	Cl2	O3	110.5(4)
N102	Cu1	N101	98.54(13)		C8	O1AA	O8	51.8(7)
O204	Cu2	Dy1	44.58(7)		C8	O8	O1AA	45.0(7)
O204	Cu2	N201	87.74(12)		O1AA	C8	O2AA	167.6(16)
O204	Cu2	N202	171.80(13)		O1AA	C8	O8	83.2(9)
O209	Cu2	Dy1	43.25(8)		O8	C8	O2AA	95.3(13)

[1]1-X,+Y,3/2-Z

Table S15: Bond Angles for **4** (La).

Atom 1	Atom 2	Atom 3	Angle/˚		Atom 1	Atom 2	Atom 3	Angle/˚
Cu1[1]	La1	Cu1	152.71(2)		O209	Cu2	La1	51.08(7)
Cu2	La1	Cu1	84.575(16)		O209	Cu2	O204	115.86(10)
Cu2[1]	La1	Cu1[1]	84.574(16)		O209	Cu2	N31	169.08(12)
Cu2[1]	La1	Cu1	103.010(15)		O209	Cu2	N35	86.21(11)
Cu2	La1	Cu1[1]	103.014(15)		N31	Cu2	La1	118.95(10)
Cu2	La1	Cu2[1]	147.86(2)		N31	Cu2	O204	73.37(12)
O104	La1	Cu1	34.43(6)		N35	Cu2	La1	122.43(9)
O104[1]	La1	Cu1[1]	34.43(6)		N35	Cu2	O204	101.67(12)
O104[1]	La1	Cu1	165.37(6)		N35	Cu2	N31	97.88(12)
O104	La1	Cu1[1]	165.38(6)		Cu1	O104	La1	99.62(10)
O104[1]	La1	Cu2	107.21(6)		C104	O104	La1	147.4(2)
O104	La1	Cu2[1]	107.20(6)		C104	O104	Cu1	109.6(2)
O104[1]	La1	Cu2[1]	62.40(6)		Cu1	O109	La1	101.89(10)
O104	La1	Cu2	62.40(6)		C109	O109	La1	145.8(2)
O104[1]	La1	O104	144.78(12)		C109	O109	Cu1	111.8(2)
O104	La1	O205	83.76(8)		C204	O204	Cu2	102.7(2)
O104[1]	La1	O205[1]	83.76(8)		Cu2	O205	La1	94.85(10)
O104	La1	O205[1]	106.92(8)		C205	O205	La1	129.6(2)
O104[1]	La1	O205	106.93(8)		C205	O205	Cu2	108.8(2)
O104[1]	La1	O209	76.72(8)		Cu2	O209	La1	93.01(9)
O104[1]	La1	O209[1]	78.77(8)		C209	O209	La1	128.9(2)
O104	La1	O209	78.77(8)		C209	O209	Cu2	110.3(2)
O104	La1	O209[1]	76.72(8)		C202	N31	Cu2	119.6(2)
O109	La1	Cu1	33.68(6)		C202	N31	C203	115.5(3)
O109	La1	Cu1[1]	119.03(6)		C203	N31	Cu2	100.4(2)
O109[1]	La1	Cu1	119.04(6)		C207	N35	Cu2	114.9(2)
O109[1]	La1	Cu1[1]	33.68(6)		C207	N35	C208	118.3(3)
O109[1]	La1	Cu2[1]	95.85(6)		C208	N35	Cu2	107.5(2)
O1091	La1	Cu2	107.77(6)		C102	N101	Cu1	115.4(2)
O109	La1	Cu2[1]	107.76(6)		C103	N101	Cu1	106.8(2)
O109	La1	Cu2	95.85(6)		C103	N101	C102	116.9(3)
O109	La1	O104	66.40(8)		C107	N102	Cu1	118.3(2)
O109	La1	O104[1]	147.68(8)		C107	N102	C108	114.9(3)
O109[1]	La1	O104	147.68(8)		C108	N102	Cu1	107.8(2)
O109[1]	La1	O104[1]	66.40(8)		O111	C18	C108	114.8(3)
O109[1]	La1	O109	85.37(11)		C107	C101	C102	114.1(3)
O109	La1	O205	79.04(8)		N101	C102	C101	111.2(3)
O109[1]	La1	O205	75.33(8)		N101	C103	C104	105.2(3)
O109	La1	O205[1]	75.33(8)		N101	C103	C105	111.1(3)
O109[1]	La1	O205[1]	79.04(8)		N101	C103	C106	112.0(3)
O109[1]	La1	O209[1]	131.06(8)		C105	C103	C104	111.4(3)
O109[1]	La1	O209	111.99(8)		C106	C103	C104	110.0(3)
O109	La1	O209[1]	111.99(8)		C106	C103	C105	107.3(3)
O109	La1	O209	131.06(8)		O104	C104	C103	112.7(3)
O205[1]	La1	Cu1	84.14(6)		O105	C105	C103	114.5(3)
O205	La1	Cu1	87.70(6)		O106	C106	C103	111.9(3)
O205[1]	La1	Cu1[1]	87.70(6)		N102	C107	C101	111.8(3)

