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SUPPLEMENTARY INFORMATION

4-Hydroxybenzoato-Rare Earth(III) Complexes – Syntheses, a Structural Goldmine from Coordination Diversity and Improved Corrosion Inhibition Behaviour

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Contents

1. Preparation of 4-Hydroxybenzoato Rare Earth Aqua Complexes

The complexes were synthesised by reaction between sodium 4-hydroxybenzoate prepared *in situ* unless noted, and a rare earth salt ($RECl_3 \cdot xH_2O$; RE = Nd, Sm) in a 3:1 mole ratio, typically on a 0.5-1.5 mmol scale (by metal salt). Reactions were conducted in aqueous media at ambient temperature. Precipitates were collected for $RE(4hob)_3$ (RE = Nd, Sm).

Characterization of the Aqua Complexes for which structures could not be obtained follow.

$Nd(4hob)_3(H_2O)_2$. Fibrous bunches of pale purple needles (yield: 63%) dec. 268 °C. $C_{21}H_{19}NdO_{11}$ (591.61) calculated: C 42.63, H 3.24, Nd 24.38%; found C 42.22, H 3.44, Nd 23.87%.
IR (cm^{-1}): 3260s, v br, 1655vw, 1601s, 1509vs, 1413vs, 1252vs, 1176s, 1102m, 1015w, 914vw, 853m, 785vs, 699s.
$Sm(4hob)_3(H_2O)_2$. White precipitate (yield: 91%) dec. 276 °C. $C_{21}H_{19}SmO_{11}$ (597.73) calculated: C 42.20, H 3.20, Sm 25.16%; found C 42.47, H 3.28, Sm 24.83%.
IR (cm^{-1}): 3299s, v br, 1698vw, 1599s, 1501s, 1397vs, 1238s, 1168vs, 1101m, 1013vw, 966vw, 854m,784vs, 699m.

Preparation of Rare Earth 4hob Complexes with 2,2′-Bipyridine

The complexes were synthesised by a reaction between sodium 4-hydroxybenzoate prepared *in situ*, 2,2′-bipyridine (bpy), and a rare earth salt ($REX_3 \cdot xH_2O$; X = Cl^- or NO_3^-, or ½ SO_4^{2-} (for Ce only) in a 3:1:1 mole ratio, on a 1 mmol scale (by metal salt). Reactions were conducted in aqueous medium at pH ~6. Precipitates were collected for complexes $RE(4hob)_3(bpy)$ (RE = La, Ce, Pr, Nd, Sm, Eu, Gd, Ho, Y, Er, Yb Lu).

Characterization of the Complexes with 2,2′-Bipyridine for which structures could not be obtained follow.

$La(4hob)_3(bpy)$. White precipitate (yield: 12%) dec. 188 °C. $C_{31}H_{23}N_2LaO_9$ (706.43) calculated: C 52.71, H 3.28, N 3.97, La 19.66%; found C 53.09, H 3.37, N 4.03, La 19.38%.
IR (cm^{-1}): 3076w, 1594m, 1525m, 1505m, 1381s, 1273m, 1239m, 1165m, 1098w, 1008w, 855m, 785m, 757m, 700w.
$Ce(4hob)_3(bpy)$. White precipitate (yield: 14%) dec. 152 °C. $C_{31}H_{23}N_2CeO_9$ (707.64) calculated: C 52.62, H 3.28, N 3.96, Ce 19.80%; found C 52.96, H 3.41, N 4.02, Ce 19.68%.
IR (cm^{-1}): 3072w, 1594m, 1526m, 1505m, 1384s, 1274m, 1239m, 1165m, 1096m, 1009w, 855w, 785m, 757m, 701w.
$Pr(4hob)_3(bpy)$. Green precipitate (yield: 31%) dec. 181 °C. $C_{31}H_{23}N_2PrO_9$ (708.43) calculated: C 52.56, H 3.27, N 3.95, Pr 19.89%; found C 51.96, H 3.41, N 4.03, Pr 19.56%.
IR (cm^{-1}): 3076w, 1596m, 1529m, 1505m, 1384s, 1275m, 1239m, 1165m, 1099w, 1062w, 1010w, 865w, 785m, 757m, 737w, 701w.
$Nd(4hob)_3(bpy)$. Blue precipitate (yield: 65%) dec. 165 °C. $C_{31}H_{23}N_2NdO_9$ (711.76) calculated: C 52.31, H 3.26, N 3.94, Nd 20.27%; found C 52.76, H 3.39, N 3.98, Nd 19.90%.

