

Supplementary Material

RE(III) 3-furoate complexes: Synthesis, structure, and corrosion inhibiting properties

Vidushi P. Vithana ¹, Zhifang Guo ¹, Glen B. Deacon ², Anthony E. Somers ³ and Peter C. Junk ^{1,*}

¹ College of Science & Engineering, James Cook University, Townsville, QLD 4811, Australia

² School of Chemistry, Monash University, Clayton, VIC 3800, Australia

³ Institute for Frontier Materials, Deakin University, Burwood, VIC 3125, Australia

* Correspondence: peter.junk@jcu.edu.au

Content:

1. **Table S1:** Crystal data and structural refinement for RE 3-furoate complexes
2. **Table S2:** Selected bond lengths and RE...RE distances (Å) for the isostructural [RE(3fur)₃(H₂O)₂]_n **1RE** series
3. **Table S3:** Selected bond angles (°) for the isostructural [RE(3fur)₃(H₂O)₂]_n **1RE** series.
4. **Table S4:** Hydrogen bonds for [Nd(3fur)₃(H₂O)₂]_n (**1Nd**) [d/Å and </°]
5. **Table S5:** Selected bond lengths and Na...RE distances (Å) for the isostructural [NaRE(3fur)₄]_n **2RE** series
6. **Table S6:** Selected bond angles (°) for the isostructural [NaRE(3fur)₄]_n **2RE** series.
7. **Figure S1:** IR spectra of [RE(3fur)₃(H₂O)₂]_n **1RE** series
8. **Figure S2:** IR spectra of [NaRE(3fur)₄]_n **2RE** series
9. **Figure S3:** TGA plots of the [RE(3fur)₃(H₂O)₂]_n **1RE** series
10. **Figure S4:** TGA plots of the [NaRE(3fur)₄]_n **2RE** series
11. **Figure S5:** IR spectra of Ce₂(CO₃)₂ from thermal decomposition of **1Ce**, reported Dy₂(CO₃)₃·4H₂O (middle) and Na₃Yb(CO₃)₃ (right) from thermal decomposition of **2Yb**
12. **Figure S6:** Mild steel coupons immersed in control and the three best inhibited solutions for 168 h (Left – Trial 1; right – Trial 2.)

Table S1. Crystal data and structural refinement for rare earth 3-furoate complexes

	1La	1Ce	1Pr	1Nd	1Gd	1Dy	1Ho
	[La(3fur)(H₂O)₂]_n	[Ce(3fur)(H₂O)₂]_n	[Pr(3fur)(H₂O)₂]_n	[Nd(3fur)(H₂O)₂]_n	[Gd(3fur)(H₂O)₂]_n	[Dy(3fur)(H₂O)₂]_n	[Ho(3fur)(H₂O)₂]_n
Formula	C ₁₅ H ₁₃ LaO ₁₁	C ₁₅ H ₁₃ CeO ₁₁	C ₁₅ H ₁₃ O ₁₁ Pr	C ₁₅ H ₁₃ NdO ₁₁	C ₁₅ H ₁₃ GdO ₁₁	C ₁₅ H ₁₃ DyO ₁₁	C ₁₅ H ₁₃ HoO ₁₁
<i>M_r</i>	508.16	509.37	510.16	513.49	526.50	531.75	534.18
Space group	C2/c	C2/c	C2/c	C2/c	C2/c	C2/c	C2/c
<i>a</i> (Å)	11.500(2)	11.513(2)	11.533(2)	11.547(2)	11.493(2)	11.461(2)	11.434(2)
<i>b</i> (Å)	27.339(6)	27.247(5)	27.173(5)	27.114(5)	26.991(5)	26.918(5)	26.886(5)
<i>c</i> (Å)	6.0950(12)	6.0820(12)	6.0720(12)	6.0560(12)	6.0220(12)	6.0140(12)	5.9990(12)
<i>α</i> (°)	90	90	90	90	90	90	90
<i>β</i> (°)	117.29(3)	117.75(3)	118.04(3)	118.27(3)	118.65(3)	118.85(3)	118.89(3)
<i>γ</i> (°)	90	90	90	90	90	90	90
<i>V</i> (Å ³)	1703.0(7)	1688.4(7)	1679.5(7)	1669.9(7)	1639.4(7)	1625.2(7)	1614.8(7)
<i>Z</i>	4	4	4	4	4	4	4
<i>ρ</i> _{calc} , g cm ⁻³	1.982	2.044	2.018	2.042	2.133	2.173	2.197
<i>μ</i> , mm ⁻¹	2.569	2.757	2.962	3.171	4.108	4.661	4.964
<i>N_τ</i>	9803	27366	9244	18672	18366	8857	8562
<i>N</i> (<i>R</i> _{int})	1473 (0.0389)	1507(0.0634)	1449(0.0360)	1462(0.0251)	1386(0.0267)	1396(0.0382)	1407(0.0753)
<i>R</i> ₁ (<i>I</i> > 2σ(<i>I</i>))	0.0230	0.0240	0.0179	0.0136	0.0156	0.0207	0.0379
<i>wR</i> ₂ (all data)	0.0612	0.0616	0.0468	0.0323	0.0410	0.0524	0.0991
GOF	1.048	1.087	1.097	1.158	1.095	1.073	1.035

