Supplementary Material

Synthesis, structure, and corrosion inhibiting properties of RE^{III} 3-thiophenecarboxylate complexes

Vidushi P. Vithana, [a] Zhifang Guo, [a] Glen B. Deacon, [b] Anthony E. Somers [c] and Peter C. Junk [a]*

[a]College of Science & Engineering, James Cook University, Townsville 4811, Qld, Australia.

[b]School of Chemistry, Monash University, Clayton 3800, Australia.

[c]Institute for Frontier Materials, Deakin University, Burwood 3125, Australia.

*Corresponding author: peter.junk@jcu.edu.au

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Table S1. Crystal data and structural refinement for lanthanoid 3-thiophenecarboxylate complexes						
	1a	**1b**	**1c**	**1d**	**1e**	**1f**
	$[La(3TPC)(H_2O)_3]_n$	**$[Ce(3TPC)(H_2O)_3]_n$**	**$[Pr(3TPC)(H_2O)_3]_n$**	**$[Nd(3TPC)(H_2O)_3]_n$**	**$[Sm(3TPC)(H_2O)_3]_n$**	**$[Gd(3TPC)(H_2O)_3]_n$**
Formula	$C_{15}H_{15}LaO_9S_3$	$C_{15}H_{15}CeO_9S_3$	$C_{15}H_{15}O_9PrS_3$	$C_{15}H_{15}NdO_9S_3$	$C_{15}H_{15}O_9S_3Sm$	$C_{15}H_{15}GdO_9S_3$
M_r	574.36	575.57	576.36	579.69	585.80	592.70
Space group	$P2_1/c$	$P2_1/c$	$P2_1/c$	$P2_1/c$	$P2_1/c$	$P2_1/c$
a (Å)	15.070(3)	15.0999(6)	15.059(3)	15.020(3)	15.042(3)	14.960(3)
b (Å)	12.120(2)	12.1722(4)	12.157(2)	12.070(2)	12.055(2)	12.000(2)
c (Å)	10.840(2)	10.8103(3)	10.775(2)	10.720(2)	10.666(2)	10.600(2)
α (°)	90	90	90	90	90	90
β (°)	100.41(3)	100.769(3)	100.81(3)	100.78(3)	101.00(3)	101.07(3)
γ (°)	90	90	90	90	90	90
V (Å^3)	1947.3(7)	1951.93(12)	1937.5(7)	1909.1(7)	1898.6(7)	1867.5(7)
Z	4	4	4	4	4	4
ρ_{calc}, g cm^{-3}	1.959	1.959	1.976	2.017	2.049	2.108
μ, mm^{-1}	2.562	2.699	22.751	3.095	3.470	3.935
N_τ	41288	11030	3776	3344	3819	39196
N (R_{int})	3420 (0.0646)	4592(0.0457)	3776	3344	3819	3298(0.0491)
$R_1(I > 2\sigma(I))$	0.0345	0.0408	0.0522	0.0342	0.0615	0.0312
wR_2 (all data)	0.0968	0.0851	0.1412	0.1060	0.1791	0.0896
GOF	1.099	1.034	1.050	1.080	1.047	1.037