O205	La1	Cu1[1]	84.14(6)		N102	C108	C18	111.2(3)
O205[1]	La1	Cu2[1]	35.57(6)		N102	C108	C109	105.1(3)
O205	La1	Cu2	35.57(6)		N102	C108	C110	110.8(3)
O205	La1	Cu2[1]	168.64(6)		C18	C108	C109	111.0(3)
O205[1]	La1	Cu2	168.63(6)		C110	C108	C18	109.1(3)
O205	La1	O205[1]	144.90(12)		C110	C108	C109	109.7(3)
O205[1]	La1	O209[1]	63.44(8)		O109	C109	C108	112.1(3)
O205	La1	O209	63.43(8)		O110	C110	C108	111.6(3)
O205	La1	O209[1]	150.49(8)		C207	C201	C202	115.4(3)
O205[1]	La1	O209	150.50(8)		N31	C202	C201	111.8(3)
O209	La1	Cu1[1]	88.48(5)		N31	C203	C204	108.5(3)
O209	La1	Cu1	110.95(5)		N31	C203	C205	104.1(3)
O209[1]	La1	Cu1[1]	110.95(5)		N31	C203	C206	115.5(3)
O209[1]	La1	Cu1	88.48(5)		C205	C203	C204	111.1(3)
O209	La1	Cu2[1]	114.93(6)		C205	C203	C206	110.9(3)
O209[1]	La1	Cu2[1]	35.91(5)		C206	C203	C204	106.7(3)
O209[1]	La1	Cu2	114.93(6)		O204	C204	C203	111.5(3)
O209	La1	Cu2	35.91(6)		O205	C205	C203	110.3(3)
O209[1]	La1	O209	90.90(12)		O206	C206	C203	116.1(3)
O104	Cu1	La1	45.95(7)		N35	C207	C201	110.0(3)
O104	Cu1	N101	86.95(11)		N35	C208	C209	104.5(3)
O104	Cu1	N102	173.28(12)		N35	C208	C210	109.7(3)
O109	Cu1	La1	44.43(7)		N35	C208	C211	109.8(3)
O109	Cu1	O104	87.87(10)		C209	C208	C211	110.3(3)
O109	Cu1	N101	173.64(12)		C210	C208	C209	110.7(3)
O109	Cu1	N102	86.16(11)		C210	C208	C211	111.6(3)
N101	Cu1	La1	129.50(9)		O209	C209	C208	112.2(3)
N101	Cu1	N102	99.20(12)		O210	C210	C208	107.0(3)
N102	Cu1	La1	129.05(9)		O211	C211	C208	110.6(3)
O204	Cu2	La1	129.21(7)		O1	Cl2	O2	109.8(4)
O205	Cu2	La1	49.58(8)		O1	Cl2	O3	107.4(7)
O205	Cu2	O204	85.67(11)		O1	Cl2	O4	113.2(6)
O205	Cu2	O209	87.71(11)		O2	Cl2	O3	112.0(7)
O205	Cu2	N31	87.22(12)		O4	Cl2	O2	112.8(6)
O205	Cu2	N35	172.00(12)		O4	Cl2	O3	101.4(8)

[1]1-X,+Y,3/2-Z

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