Supporting Information

Two Pairs of Chiral Lanthanide-oxo Clusters Ln_{14} Induced by Amino Acid Derivative

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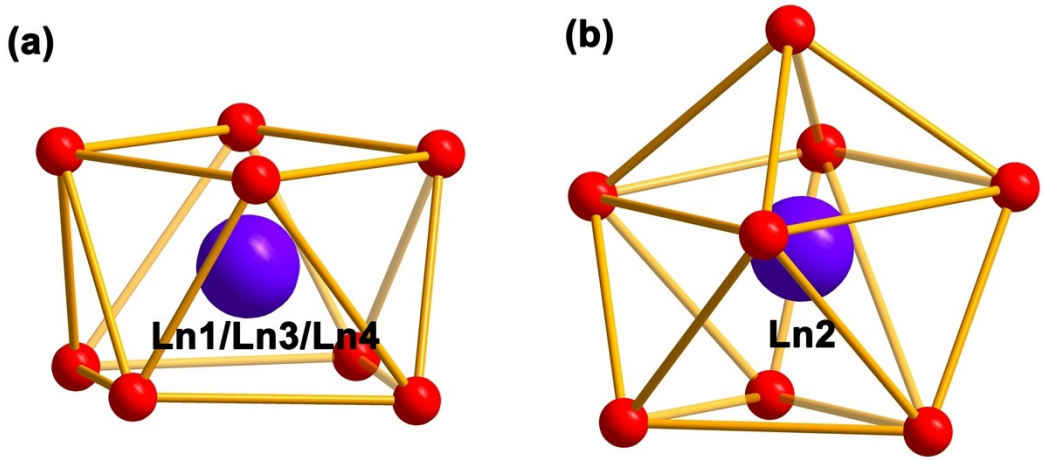

Fig. S1 The coordination modes of Ln^{3+} ions in compounds **L-/D-Y$_{14}$** and **L-/D-Dy$_{14}$**.

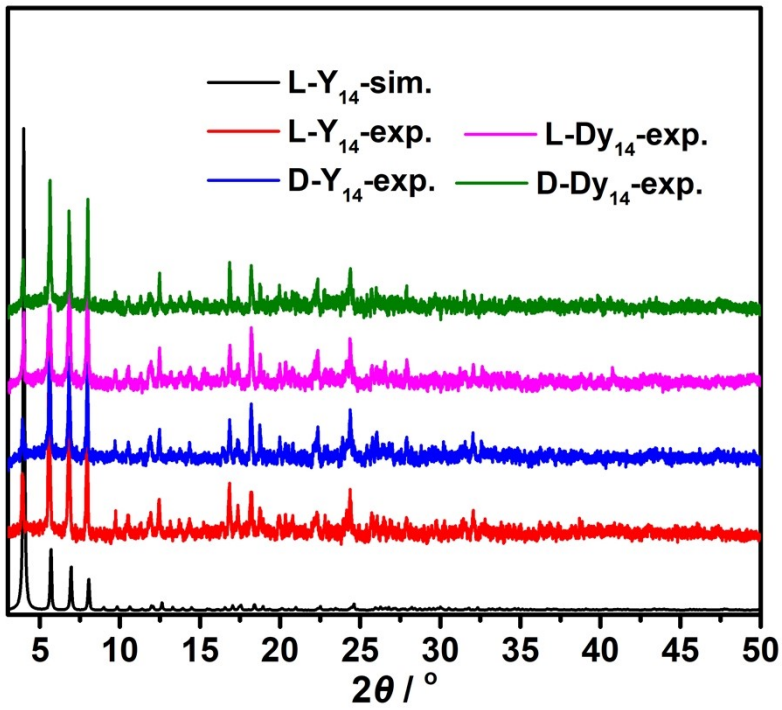

Fig. S2 PXRD curves of compounds **L-/D-Y$_{14}$** and **L-/D-Dy$_{14}$**.

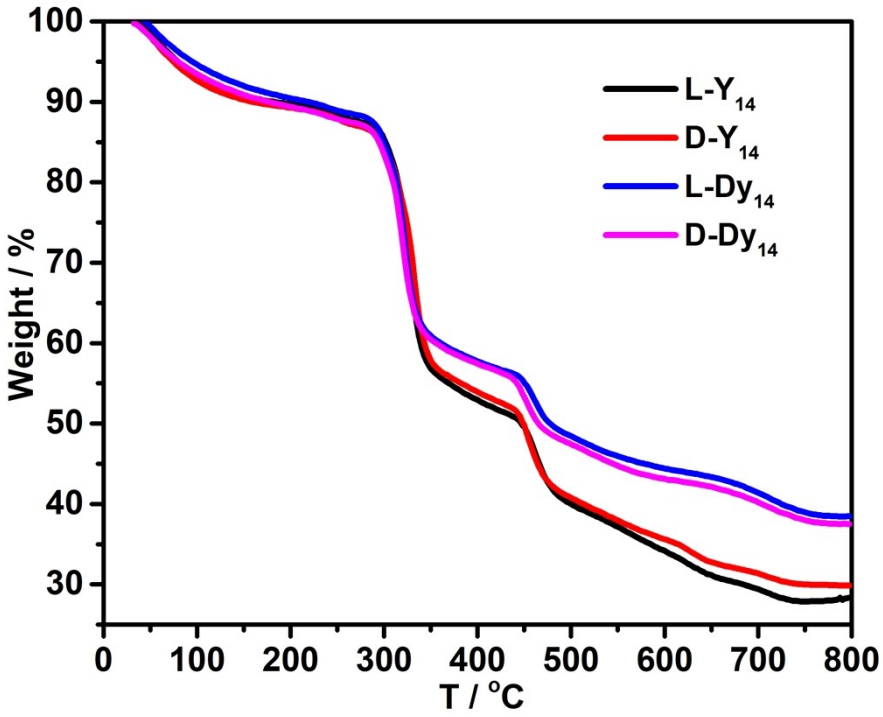

Fig. S3 The TGA of compounds **L-/D-Y$_{14}$** and **L-/D-Dy$_{14}$** under air atmosphere.