	2a	**2b**	**2c**	**2d**	**2e**
	$[Dy_2(3TPC)_3(H_2O)_4]\cdot H_2O$	**$[Ho_2(3TPC)_3(H_2O)_4]\cdot H_2O$**	**$[Y_2(3TPC)_3(H_2O)_4]\cdot H_2O$**	**$[Er_2(3TPC)_3(H_2O)_4]\cdot H_2O$**	**$[Lu_2(3TPC)_3(H_2O)_4]\cdot H_2O$**
Formula	$C_{30}H_{28}Dy_2O_{17}S_6$	$C_{30}H_{28}Ho_2O_{17}S_6$	$C_{30}H_{28}O_{17}S_6Y_2$	$C_{30}H_{28}Er_2O_{17}S_6$	$C_{30}H_{28}Lu_2O_{17}S_6$
M_r	1177.88	1182.74	1030.70	1187.40	1202.82
Space group	$P2_1/c$	$P2_1/c$	$P2_1/c$	$P2_1/c$	$P2_1/n$
a (Å)	9.9091(7)	9.9388(6)	9.920(2)	9.9187(7)	9.8729(3)
b (Å)	19.1194(7)	19.2401(11)	19.170(4)	19.1800(7)	19.2032(5)
c (Å)	11.0210(7)	11.0949(8)	11.080(2)	11.0843(7)	11.0534(4)
α (°)	90	90	90	90	90
β (°)	115.932(8)	116.176(8)	116.41(3)	116.458(8)	116.308(4)
γ (°)	90	90	90	90	90
V (Å^3)	1877.8(2)	1904.0(2)	1887.1(8)	1887.8(2)	1878.57(12)
Z	2	2	2	2	2
ρ_{calc}, g cm^{-3}	2.083	2.063	1.814	2.089	2.126
μ, mm^{-1}	4.357	4.528	3.466	4.821	5.633
N_τ	12382	8447	30379	36686	26278
N (R_{int})	3996(0.0339)	4364(0.0345)	3313(0.0407)	4315(0.0846)	5615(0.0460)
$R_1(I > 2\sigma(I))$	0.0256	0.0484	0.0357	0.0235	0.0303
wR_2 (all data)	0.0581	0.0905	0.0978	0.0546	0.0620
GOF	1.051	1.136	1.073	1.036	1.051

Table S2. Selected bond lengths and distances (Å) for the isostructural $[Ln(3TPC)_3(H_2O)_3]_n$ series.

	La1 (**1a**)	Ce1 (**1b**)	Pr1 (**1c**)	Nd1 (**1d**)	Sm1 (**1e**)	Gd1 (**1f**)
RE1#1 =RE1#2	6.3117(9)	6.2961(3)	6.2763(9)	6.2360(9)	6.2060(9)	6.1655(9)
O1	2.610(3)	2.598(3)	2.570(5)	2.529(4)	2.525(5)	2.478(4)
O2	2.583(3)	2.552(3)	2.531(5)	2.553(3)	2.464(5)	2.494(3)
O3	2.568(3)	2.602(3)	2.577(5)	2.555(4)	2.518(4)	2.451(3)
O4	2.620(3)	2.550(3)	2.523(5)	2.502(3)	2.499(5)	2.514(3)
O5	2.501(3)	2.484(3)	2.468(5)	2.464(3)	2.430(4)	2.413(3)
O6#1	2.510(3)	2.504(3)	2.489(5)	2.456(3)	2.441(4)	2.421(3)
O7	2.577(3)	2.518(3)	2.538(5)	2.461(3)	2.434(5)	2.410(3)
O8	2.524(3)	2.499(3)	2.485(5)	2.469(3)	2.452(4)	2.418(3)
O9	2.518(3)	2.557(3)	2.495(5)	2.523(3)	2.493(4)	2.471(3)

Table S3. Hydrogen bonds for $[Pr(3TPC)_3(H_2O)_3]_n$ (**1c**) [d/Å and </°].

D-H…A	d(D-H)	d(H…A)	d(D…A)	<(DHA)
O7#1-H7B#1…O5	0.8699	2.2476	2.9587	138.882
C10-H10…O2	0.9502	2.1510	3.0093	149.599

Table S4. Selected bond lengths and distances (Å) for the isostructural $[Ln_2(3TPC)_6(H_2O)_4]\cdot H_2O$ series.

	Dy1 (**2a**)	Ho1 (**2b**)	Y1 (**2c**)	Er1 (**2d**)	Lu1 (**2e**)
RE1#1 =RE1#2	4.3346(5)	4.4325(6)	4.4708(10)	4.4809(4)	4.5153(2)
O1	2.446(2)	2.435(4)	2.405(19)	2.426(2)	2.367(2)
O2	2.423(2)	2.410(4)	2.435(2)	2.398(2)	2.409(2)
O3	2.459(2)	2.455(4)	2.437(2)	2.433(2)	2.368(2)
O4	2.400(2)	2.401(4)	2.402(19)	2.394(2)	2.396(2)
O5	2.285(3)	2.249(4)	2.235(2)	2.229(2)	2.187(2)
O6#1	2.325(2)	2.294(5)	2.290(2)	2.283(2)	2.240(3)
O7	2.325(2)	2.395(4)	2.392(2)	2.385(2)	2.299(2)
O8	2.361(2)	2.342(4)	2.341(18)	2.330(2)	2.355(2)

Table S5. Hydrogen bonds for $[Er_2(3TPC)_6(H_2O)_4]\cdot H_2O$ (**2d**) [d/Å and </°].