IR (cm^{-1}): 3194w, 1595m, 1531m, 1505m, 1392s, 1247m, 1240m, 1167m, 1099w, 1011w, 856w, 786w, 753s, 686s.
Sm(4hob)$_3$(bpy). White precipitate (yield: 72%) dec. 180 °C. $C_{31}H_{23}N_2SmO_9$ (717.88) calculated: C 51.87, H 3.23, N 3.90, Sm 20.94%; found C 52.34, H 3.38, N 3.95, Sm 20.67%.
IR (cm^{-1}): 3160w, 1595m, 1531m, 1505m, 1392s, 1273m, 1240m, 1166m, 1099w, 1063w, 1011w, 856m, 786m, 758m, 737w, 699w.
Eu(4hob)$_3$(bpy). White precipitate (yield: 80%) dec. 180 °C. $C_{31}H_{23}N_2EuO_9$ (719.49) calculated: C 50.62, H 3.15, N 3.88, Eu 20.66%; found C 51.21, H 3.25, N 3.94, Eu 20.33%.
IR (cm^{-1}): 3161w, 1595m, 1531m, 1505m, 1386s, 1240m, 1166m, 1098w, 1011w, 855w, 785m, 757m, 699m.
Gd(4hob)$_3$(bpy). White precipitate (yield: 90%) dec. 205 °C. $C_{31}H_{23}N_2GdO_9$ (724.77) calculated: C 50.26, H 3.13, N 3.85, Gd 21.23%; found C 50.79, H 3.30, N 3.90, Gd 21.10%.
IR (cm^{-1}): 3182w, 1595m, 1531m, 1393s, 1245m, 1166m, 1098w, 1012w, 856m, 785m, 757m, 700w.
Ho(4hob)$_3$(bpy). Pink precipitate (yield: 55%) dec. 190 °C. $C_{31}H_{23}N_2HoO_9$ (732.45) calculated: C 50.83, H 3.17, N 3.82, Ho 22.52%; found C 51.31, H 3.39, N 3.97, Ho 21.70%.
IR (cm^{-1}): 3535m, 3518m, 3015w, 2969w, 1735s, 1598w, 1538w, 1418w, 1370m, 1216m, 1092w, 744m.
Y(4hob)$_3$(bpy). White precipitate (yield: 38%) dec. 162 °C. $C_{31}H_{23}N_2YO_9$ (656.43) calculated: C 56.72, H 3.53, N 4.27, Y 13.54%; found C 57.15, H 3.74, N 4.43, Y 13.21%.
IR (cm^{-1}): 3075w, 1632w, 1595m, 1531w, 1506w, 1457w, 1393s, 1274m, 1240m, 1167m, 1098w, 1063w, 1013w, 856w, 786m, 758m, 737w, 701w.
Er(4hob)$_3$(bpy). Pink microcrystals (yield: 86%) dec. 150 °C. $C_{31}H_{23}N_2ErO_9$ (734.78) calculated: C 50.67, H 3.16, N 3.81, Er 22.76%; found C 50.99, H 3.31, N 3.94, Er 22.43%.
IR (cm^{-1}): 3533w, 3113w, 1596m, 1531m, 1505m, 1397s, 1276m, 1242m, 1167m, 1098w, 1014w, 856w, 815w, 786m, 757s, 701m.
Yb(4hob)$_3$(bpy). White precipitate (yield: 86%) dec. 173 °C. $C_{31}H_{23}N_2YbO_9$ (740.56) calculated: C 50.28, H 3.13, N 3.78, Yb 23.37%; found C 49.79, H 3.24, N 3.90, Yb 23.87%.
IR (cm^{-1}): 3168w, 1596m, 1531m, 1508m, 1408s, 1275m, 1243m, 1167m, 1099w, 1063w, 1016w, 857w, 787m, 759m, 737w, 701w.
Lu(4hob)$_3$(bpy). White precipitate (yield: 91%) dec. 160 °C. $C_{31}H_{23}N_2LuO_9$ (742.49) calculated: C 50.15, H 3.12, N 3.77, Lu 23.56%; found C 50.59, H 3.90, N 3.87, Lu 23.18%.
IR (cm^{-1}): 3188w, 2888w, 1596m, 1531m, 1402s, 1246m, 1167m, 1099w, 1017w, 856m, 786m, 759m, 700w.