From the results of TGA, it found that the mass losses of compounds **L-/D-Y$_{14}$** and **L-/D-Dy$_{14}$** at 300 °C were about 15.7 %, respectively, which were close to the calculated values of 16.8 % for the removal of guest water molecules. As the temperature increased, the metal frameworks drastically collapsed. The final residues of **L-/D-Y$_{14}$** (28.1 % ~ 30.0 %) and **L-/D-Dy$_{14}$** (37.5 % ~ 38.7 %) were slightly higher than the calculated values based on Y_2O_3 (26.5 %) and Dy_2O_3 (36.3 %), respectively, which might be due to the formation of lanthanide oxychlorides caused by the presence of perchlorates.

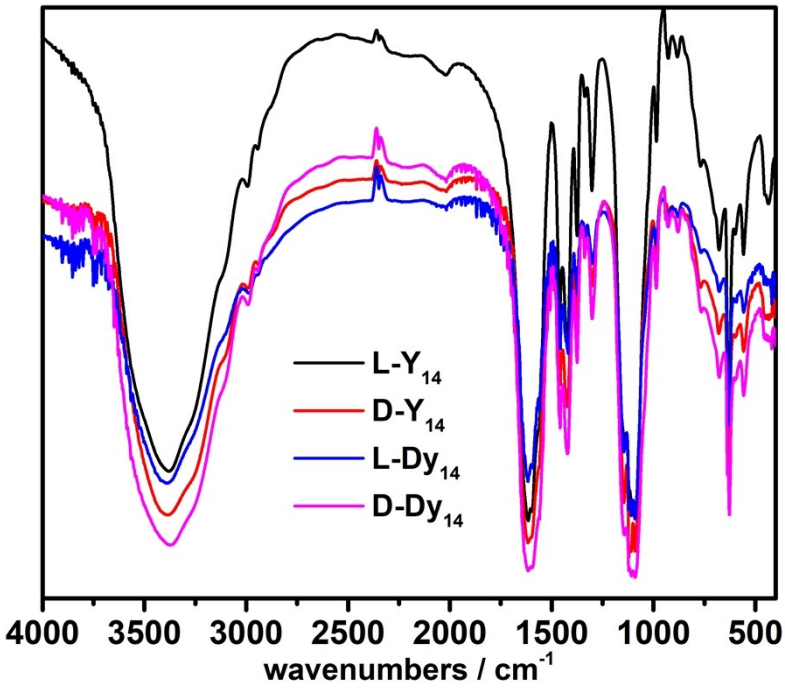

Fig. S4 IR spectra in 500-4000 cm^{-1} for compounds **L-/D-Y$_{14}$** and **L-/D-Dy$_{14}$**.

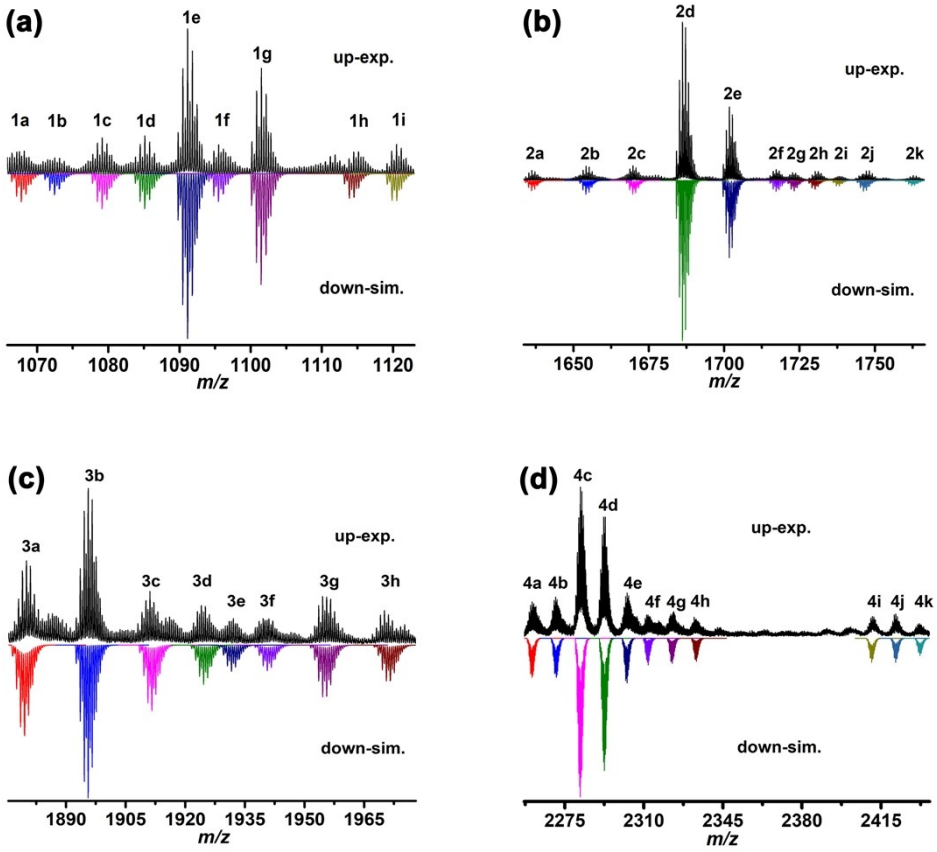

Fig. S5 Positive HRESI-MS data of **L-Y$_{14}$** in the mixed solution of DCM and MeOH.