D-H…A	d(D-H)	d(H…A)	d(D…A)	<(DHA)
O7-H7B …O9	0.8628(2)	1.9557(6)	2.7291(6)	148.551(2)
O7-H7A …O4#1	0.8615(2)	1.8623(2)	2.7107(3)	167.887(16)

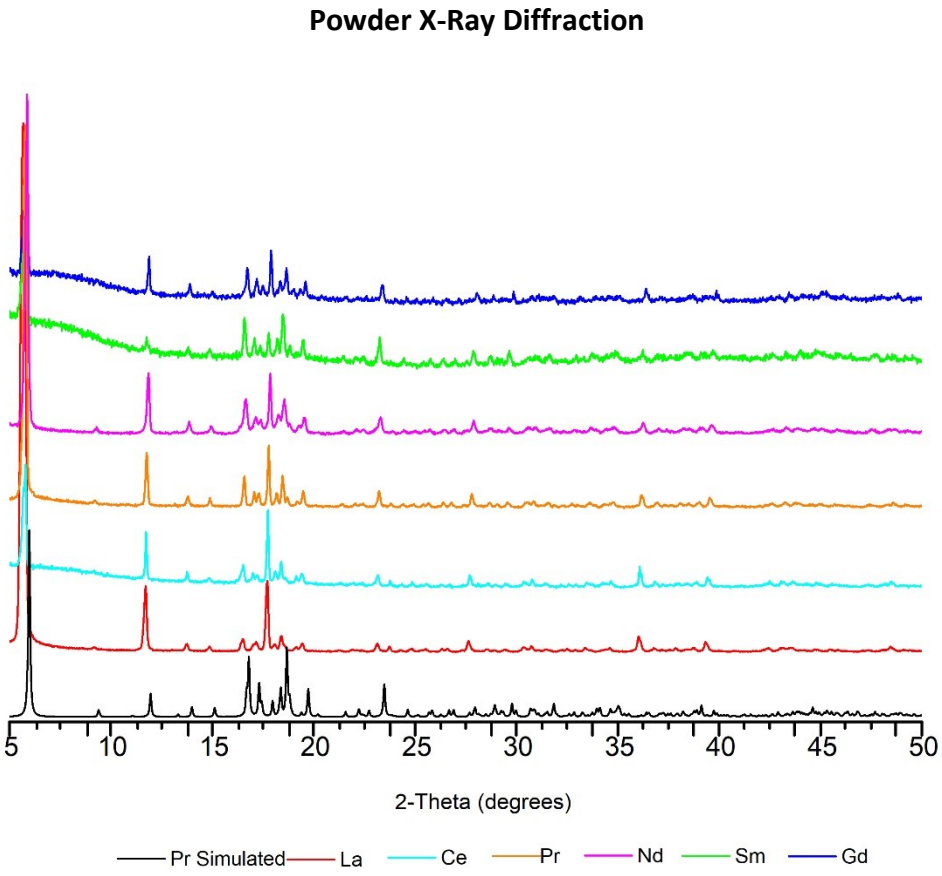


Figure S1. PXRD traces of the $[Ln(3TPC)_3(H_2O)_3]$ **(1a-f)** series at room temperature compared to the simulated pattern of $[Pr(3TPC)_3(H_2O)_3]_n$ (**1c**)