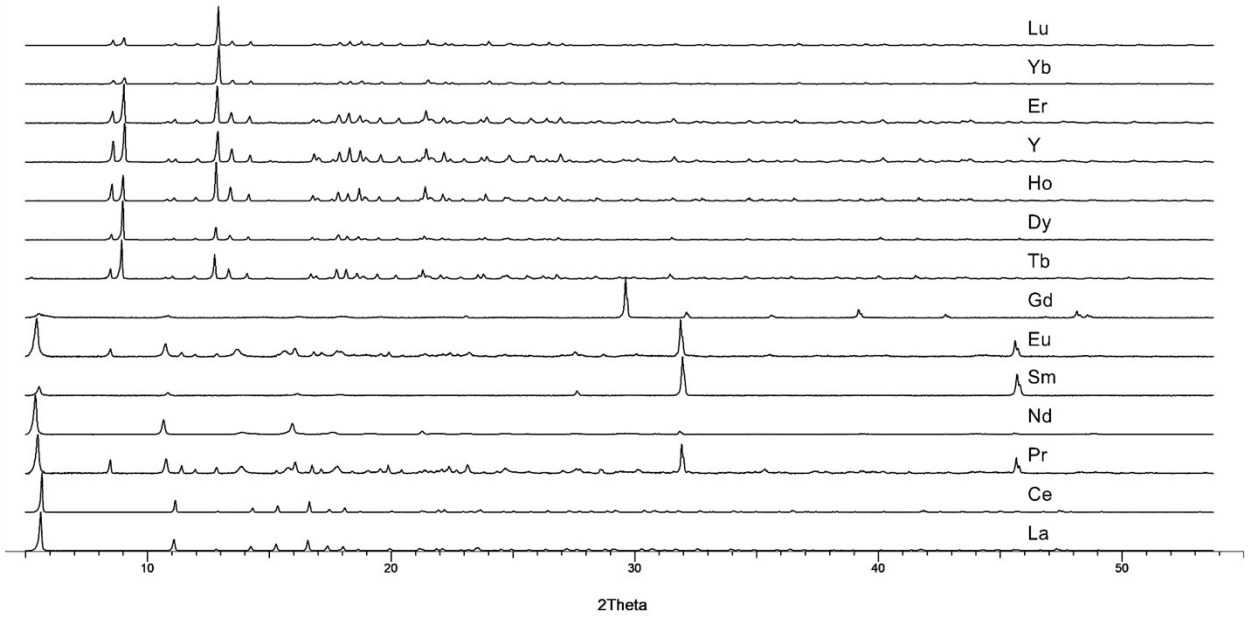

Figure S1. PXRD traces of the bulk products for the aqua reactions (2θ range: 5-55°). All traces are normalized to facilitate comparison.

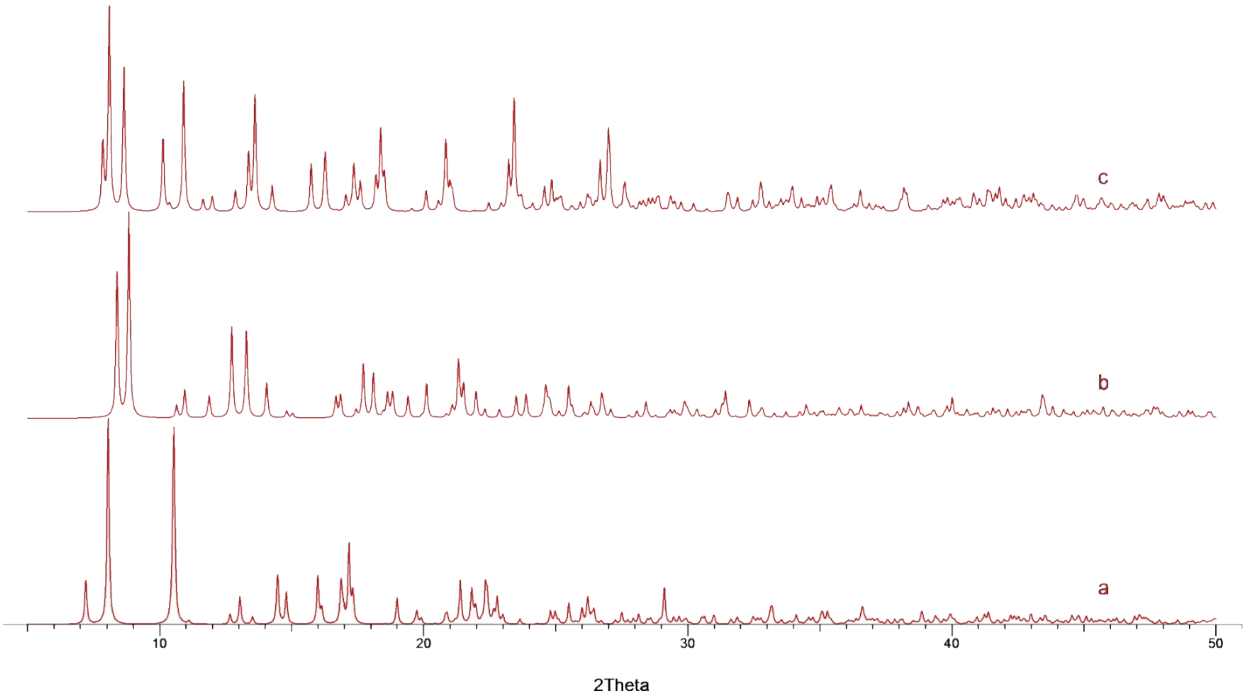

Figure S2. Comparison of the PXRD traces for types **a**, **b** and **c** dimers, generated from the crystal data for RE = Tb (2θ range 5-50°). The data for **c** was drawn from the CCDC (DUPWUH).