Table S1. The formula of each species for **L-Y_{14}**.

Peaks	Species	Exp. m/z	Cal. m/z
	+3 charge species		
1	$\{[Y_{12}(C_5H_8NO_3)_9(OH)_8(O)_8]\cdot 13H_2O\cdot 4CH_3OH\cdot 4CH_2Cl_2\}^{3+}$	1067.800	1067.785
2	$\{[Y_{12}(C_5H_8NO_3)_9(OH)_8(O)_8]\cdot 12H_2O\cdot 5CH_3OH\cdot 4CH_2Cl_2\}^{3+}$	1072.472	1072.457
3	$\{[Y_{12}(C_5H_8NO_3)_9(OH)_8(O)_8]\cdot 6H_2O\cdot 9CH_3OH\cdot 4CH_2Cl_2\}^{3+}$	1079.133	1079.137
4	$\{[Y_{12}(C_5H_8NO_3)_9(OH)_8(O)_8]\cdot 7H_2O\cdot 9CH_3OH\cdot 4CH_2Cl_2\}^{3+}$	1085.127	1085.141
5	$\{[Y_{12}(C_5H_8NO_3)_9(OH)_8(O)_8]\cdot 8H_2O\cdot 5CH_3OH\cdot 4CH_2Cl_2\}^{3+}$	1091.145	1091.144
6	$\{[Y_{12}(C_5H_8NO_3)_9(OH)_8(O)_8]\cdot 7H_2O\cdot 10CH_3OH\cdot 4CH_2Cl_2\}^{3+}$	1095.815	1095.816
7	$\{[Y_{12}(C_5H_8NO_3)_9(OH)_8(O)_8]\cdot 8H_2O\cdot 10CH_3OH\cdot 4CH_2Cl_2\}^{3+}$	1101.824	1101.820
8	$\{[Y_{12}(C_5H_8NO_3)_9(OH)_8(O)_8]\cdot 13H_2O\cdot 11CH_3OH\cdot 3CH_2Cl_2\}^{3+}$	1114.519	1114.528
9	$\{[Y_{12}(C_5H_8NO_3)_9(OH)_8(O)_8]\cdot 14H_2O\cdot 11CH_3OH\cdot 4CH_2Cl_2\}^{3+}$	1120.527	1120.532
	+2 charge species		
1	$\{[Y_{12}(C_5H_8NO_3)_9(OH)_8(O)_8(ClO_4)_1]\cdot 6H_2O\cdot 7CH_3OH\cdot 4CH_2Cl_2\}^{2+}$	1636.169	1636.154
2	$\{[Y_{12}(C_5H_8NO_3)_9(OH)_8(O)_8(ClO_4)_1]\cdot 8H_2O\cdot 7CH_3OH\cdot 4CH_2Cl_2\}^{2+}$	1654.179	1654.165
3	$\{[Y_{12}(C_5H_8NO_3)_{10}(OH)_9(O)_7(ClO_4)_1]\cdot 6H_2O\cdot 5CH_3OH\cdot 4CH_2Cl_2\}^{2+}$	1669.668	1669.657
4	$\{[Y_{12}(C_5H_8NO_3)_9(OH)_8(O)_8(ClO_4)_1]\cdot 8H_2O\cdot 9CH_3OH\cdot 4CH_2Cl_2\}^{2+}$	1686.180	1686.191
5	$\{[Y_{12}(C_5H_8NO_3)_{10}(OH)_9(O)_7(ClO_4)_1]\cdot 6H_2O\cdot 7CH_3OH\cdot 4CH_2Cl_2\}^{2+}$	1701.696	1701.683
6	$\{[Y_{12}(C_5H_8NO_3)_{11}(OH)_9(O)_7]\cdot 6H_2O\cdot 7CH_3OH\cdot 4CH_2Cl_2\}^{2+}$	1717.230	1717.234
7	$\{[Y_{12}(C_5H_8NO_3)_{11}(OH)_{10}(O)_6(ClO_4)_1]\cdot 4H_2O\cdot 8CH_3OH\cdot 3CH_2Cl_2\}^{2+}$	1723.240	1723.239
8	$\{[Y_{12}(C_5H_8NO_3)_{11}(OH)_{12}(O)_4(ClO_4)_3]\cdot 9H_2O\cdot 2CH_3OH\cdot 2CH_2Cl_2\}^{2+}$	1730.176	1730.166
9	$\{[Y_{12}(C_5H_8NO_3)_{11}(OH)_{11}(O)_5(ClO_4)_2]\cdot 19H_2O\cdot 2CH_2Cl_2\}^{2+}$	1738.227	1738.215
10	$\{[Y_{12}(C_5H_8NO_3)_{11}(OH)_{10}(O)_6(ClO_4)_1]\cdot 9H_2O\cdot 4CH_3OH\cdot 4CH_2Cl_2\}^{2+}$	1746.182	1746.189