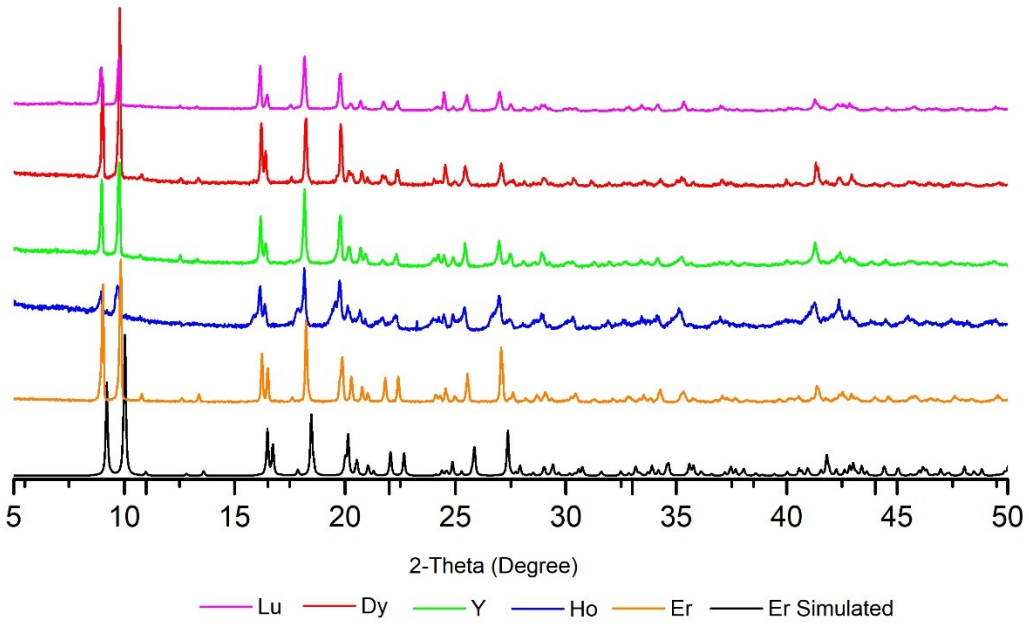


Figure S2. PXRD traces of the $[Ln_2(3TPC)_6(H_2O)_4]\cdot H_2O$ **(2a-e)** series at room temperature compared to the simulated pattern of $[Er_2(3TPC)_6(H_2O)_4]\cdot H_2O$ (**2d**)