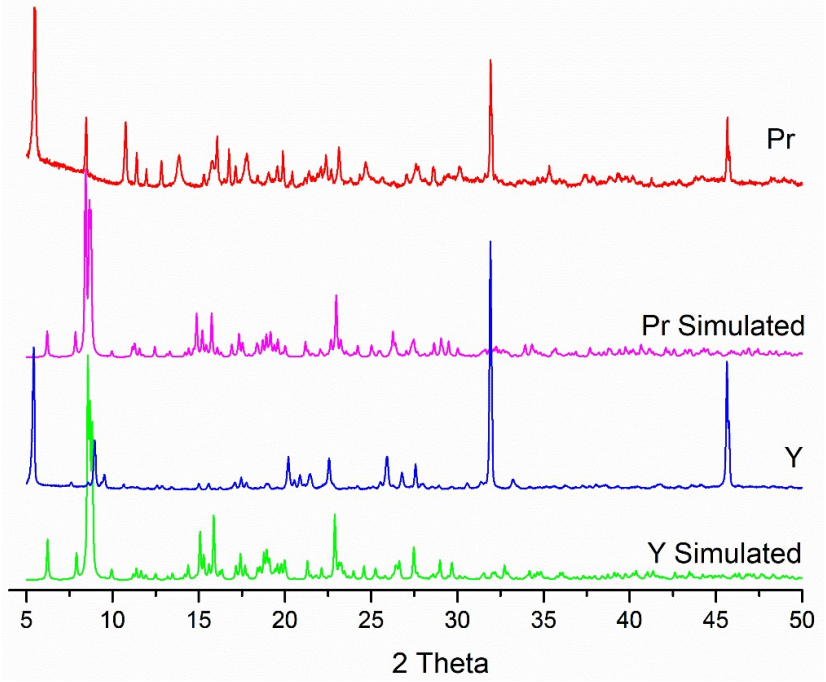

Figure S3 PXRD traces of (4-hydroxybenzoato)Ln(III) complexes (Ln = Pr and Y) at room temperature compared to their simulated patterns (2θ range 5-50°). The data for Y Simulated was drawn from the CCDC (BEWBAG).

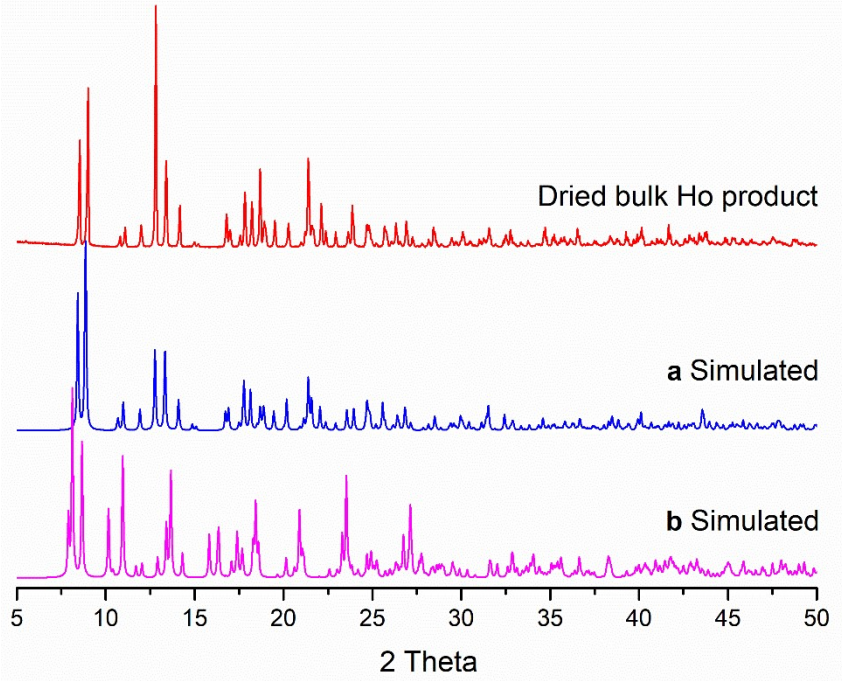

Figure S4 PXRD traces of dried bulk Ho product at room temperature compared to it simulated patterns (2θ range 5-50°): **$[Ho_2(4hob)_6(H_2O)_4]\cdot 2H_2O$** (**a** Simulated) and **$[Ho_2(4hob)_6(H_2O)_4]\cdot 10H_2O$** (**b** Simulated).