11	$\{[Y_{12}(C_5H_8NO_3)_{11}(OH)_{10}(O)_6(ClO_4)_1]\cdot 9H_2O\cdot 5CH_3OH\cdot 4CH_2Cl_2\}^{2+}$	1762.206	1762.202
	+2 charge species		
1	$\{[Y_{12}(C_5H_8NO_3)_{12}(OH)_{15}(O)_1(ClO_4)_5]\cdot 6H_2O\cdot 3CH_2Cl_2\}^{2+}$	1879.589	1879.585
2	$\{[Y_{12}(C_5H_8NO_3)_{12}(OH)_{15}(O)_1(ClO_4)_5]\cdot 6H_2O\cdot 1CH_3OH\cdot 3CH_2Cl_2\}^{2+}$	1895.587	1895.598
3	$\{[Y_{12}(C_5H_8NO_3)_{12}(OH)_{15}(O)_1(ClO_4)_5]\cdot 6H_2O\cdot 2CH_3OH\cdot 3CH_2Cl_2\}^{2+}$	1911.608	1911.611
4	$\{[Y_{12}(C_5H_8NO_3)_{12}(OH)_{14}(O)_2(ClO_4)_4]\cdot 3H_2O\cdot 5CH_3OH\cdot 4CH_2Cl_2\}^{2+}$	1924.617	1924.633
5	$\{[Y_{12}(C_5H_8NO_3)_{12}(OH)_{14}(O)_2(ClO_4)_5]\cdot 2H_2O\cdot 6CH_3OH\cdot 4CH_2Cl_2\}^{2+}$	1931.620	1931.641
6	$\{[Y_{12}(C_5H_8NO_3)_{12}(OH)_{14}(O)_2(ClO_4)_5]\cdot 3H_2O\cdot 6CH_3OH\cdot 4CH_2Cl_2\}^{2+}$	1940.632	1940.646
7	$\{[Y_{12}(C_5H_8NO_3)_{12}(OH)_{14}(O)_2(ClO_4)_5]\cdot 7H_2O\cdot 2CH_3OH\cdot 5CH_2Cl_2\}^{2+}$	1955.585	1955.590
8	$\{[Y_{12}(C_5H_8NO_3)_{12}(OH)_{14}(O)_2(ClO_4)_5]\cdot 7H_2O\cdot 3CH_3OH\cdot 5CH_2Cl_2\}^{2+}$	1971.614	1971.603
	+3 charge species		
1	$\{[Y_{24}(C_5H_8NO_3)_{24}(OH)_{28}(O)_4(ClO_4)_9]\ 5H_2O\}^{3+}$	2260.545	2260.531
2	$\{[Y_{24}(C_5H_8NO_3)_{24}(OH)_{28}(O)_4(ClO_4)_9]\ 5H_2O\ 1CH_3OH\}^{3+}$	2271.224	2271.206
3	$\{[Y_{24}(C_5H_8NO_3)_{24}(OH)_{28}(O)_4(ClO_4)_9]\ 5H_2O\ 2CH_3OH\}^{3+}$	2281.886	2281.881
4	$\{[Y_{24}(C_5H_8NO_3)_{24}(OH)_{28}(O)_4(ClO_4)_9]\ 5H_2O\ 3CH_3OH\}^{3+}$	2292.554	2292.557
5	$\{[Y_{24}(C_5H_8NO_3)_{24}(OH)_{27}(O)_5(ClO_4)_8]\ 14H_2O\ 2CH_3OH\}^{3+}$	2302.596	2302.595
6	$\{[Y_{24}(C_5H_8NO_3)_{24}(OH)_{27}(O)_5(ClO_4)_8]\ 12H_2O\ 4CH_3OH\}^{3+}$	2311.922	2311.938
7	$\{[Y_{24}(C_5H_8NO_3)_{24}(OH)_{27}(O)_5(ClO_4)_8]\ 12H_2O\ 5CH_3OH\}^{3+}$	2322.594	2322.614
8	$\{[Y_{24}(C_5H_8NO_3)_{24}(OH)_{27}(O)_5(ClO_4)_8]\ 12H_2O\ 6CH_3OH\}^{3+}$	2333.583	2333.589
9	$\{[Y_{24}(C_5H_8NO_3)_{24}(OH)_{20}(O)_{12}(ClO_4)_1]\ 22H_2O\ 19CH_3OH\cdot 4CH_2Cl_2\}^{3+}$	2410.793	2410.811
10	$\{[Y_{24}(C_5H_8NO_3)_{24}(OH)_{20}(O)_{12}(ClO_4)_1]\ 22H_2O\ 20CH_3OH\cdot 4CH_2Cl_2\}^{3+}$	2421.497	2421.487
11	$\{[Y_{24}(C_5H_8NO_3)_{24}(OH)_{20}(O)_{12}(ClO_4)_1]\ 22H_2O\ 21CH_3OH\cdot 4CH_2Cl_2\}^{3+}$	2432.172	2432.162

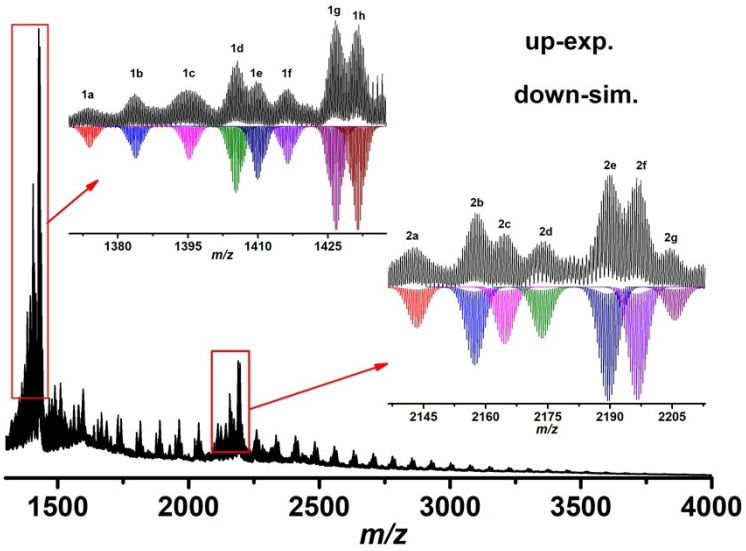

Fig. S6 Positive HRESI-MS data of **L-Dy$_{14}$** in the mixed solution of DCM and MeOH.