Infrared Spectroscopy

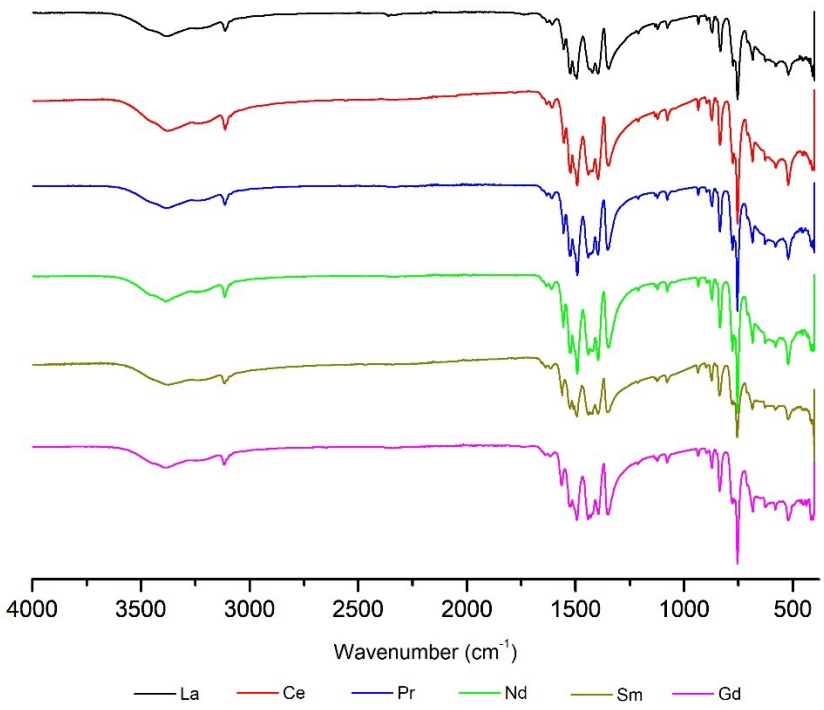


Figure S3. IR spectra of $[Ln(3TPC)_3(H_2O)_3]_n$ **(1a-f)** series

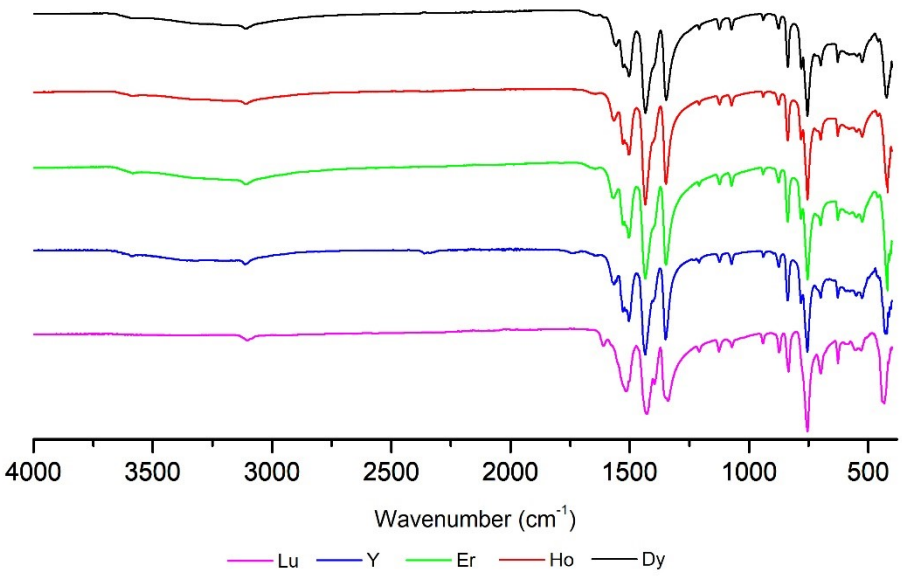


Figure S4. IR spectra of $[Ln_2(3TPC)_6(H_2O)_4]\cdot H_2O$ **(2a-e)** series

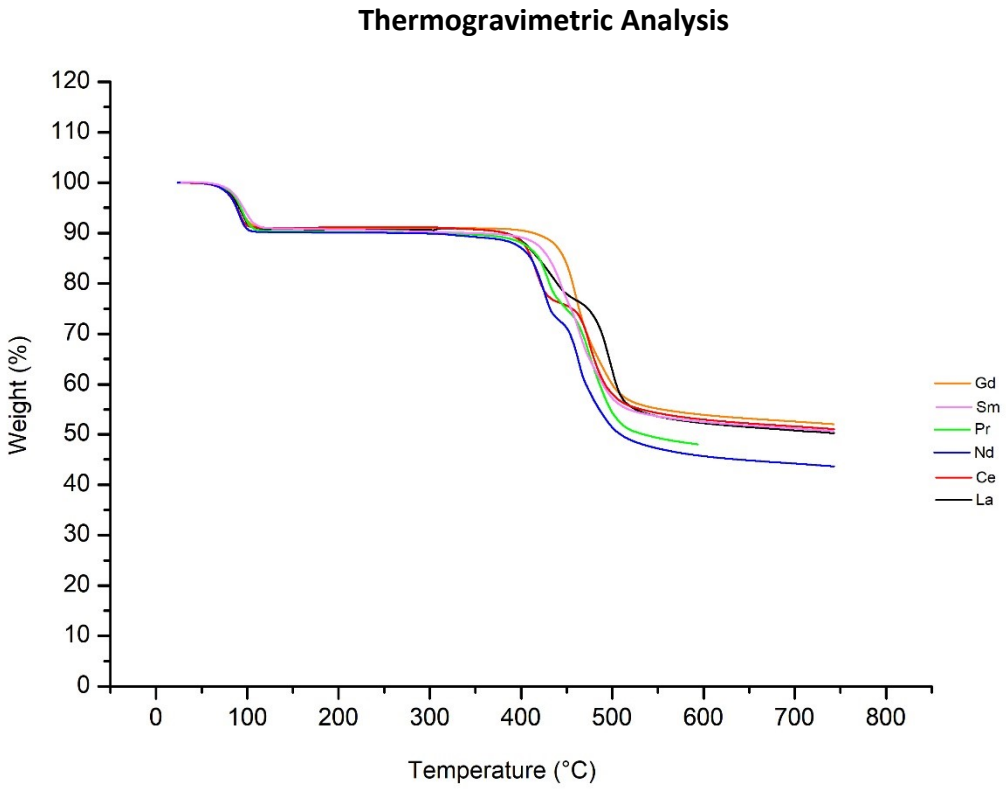