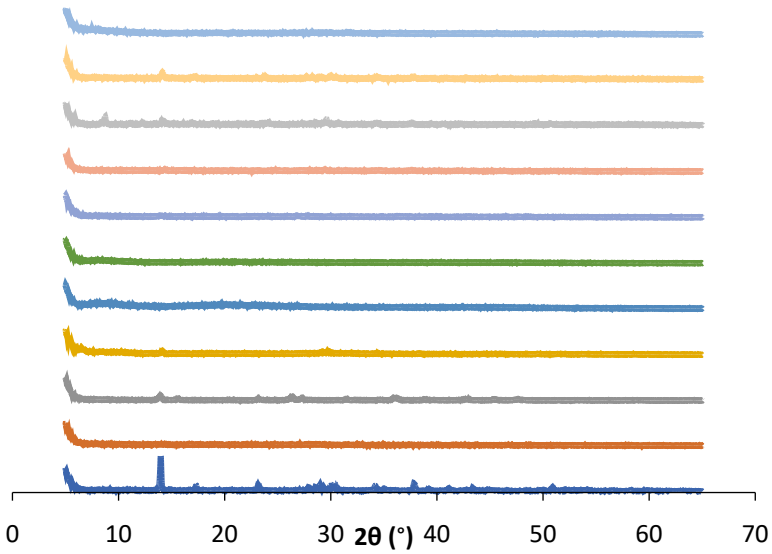

Figure S5. PXRD traces for $[RE(4hob)_3(bpy)]_2$ (RE = Pr, Nd, Sm, Eu, Gd, Tb, Dy, Er, Yb, Lu, Y) bulk products at room temperature (2θ range: 5-55°).

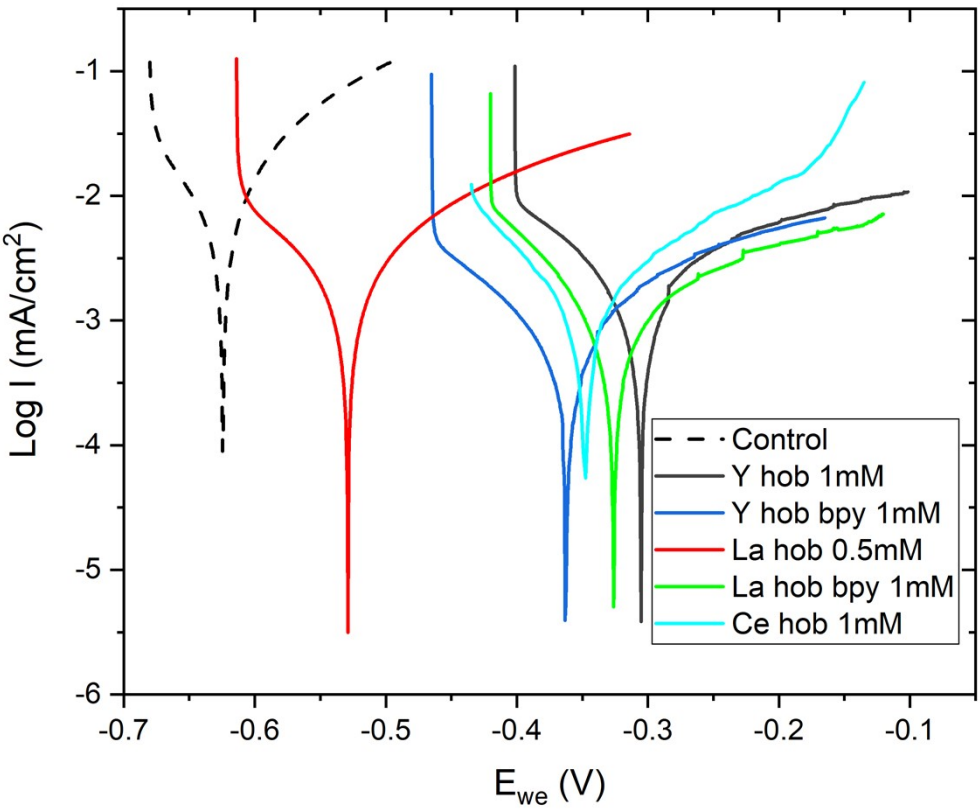

Figure S6. Tafel plots for AS1020 mild steel after 24 h in control and inhibitor solutions.

Table S1. Hydrogen bonding Parameters [d/Å and </°] for the compounds

D-H…A	d(D-H)	d(H…A)	d(D…A)	<(DHA)
a. $[La(4hob)_3(H_2O)_2]_n$				
O2-H2A…O7*	0.8710(15)	1.9584(15)	2.806(2)	164.2(1)
O2-H2B…O7#	0.8711(15)	2.0779(15)	2.873(2)	151.46(11)
b. $[Pr_4(4hob)_{12}(H_2O)_8]\cdot 4H_2O$				
O4-H4B…O16*	0.9905(16)	1.7526(14)	2.738(2)	172.89(13)
O3-H3A…O5#	0.8506(16)	1.8291(16)	2.677(2)	174.61(14)
O2#-H2B#...O15	0.8539(16)	1.9799(16)	2.833(2)	177.52(13)
c. $[Tb_2(4hob)_6(H_2O)_4]\cdot 4H_2O$				
O12-H12A…O3*	0.850(3)	1.8774(17)	2.721(3)	171.0(2)
d. $[Dy_2(4hob)_6(H_2O)_4]\cdot 2H_2O$				
O1-H1B…O8	0.861(2)	1.934(2)	2.741(3)	155.53(18)
e. $[Y_2(4hob)_6(H_2O)_6]\cdot 10H_2O$				
O2-H2B…O6′	0.850(2)	2.1701(18)	2.93(3)	149.30(13)

Table S2. Selected distances and bond lengths (Å) for the type **b** dimers, $[RE_2(4hob)_6(H_2O)_4]\cdot 2H_2O$.