Table S2. The formula of each species for **L-Dy$_{14}$**.

Peaks	Species	Exp. m/z	Cal. m/z
	+3 charge species		
1	$\{[Dy_{12}(C_5H_8NO_3)_{12}(OH)_{11}(O)_5]\ 9H_2O{\cdot}3CH_3OH{\cdot}1CH_2Cl_2\}^{3+}$	1373.949	1373.957
2	$\{[Dy_{12}(C_5H_8NO_3)_{12}(OH)_{12}(O)_4(ClO_4)_1]\ 8H_2O{\cdot}4CH_3OH\}^{3+}$	1383.629	1383.630
3	$\{[Dy_{12}(C_5H_8NO_3)_{12}(OH)_{12}(O)_4(ClO_4)_1]\ 7H_2O{\cdot}3CH_3OH{\cdot}1CH_2Cl_2\}^{3+}$	1395.274	1395.268
4	$\{[Dy_{12}(C_5H_8NO_3)_{12}(OH)_{12}(O)_4(ClO_4)_1]\ 14H_2O{\cdot}1CH_2Cl_2\}^{3+}$	1405.275	1405.267
5	$\{[Dy_{12}(C_5H_8NO_3)_{12}(OH)_{12}(O)_4(ClO_4)_1]\ 13H_2O{\cdot}1CH_3OH{\cdot}1CH_2Cl_2\}^{3+}$	1409.934	1409.939
6	$\{[Dy_{12}(C_5H_8NO_3)_{12}(OH)_{12}(O)_4(ClO_4)_1]\ 4H_2O{\cdot}4CH_3OH{\cdot}2CH_2Cl_2\}^{3+}$	1416.256	1416.250
7	$\{[Dy_{12}(C_5H_8NO_3)_{12}(OH)_{12}(O)_4(ClO_4)_1]\ 13H_2O{\cdot}3CH_3OH{\cdot}1CH_2Cl_2\}^{3+}$	1426.625	1426.617
8	$\{[Dy_{12}(C_5H_8NO_3)_{12}(OH)_{12}(O)_4(ClO_4)_1]\ 14H_2O{\cdot}2CH_3OH{\cdot}1CH_2Cl_2\}^{3+}$	1431.296	1431.289
	+2 charge species		
1	$\{[Dy_{12}(C_5H_8NO_3)_{12}(OH)_{12}(O)_4(ClO_4)_2]\ 10H_2O{\cdot}4CH_3OH\}^{2+}$	2143.434	2143.430
2	$\{[Dy_{12}(C_5H_8NO_3)_{12}(OH)_{12}(O)_4(ClO_4)_2]\ 8H_2O{\cdot}6CH_3OH\}^{2+}$	2157.442	2157.446
3	$\{[Dy_{12}(C_5H_8NO_3)_{12}(OH)_{13}(O)_3(ClO_4)_3]\ 5H_2O{\cdot}5CH_3OH\}^{2+}$	2164.409	2164.394
4	$\{[Dy_{12}(C_5H_8NO_3)_{12}(OH)_{13}(O)_3(ClO_4)_3]\ 6H_2O{\cdot}5CH_3OH\}^{2+}$	2173.402	2173.400
5	$\{[Dy_{12}(C_5H_8NO_3)_{12}(OH)_{13}(O)_3(ClO_4)_3]\ 6H_2O{\cdot}6CH_3OH\}^{2+}$	2189.424	2189.413
6	$\{[Dy_{12}(C_5H_8NO_3)_{12}(OH)_{13}(O)_3(ClO_4)_3]\ 5H_2O{\cdot}7CH_3OH\}^{2+}$	2196.414	2196.421
7	$\{[Dy_{12}(C_5H_8NO_3)_{12}(OH)_{13}(O)_3(ClO_4)_3]\ 6H_2O{\cdot}7CH_3OH\}^{2+}$	2205.419	2205.426

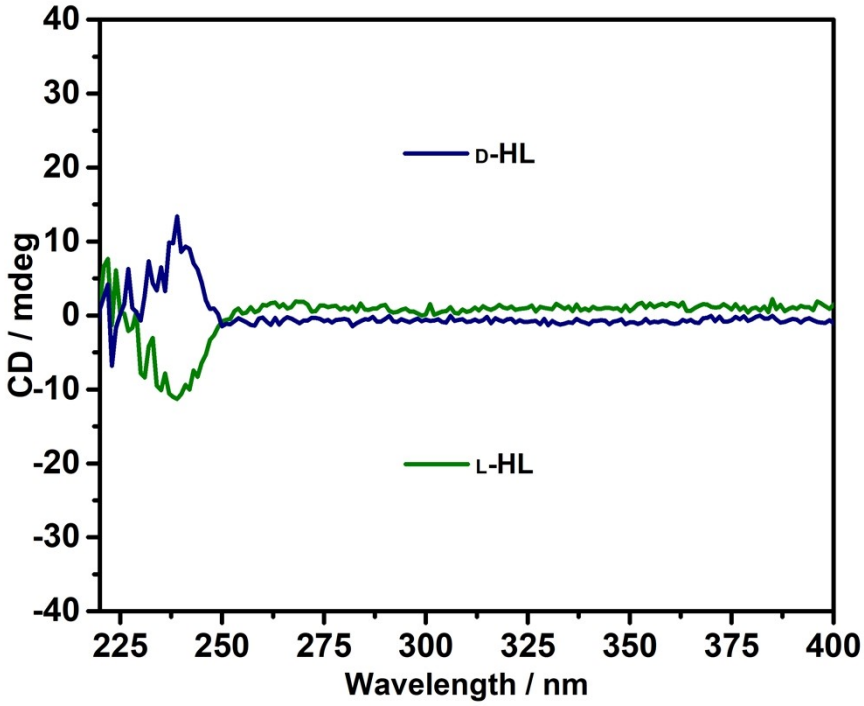

Fig. S7 The solid-state CD spectra of ligands $_{L}$-/$_{D}$-HL.