Figure S5. TGA plots of the $[Ln(3TPC)_3(H_2O)_3]_n$ **(1a-f)** series

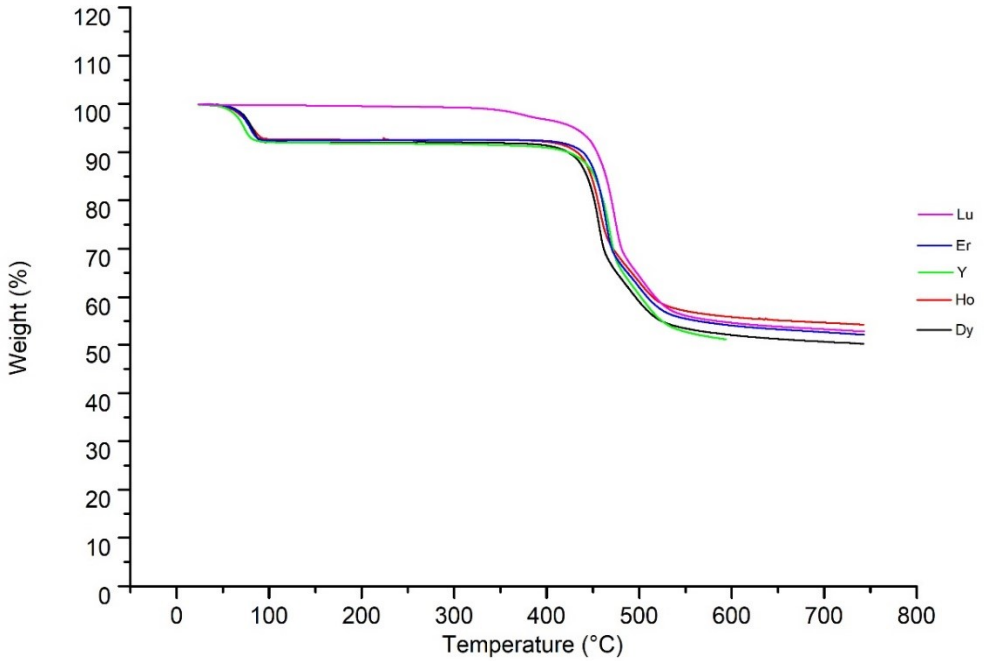


Figure S6. TGA plots of the $[Ln_2(3TPC)_6(H_2O)_4]\cdot H_2O$ **(2a-e)** series

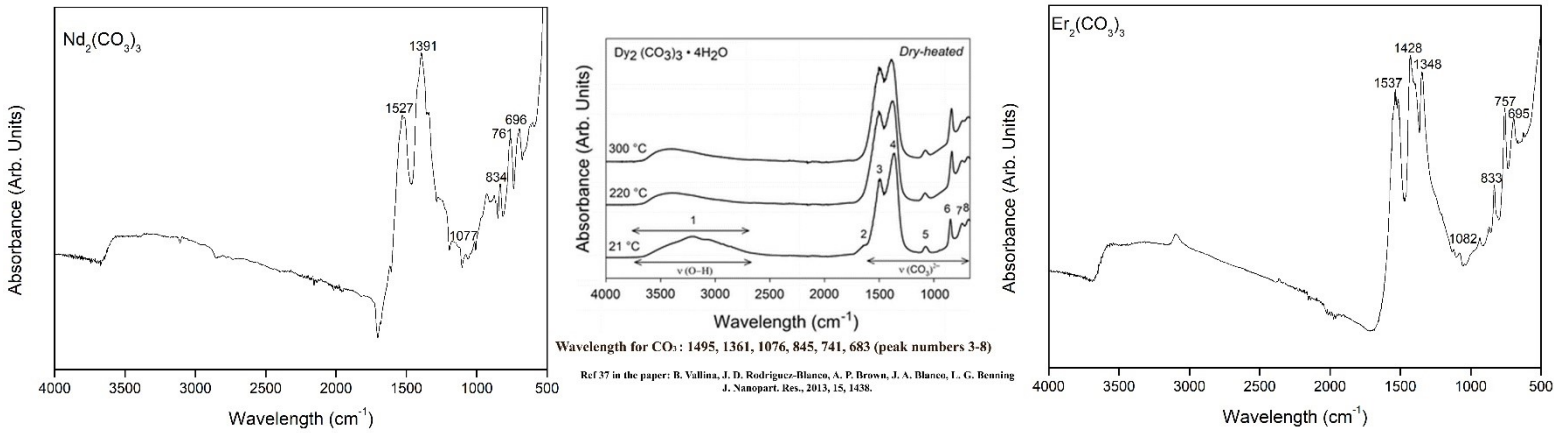
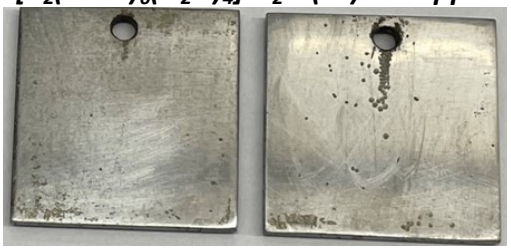