RE:	Eu	Gd	Tb	Dy	Ho	Y	Er	Yb	Lu
RE-RE	5.0393(3)	5.0331(9)	5.0167(3)	5.0067(6)	4.9931(3)	4.9876(3)	4.9718(5)	4.9402(4)	4.9358(3)
RE-O1	2.359(2)	2.3607(17)	2.3397(17)	2.330(3)	2.325(2)	2.3179(12)	2.308(2)	2.283(3)	2.281(3)
RE-O2	2.418(2)	2.4206(17)	2.4007(17)	2.406(3)	2.386(2)	2.3779(12)	2.373(3)	2.346(3)	2.347(3)
RE-O3	2.412(2)	2.4114(16)	2.3986(17)	2.376(2)	2.369(2)	2.3668(12)	2.350(2)	2.332(3)	2.324(2)
RE-O4	2.444(2)	2.4492(18)	2.4281(17)	2.415(2)	2.402(2)	2.4063(12)	2.390(2)	2.365(3)	2.368(2)
RE-O5	2.479(2)	2.4748(17)	2.4648(18)	2.451(2)	2.436(2)	2.4468(12)	2.426(3)	2.413(3)	2.414(2)
RE-O6	2.393(2)	2.3987(17)	2.3730(18)	2.368(2)	2.355(2)	2.3532(12)	2.342(3)	2.317(3)	2.313(2)
RE-O7	2.327(2)	2.3278(17)	2.3073(17)	2.292(2)	2.283(2)	2.2829(12)	2.267(2)	2.239(3)	2.243(2)
RE-O8′	2.349(2)	2.3482(17)	2.3312(18)	2.316(2)	2.3045(19)	2.3006(12)	2.288(2)	2.273(3)	2.263(2)

Table S3. Selected distances and bond lengths (Å) for the type **c** dimers, $[RE_2(4hob)_6(H_2O)_6]\cdot 10H_2O$. Data for RE = Tb is drawn from CCDC code DUPWUH.

RE:	Tb	Ho	Y	Er
RE-O1	2.4482(19)	2.4205(17)	2.4316(17)	2.3132(14)
RE-O2	2.423(2)	2.3991(16)	2.4118(16)	2.3923(14)

RE-O3	2.4042(17)	2.3789(17)	2.3807(18)	2.3697(14)
RE-O4	2.4276(19)	2.4026(17)	2.3974(19)	2.3908(14)
RE-O5	2.4387(17)	2.4167(17)	2.4246(19)	2.4103(15)
RE-O6	2.3161(14)	2.2930(16)	2.3004(15)	2.2848(13)
RE-O7′	2.3276(18)	2.3012(16)	2.2985(19)	2.2973(14)
RE-O8	2.2790(17)	2.2593(16)	2.2569(17)	2.2511(14)

X-ray crystallography

Complexes $[Pr_4(4hob)_{12}(H_2O)_8]\cdot 4H_2O$, $[Tb_2(4hob)_6(H_2O)_4]\cdot 4H_2O$, $[Dy_2(4hob)_6(H_2O)_4]\cdot 2H_2O$, $[Y_2(4hob)_6(H_2O)_6]\cdot 10H_2O$, $[Er_2(4hob)_6(H_2O)_4]\cdot 2H_2O$, $[Yb_2(4hob)_6(H_2O)_4]\cdot 2H_2O$, $[Lu_2(4hob)_6(H_2O)_4]\cdot 2H_2O$, $[Tb_2(4hob)_6(bpy)_2]\cdot 2bpy\cdot 4H_2O$ and $[Dy_2(4hob)_6(bpy)_2]\cdot 2bpy\cdot 4H_2O$ were measured on a Bruker APEX-II CCD diffractometer equipped with graphite-monochromated Mo-Ka radiation (λ = 0.71073 Å) at 123 K. Absorption corrections were completed using Apex II program suite using SADABS.[1] Complexes $[La(4hob)_3(H_2O)_2]_n$ and $[Gd_2(4hob)_6(H_2O)_4]\cdot 2H_2O$ were measured at the Australian Synchrotron on the MX1 beamline, data integration was completed using Blue-ice[2] and XDS[3] software programs. Others were measured on a Rigaku SynergyS diffractometer at 123 K. The SynergyS operated using microsource Mo-Kα radiation (λ = 0.71073 Å) for complex $[Er_2(4hob)_6(H_2O)_6]\cdot 10H_2O$ or Cu-Kα radiation (λ = 1.54184Å) for complexes $\{[Ce(4hob)_3(H_2O)_2]\cdot 3H_2O\}_n$, $[\{Y(4hob)_3\}\cdot H_2O]_n$, $[Eu_2(4hob)_6(H_2O)_4]\cdot 2H_2O$, $[Tb_2(4hob)_6(H_2O)_4]\cdot 2H_2O$, $[Ho_2(4hob)_6(H_2O)_4]\cdot 2H_2O$, $[Ho_2(4hob)_6(H_2O)_6]\cdot 10H_2O$, $[Y_2(4hob)_6(H_2O)_4]\cdot 2H_2O$. Data processing was conducted using CrysAlisPro.55 software suite.[4] Structural solutions were obtained by either direct methods [5] or charge flipping [6] methods and refined using full-matrix least-squares methods against F^2 using SHELX2018,[7] in conjunction with the Olex2 [8] graphical user interface. All hydrogen atoms were placed in calculated positions using the riding model. Crystal data and refinement details are given in **Table S3**.