Table S3. Crystallographic Data for Compounds **L-/D-Y_{14}**.

compound	**L-Y_{14}**	**D-Y_{14}**
Formula	$C_{80}H_{294}Cl_{10}N_{16}O_{179}Y_{14}$	$C_{80}H_{294}Cl_{10}N_{16}O_{179}Y_{14}$
FW	5944.53	5944.53
T/K	120(1)	120(1)
Cry. system	tetragonal	tetragonal
Space group	$I4_122$	$I4_122$
a /Å	30.983(4)	31.008(4)
b /Å	30.983(4)	31.008(4)
c /Å	31.523(7)	30.850(4)
α/°	90	90
β/°	90	90
γ/°	90	90
V /Å^3	30259.0(1)	29663.0(8)
Z	4	4
Dc/g cm^{-3}	1.305	1.331
μ/ mm^{-1}	5.065	5.167
Data/parameters	13991/528	13571/528
2θ/°	8.058–143.326	6.994–140.622
Obs. reflections	61086	50227
F (000)	12136.0	12136.0
GOF	1.006	1.032
R_1[I> 2σ(I)][a]	0.0631	0.0432
wR_2(All data)[b]	0.1943	0.1296

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

Table S4. Crystallographic Data for Compounds **L-/D-Dy$_{14}$**.

compound	**L-Dy$_{14}$**	**D-Dy$_{14}$**
Formula	$C_{80}H_{318}Cl_{10}Dy_{14}N_{16}O_{191}$	$C_{80}H_{318}Cl_{10}Dy_{14}N_{16}O_{191}$
FW	7190.98	7190.98
T/K	120(1)	120(1)
Cry. system	tetragonal	tetragonal
Space group	$I4_122$	$I4_122$
a /Å	31.0292(5)	31.0353(11)
b /Å	31.0292(5)	31.0353(11)
c /Å	31.3898(6)	31.3981(12)
α/°	90	90
β/°	90	90
γ/°	90	90
V /Å^3	30222.5(11)	30242.0(2)
Z	4	4
Dc/g cm^{-3}	1.580	1.579
μ/ mm^{-1}	3.600	19.819
Data/parameters	20269/528	13871/527
2θ/°	4.908–59.942	8.012–139.416
Obs. reflections	50959	32609
F (000)	14128.0	14128.0
GOF	0.807	1.068
R_1[I> 2σ(I)][a]	0.0427	0.0976
wR_2(All data)[b]	0.0895	0.2673

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

Table S5. Selected bond distances (Å) and band angles (°) of **L-Y_{14}.**

Y1-O2	2.349(9)	Y2-O14	2.315(9)
Y1-O13	2.352(10)	Y3-O1[1]	2.392(9)
Y1-O14	2.360(7)	Y3-O2W	2.408(10)
Y1-O13[2]	2.325(10)	Y3-O6	2.259(17)
Y1-O15	2.374(10)	Y3-O9	2.217(10)
Y1-O16[1]	2.365(9)	Y3-O15	2.553(9)
Y1-O17	2.332(8)	Y3-O16	2.356(8)
Y1-O17[1]	2.345(8)	Y3-O16[1]	2.327(8)
Y2-O1W	2.406(10)	Y3-O17	2.393(9)
Y2-O2	2.590(10)	Y4-O3W[2]	2.392(13)
Y2-O3	2.285(10)	Y4-O4W	2.387(16)
Y2-O12	2.272(9)	Y4-O5W[2]	2.377(17)
Y2-O13	2.381(7)	Y4-O10	2.255(10)

O13[1]-Y1-O2	129.2(3)	O1[2]-Y3-O15	127.7(3)
O13-Y1-O2	70.7(3)	O2W-Y3-O1[2]	139.9(4)
O13[1]-Y1-O13	70.0(3)	O2W-Y3-O15	77.3(3)
O13[1]-Y1-O14	70.3(3)	O6-Y3-O1[2]	75.2(5)
O13[1]-Y1-O17	78.4(3)	O6-Y3-O2W	70.7(5)
O3-Y2-O1W	80.9(3)	O6-Y3-O17	146.2(5)
O3-Y2-O2	75.1(3)	O4W-Y4-O3W	143.2(6)
O3-Y2-O13	102.2(3)	O5W-Y4-O3W	119.6(6)
O3-Y2-O14	138.7(4)	O10-Y4-O3W	74.4(4)
O12-Y2-O2	150.4(3)	O10-Y4-O4W	141.9(6)
O12-Y2-O3	98.0(4)	O10-Y4-O5W	71.7(5)

Symmetry code: [1]+Y,+X,-Z; [2]1-X,1-Y,+Z; [3]1-Y,1-X,-Z

Table S6. Selecte d bond distances (Å) and band angles (°) of **D-Y_{14}**.