Figure S7: IR spectra of $Nd_2(CO_3)_3$ (Left) from thermal decomposition of **1d**, reported $Dy_2(CO_3)_3\cdot 4H_2O$ (middle) and $Er_2(CO_3)_3$ (right) from thermal decomposition of **2d**

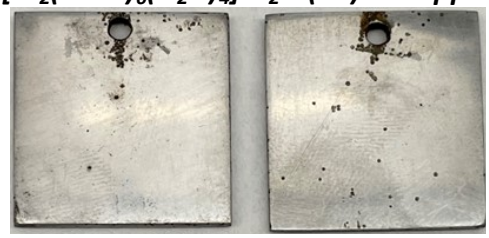
Weight loss experiments

NaCl 0.01 M control

$[Y_2(3TPC)_6(H_2O)_4]\cdot H_2O$ (2c) -500 ppm



$[Er_2(3TPC)_6(H_2O)_4]\cdot H_2O$ (2d) -500 ppm



$[Gd(3TPC)_3(H_2O)_3]_n$ (1f)- 500 ppm

$[La(3TPC)_3(H_2O)_3]_n$ (1a)- 500 ppm

Figure S8: Visual comparisons pictures of few sample coupons after 7 days immersion in inhibitor solutions in NaCl 0.01M. (Left – Trial 1; right – Trial 2.)

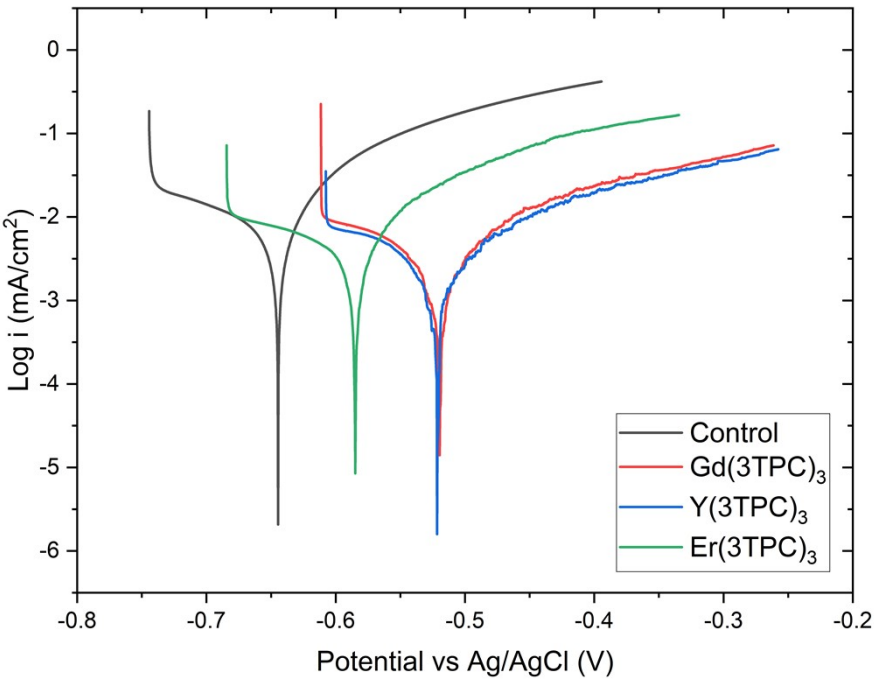


Figure S9: Representative potentiodynamic polarisation scans after 24 hours for 0.01 M NaCl control, and solutions with 0.01 M NaCl and 500ppm of $[Gd(3TPC)_3(H_2O)_3]_n$ **(1f)**, $[Y_2(3TPC)_6(H_2O)_4]\cdot H_2O$ **(2c)** or $[Er_2(3TPC)_6(H_2O)_4]$. H_2O **(2d)**