Table S4. Structural and refinement data for RE-4hob species.

	$[La(4hob)_3(H_2O)_2]_n$	$\{[Ce(4hob)_3(H_2O)_2]\cdot 3H_2O\}_n$	$[Pr_4(4hob)_{12}(H_2O)_8]\cdot 4H_2O$	$[Tb_2(4hob)_6(H_2O)_4]\cdot 4H_2O$	$[Eu_2(4hob)_6(H_2O)_4]\cdot 2H_2O$
Formula	$C_{21}H_{19}LaO_{11}$	$C_{21}H_{25}CeO_{14}$	$C_{84}H_{84}O_{48}Pr_4$	$C_{42}H_{46}O_{26}Tb_2$	$C_{42}H_{42}Eu_2O_{24}$
M_r	586.27	641.53	2425.15	1284.63	1234.67
Space group	$P2_1/c$	P-1	P-1	P-1	$P2_1/c$
a (Å)	16.215(3)	6.36120(10)	12.0467(3)	9.0067(7)	10.4168(3)
b (Å)	12.467(3)	10.0317(2)	14.1840(4)	11.0069(9)	14.9277(5)
c (Å)	10.233(2)	19.6952(9)	14.6821(4)	12.9695(10)	15.5044(5)
α (°)	90	104.267(3)	93.1860(10)	91.8950(10)	90
β (°)	94.01(3)	93.474(3)	102.7450(10)	108.879(2)	105.9590(10)
γ (°)	90	96.567(2)	105.5620(10)	93.5260(10)	90
V (Å^3)	2063.6(7)	1204.91(7)	2339.57(11)	1212.36(17)	2318.00(13)
Z	4	2	1	1	2
ρ_{calc}, g cm^{-3}	1.887	1.768	1.721	1.760	1.769
μ, mm^{-1}	2.134	15.248	2.145	2.982	19.940
N_τ	26356	4963	51444	8275	24759
N (R_{int})	4444(0.0259)	4963	13334(0.0539)	5757(0.0230)	4842(0.0595)
$R_1(I > 2\sigma(I))$	0.0207	0.1128	0.0314	0.0278	0.0355
wR_2 (all data)	0.0540	0.2855	0.0785	0.0723	0.0988
GOF	1.096	1.358	1.027	1.071	1.060

	$[Gd_2(4hob)_6(H_2O)_4]\cdot 2H_2O$	$[Tb_2(4hob)_6(H_2O)_4]\cdot 2H_2O$	$[Dy_2(4hob)_6(H_2O)_4]\cdot 2H_2O$	$[Ho_2(4hob)_6(H_2O)_4]\cdot 2H_2O$	$[Y_2(4hob)_6(H_2O)_4]\cdot 2H_2O$
Formula	$C_{42}H_{42}Gd_2O_{24}$	$C_{42}H_{42}O_{24}Tb_2$	$C_{42}H_{42}Dy_2O_{24}$	$C_{42}H_{42}Ho_2O_{24}$	$C_{42}H_{42}O_{24}Y_2$
M_r	1245.25	1248.59	1255.75	1260.61	1108.57
Space group	$P2_1/c$	$P2_1/c$	$P2_1/c$	$P2_1/c$	$P2_1/c$
a (Å)	10.4100(3)	10.39280(10)	10.4033(3)	10.3692(3)	10.37330(10)
b (Å)	14.9000(5)	14.9032(2)	14.8810(5)	14.8578(5)	14.88310(10)
c (Å)	15.5100(5)	15.4634(2)	15.5628(5)	15.4168(5)	15.43080(10)
α (°)	90	90	90	90	90
β (°)	105.9610(10)	105.8680(10)	105.9720(10)	105.8910(10)	105.8630(10)
γ (°)	90	90	90	90	90
V (Å^3)	2313.00(13)	2303.80(5)	2316.29(13)	2284.40(13)	2291.59(3)
Z	2	2	2	2	2
ρ_{calc}, g cm^{-3}	1.788	1.800	1.800	1.833	1.607
μ, mm^{-1}	2.930	15.670	3.289	7.048	4.163
N_τ	38190	24578	34051	24375	42965
N (R_{int})	4213(0.0358)	4808(0.0437)	5313(0.0701)	4773(0.0397)	4773(0.0338)
$R_1(I > 2\sigma(I))$	0.0199	0.0256	0.0319	0.0277	0.0253
wR_2 (all data)	0.0520	0.0649	0.0820	0.0750	0.0702
GOF	1.138	1.050	1.119	1.120	1.106