Y1-O2	2.379(5)	Y2-O14	2.296(5)
Y1-O13	2.331(5)	Y3-O1[1]	2.371(5)
Y1-O14	2.358(5)	Y3-O2W	2.396(6)
Y1-O15	2.383(5)	Y3-O6	2.252(13)
Y1-O16[1]	2.356(5)	Y3-O9	2.247(6)
Y1-O17[1]	2.351(5)	Y3-O15	2.533(5)
Y1-O17	2.333(4)	Y3-O16	2.363(5)
Y2-O1W	2.380(6)	Y3-O16[1]	2.327(5)
Y2-O2	2.565(5)	Y3-O17	2.373(5)
Y2-O3	2.283(6)	Y4-O3W[2]	2.417(9)
Y2-O8[2]	2.335(5)	Y4-O4W[2]	2.379(10)
Y2-O12	2.282(5)	Y4-O5W[2]	2.268(13)
Y2-O13	2.380(4)	Y4-O10	2.234(6)

O13-Y1-O2	69.89(18)	O6-Y3-O2W	71.8(4)
O13[1]-Y1-O2	128.92(17)	O6-Y3-O15	147.4(4)
O13[1]-Y1-O13	70.66(19)	O6-Y3-O16	81.9(4)
O13[1]-Y1-O14	70.35(16)	O9-Y3-O15	73.9(2)
O13-Y1-O14	74.74(16)	O9-Y3-O16	151.53(19)
O17-Y1-O2	150.27(17)	O9-Y3-O17	102.8(2)
O17-Y1-O14	139.60(17)	O16-Y3-O15	124.00(16)
O3-Y2-O1W	80.7(2)	O3W-Y4-O3W[1]	138.2(3)
O3-Y2-O2	75.20(19)	O4W-Y4-O3W	144.7(4)
O3-Y2-O13	102.60(18)	O5W-Y4-O3W	117.6(4)
O3-Y2-O14	139.32(19)	O10-Y4-O5W	73.4(3)

Symmetry code:[1]1-Y,1-X,1-Z; [2]1-X,1-Y,+Z; [3]+Y,+X,1-Z

Table S7. Selected bond distances (Å) and band angles (°) of **L-Dy$_{14}$.**

Dy1-O2	2.370(6)	Dy2-O14	2.309(6)
Dy1-O13	2.374(6)	Dy2-O14^{2}	2.391(6)
Dy1-O13^{2}	2.324(6)	Dy3-O1^{1}	2.381(6)
Dy1-O14	2.356(5)	Dy3-O2W	2.419(6)
Dy1-O15	2.403(6)	Dy3-O6	2.253(12)
Dy1-O16^{1}	2.410(6)	Dy3-O15	2.576(6)
Dy1-O17	2.342(6)	Dy3-O16	2.356(6)
Dy1-O17^{1}	2.397(6)	Dy3-O16^{1}	2.304(6)
Dy2-O2	2.590(6)	Dy3-O17	2.412(6)
Dy2-O3	2.296(6)	Dy4-O3W	2.344(9)
Dy2-O8^{2}	2.344(7)	Dy4-O4W^{2}	2.463(10)
Dy2-O12	2.315(7)	Dy4-O5W^{2}	2.382(12)
Dy2-O13	2.379(6)	Dy4-O10	2.242(7)

O2-Dy1-O15	114.9(2)	O8^{1}-Dy2-O2	128.6(2)
O2-Dy1-O16^{2}	81.7(2)	O8^{1}-Dy2-O13	78.5(2)
O13^{1}-Dy1-O2	128.7(2)	O8^{1}-Dy2-O14^{1}	74.8(2)
O13^{1}-Dy1-O13	69.8(2)	O9-Dy3-O1^{2}	75.4(2)
O13^{1}-Dy1-O14	69.9(2)	O9-Dy3-O2W	85.0(3)
O13-Dy1-O15	147.9(2)	O9-Dy3-O6	90.7(4)
O13-Dy1-O16^{2}	141.6(2)	O9-Dy3-O15	74.8(2)
O3-Dy2-O1W	80.3(2)	O3W-Dy4-O4W	142.3(3)
O3-Dy2-O8^{1}	76.2(2)	O3W-Dy4-O4W^{1}	73.1(4)
O3-Dy2-O12	98.3(2)	O3W^{1}-Dy4-O5W	75.7(4)
O3-Dy2-O13	103.2(2)	O10-Dy4-O3W	74.2(3)

Symmetry code: ^{1}+Y,+X,-Z; ^{2}1-X,1-Y,+Z; ^{3}1-Y,1-X,-Z

Table S8. Selected bond distances (Å) and band angles (°) of **D-Dy$_{14}$**.

Dy1-O2	2.388(15)	Dy2-O3	2.318(17)
Dy1-O13	2.368(14)	Dy3-O1^{1}	2.373(14)
Dy1-O13^{2}	2.295(13)	Dy3-O2W	2.390(17)
Dy1-O14	2.380(12)	Dy3-O6	2.24(3)
Dy1-O15	2.385(15)	Dy3-O15	2.536(16)
Dy1-O16^{2}	2.384(13)	Dy3-O9	2.252(17)
Dy2-O2	2.614(15)	Dy3-O16	2.346(15)
Dy2-O1W	2.410(16)	Dy3-O17	2.401(13)
Dy2-O8^{2}	2.325(15)	Dy3-O16^{1}	2.320(14)
Dy2-O12	2.284(14)	Dy4-O3W	2.41(2)
Dy2-O13	2.417(11)	Dy4-O4W	2.34(3)
Dy2-O14	2.357(14)	Dy4-O5W	2.48(4)
Dy2-O14^{2}	2.352(14)	Dy4-O10	2.207(15)