	$[Er_2(4hob)_6(H_2O)_4]\cdot 2H_2O$	$[Yb_2(4hob)_6(H_2O)_4]\cdot 2H_2O$	$[Lu_2(4hob)_6(H_2O)_4]\cdot 2H_2O$	$[Ho_2(4hob)_6(H_2O)_6]\cdot 10H_2O$	$[Y_2(4hob)_6(H_2O)_6]\cdot 10H_2O$
Formula	$C_{42}H_{42}Er_2O_{24}$	$C_{42}H_{42}O_{24}Yb_2$	$C_{42}H_{42}Lu_2O_{24}$	$C_{42}H_{62}Ho_2O_{34}$	$C_{42}H_{62}O_{34}Y_2$
M_r	1265.27	1276.83	1280.69	1440.77	1288.73
Space group	$P2_1/c$	$P2_1/c$	$P2_1/c$	P-1	P-1
a (Å)	10.3698(3)	10.3616(3)	10.3683(3)	10.8167(2)	10.7986(9)
b (Å)	14.8378(5)	14.8065(5)	14.8139(5)	11.3009(2)	11.4256(9)
c (Å)	15.5102(5)	15.4569(5)	15.4882(5)	11.45320(10)	11.6045(9)
α (°)	90	90	90	90.5010(10)	90.629(2)
β (°)	106.0290(10)	105.8930(10)	105.9210(10)	101.7230(10)	100.564(2)
γ (°)	90	90	90	105.3020(10)	105.4750(10)
V (Å^3)	2293.70(13)	2280.74(13)	2287.66(13)	1319.33(4)	1353.76(19)
Z	2	2	2	1	1
ρ_{calc}, g cm^{-3}	1.832	1.859	1.859	1.813	1.581
μ, mm^{-1}	3.722	4.164	4.379	6.333	2.233
N_τ	25669	24650	36496	26548	9360
N (R_{int})	5273(0.0675)	4017(0.0737)	5243(0.0661)	5499(0.0434)	6426(0.0153)
$R_1(I > 2\sigma(I))$	0.0325	0.0333	0.0305	0.0318	0.0351
wR_2 (all data)	0.0872	0.0874	0.0844	0.0826	0.0969
GOF	1.070	1.046	1.057	1.083	1.052

	$[Er_2(4hob)_6(H_2O)_6]\cdot 10H_2O$	$[\{Y(4hob)_3\}\cdot H_2O]_n$	$[Tb_2(4hob)_6(bpy)_2]\cdot 2bpy\cdot 4H_2O$	$[Dy_2(4hob)_6(bpy)_2]\cdot 2bpy\cdot 4H_2O$
Formula	$C_{42}H_{62}Er_2O_{34}$	$C_{21}H_{17}O_{10}Y$	$C_{82}H_{70}N_8O_{22}Tb_2$	$C_{82}H_{70}Dy_2N_8O_{22}$
M_r	1445.43	518.26	1837.30	1844.46
Space group	*P*-1	*P*-1	$P2_1/n$	*P*-1
a (Å)	10.8172(2)	5.29940(10)	17.3213(6)	17.3138(5)
b (Å)	11.3109(2)	12.1464(2)	13.1760(4)	13.1899(4)
c (Å)	11.44570(10)	17.0480(3)	19.1799(6)	19.1424(6)
α (°)	90.5310(10)	92.421(2)	90	90
β (°)	101.7250(10)	97.081(2)	113.2410(10)	113.1660(10)
γ (°)	105.3210(10)	101.336(2)	90	90
V (Å^3)	1319.51(4)	1065.25(3)	4022.1(2)	4019.0(2)
Z	1	2	2	2
ρ_{calc}, g cm^{-3}	1.819	1.616	1.517	1.524
μ, mm^{-1}	3.261	4.363	1.823	1.924
N_τ	36333	20531	56091	48794
N (R_{int})	8024(0.0481)	4365(0.0573)	11752(0.0601)	9227(0.0723)
$R_1(I > 2\sigma(I))$	0.0242	0.0386	0.0350	0.0367
wR_2 (all data)	0.0511	0.1076	0.0836	0.1014
GOF	1.037	1.093	1.000	1.047

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