O13^{2}-Dy1-O2	129.5(5)	O8^{2}-Dy2-O14	140.9(5)
O13-Dy1-O2	72.0(5)	O13-Dy2-O2	67.4(4)
O13^{2}-Dy1-O13	68.8(5)	O6-Dy3-O1^{1}	73.5(10)
O13^{2}-Dy1-O14	70.1(4)	O6-Dy3-O2W	72.7(10)
O13-Dy1-O14	75.8(4)	O6-Dy3-O9	92.1(10)
O13-Dy1-O15	148.2(5)	O6-Dy3-O15	148.3(9)
O14-Dy1-O2	70.4(5)	O6-Dy3-O16	82.8(9)
O14-Dy1-O15	79.3(5)	O3W^{2}-Dy4-O3W	139.1(8)
O8^{2}-Dy2-O1W	137.7(5)	O3W-Dy4-O5W^{2}	75.5(11)
O8^{2}-Dy2-O2	128.1(5)	O4W-Dy4-O3W	139.8(12)
O8^{2}-Dy2-O13	79.3(5)	O10-Dy4-O3W^{2}	76.4(7)

Symmetry code:^{1}1-X,1-Y,+Z; ^{2}1-Y,1-X,1-Z; ^{3}+Y,+X,1-Z

Table S9. The CShM (Continuous Shape Measurements) values of Y^{3+} with octa-coordinate mode in compounds **L-/D-Y_{14}**.

Com.[b] / Refcode[a]	**L-Y_{14}** Y1/Y2/Y3/Y4	**D-Y_{14}** Y1/Y2/Y3/Y4
OP-8	26.856/29.595/28.360/29.432	26.849/29.238/28.677/30.014
HPY-8	22.987/23.383/23.951/23.315	23.123/23.512/24.149/23.904
HBPY-8	15.332/15.380/15.605/17.183	15.270/15.679/15.298/16.349
CU-8	7.778/8.565/9.640/9.748	7.750/8.840/9.132/8.779
SAPR-8	**0.642**/1.705/**1.315**/**0.486**	**0.707**/1.682/**1.242**/**0.469**
TDD-8	2.345/**0.893**/1.378/1.368	2.342/**0.893**/1.288/1.563
JGBF-8	15.894/14.965/13.721/15.593	15.792/14.610/14.299/16.753
JETBPY-8	26.762/28.500/27.523/27.528	26.626/28.430/28.036/28.409
JBTPR-8	3.238/5.545/1.683/2.310	3.294/2.363/1.887/2.669
BTPR-8	2.712/2.211/1.606/1.891	2.772/2.195/1.691/2.669
JSD-8	5.402/3.243/3.203/3.658	5.469/3.012/3.378/4.339
TT-8	8.416/9.036/9.916/10.444	8.314/9.248/9.518/9.507
ETBPY-8	21.332/22.943/22.224/23.429	21.237/23.204/22.274/24.609

[a] OP-8, Octagon; HPY-8, Heptagonal pyramid; HBPY-8, Heptagonal bipyramid; CU-8, Cube; SAPR-8, Square antiprism; TDD-8, Triangular dodecahedron; JGBF-8, Johnson gyrobifastigium J26; JETBPY-8, Johnson elongated triangular bipyramid J14; JBTPR-8, Biaugmented trigonal prism J50; BTPR-8, Biaugmented trigonal prism; JSD-8, Snub diphenoid J84; TT-8, Triakis tetrahedron; ETBPY-8, Elongated trigonal bipyramid. [b] The lanthanide ion in each asymmetric unit of compounds **L-/D-Y_{14}.**

Table S10. The CShM (Continuous Shape Measurements) values of Dy^{3+} with octa-coordinate mode in compounds **L-/D-Dy$_{14}$**.

Com.[b] / Refcode[a]	**L-Dy$_{14}$** Dy1/Dy2/Dy3/Dy4	**D-Dy$_{14}$** Dy1/Dy2/Dy3/Dy4
OP-8	26.941/29.113/28.856/30.389	26.805/29.087/28.183/30.987
HPY-8	23.028/23.875/23.992/23.088	23.088/23.410/23.811/22.181
HBPY-8	15.111/15.483/15.533/17.195	15.248/15.408/15.536/16.463
CU-8	7.859/8.663/9.655/9.979	7.872/8.778/9.168/9.999
SAPR-8	**0.692**/1.765/**1.363/0.582**	**0.705**/1.592/**1.284/0.783**
TDD-8	2.220/**0.938**/1.363/1.495	2.442/**0.892**/1.330/2.189
JGBF-8	15.581/14.986/13.664/15.883	15.966/14.764/14.110/14.780
JETBPY-8	26.580/28.323/28.270/28.109	26.394/28.374/27.938/27.771
JBTPR-8	3.080/2.508/1.739/2.591	3.325/2.475/1.902/2.361
BTPR-8	2.521/2.229/1.674/2.021	2.759/2.201/1.746/2.285
JSD-8	5.282/3.106/3.214/4.137	5.391/3.255/3.388/3.660
TT-8	8.4479/9.084/9.927/10.826	8.537/9.343/9.547/10.853
ETBPY-8	21.430/23.271/22.531/23.543	21.119/22.851/22.006/24.502

[a] OP-8, Octagon; HPY-8, Heptagonal pyramid; HBPY-8, Heptagonal bipyramid; CU-8, Cube; SAPR-8, Square antiprism; TDD-8, Triangular dodecahedron; JGBF-8, Johnson gyrobifastigium J26; JETBPY-8, Johnson elongated triangular bipyramid J14; JBTPR-8, Biaugmented trigonal prism J50; BTPR-8, Biaugmented trigonal prism; JSD-8, Snub diphenoid J84; TT-8, Triakis tetrahedron; ETBPY-8, Elongated trigonal bipyramid. [b] The lanthanide ion in each asymmetric unit of compounds **L-/D-Dy$_{14}$.**