	1Y	2Ho	2Y	2Er	2Yb	2Lu
	[Y(3fur)(H₂O)₂]_n	[NaHo(3fur)₄]_n	[NaY(3fur)₄]_n	[NaEr(3fur)₄]_n	[NaYb(3fur)₄]_n	[NaLu(3fur)₄]_n
Formula	C ₁₅ H ₁₃ O ₁₁ Y	C ₂₀ H ₁₂ HoNaO ₁₂	C ₂₀ H ₁₂ NaO ₁₂ Y	C ₂₀ H ₁₂ ErNaO ₁₂	C ₂₀ H ₁₂ NaO ₁₂ Yb	C ₂₀ H ₁₂ LuNaO ₁₂
<i>M_r</i>	458.16	632.22	556.20	634.55	640.33	642.26
Space group	C2/c	P-4n2	P-4n2	P-4n2	P-4n2	P-4n2
<i>a</i> (Å)	11.446(2)	14.257(2)	14.240(2)	14.2457(2)	14.184(2)	14.177(2)
<i>b</i> (Å)	26.889(5)	14.257(2)	14.240(2)	14.2457(2)	14.184(2)	14.177(2)
<i>c</i> (Å)	6.0030(12)	21.587(4)	21.691(4)	21.5746(5)	21.501(4)	21.541(4)
<i>α</i> (°)	90	90	90	90	90	90
<i>β</i> (°)	118.84(3)	90	90	90	90	90
<i>γ</i> (°)	90	90	90	90	90	90
<i>V</i> (Å ³)	1618.4(7)	4387.8(15)	4398.4(15)	4378.35(16)	4326.0(15)	4329.5(15)
<i>Z</i>	4	8	8	8	8	8
<i>ρ</i> _{calc} , g cm ⁻³	1.880	1.914	1.680	1.925	1.966	1.971
<i>μ</i> , mm ⁻¹	3.667	3.691	2.736	3.918	4.409	4.646
<i>N_τ</i>	18244	50797	53087	28175	49021	50096
<i>N</i> (<i>R</i> _{int})	1417(0.0501)	4167(0.0478)	4496(0.0565)	6598(0.0738)	3815(0.0390)	4128(0.0521)
<i>R</i> ₁ (<i>I</i> > 2σ(<i>I</i>))	0.0201	0.0201	0.0296	0.0377	0.0129	0.0202
<i>wR</i> ₂ (all data)	0.0544	0.0549	0.0817	0.0934	0.0358	0.0522
GOF	1.077	1.068	1.043	1.047	1.095	1.090

Table S2. Selected bond lengths and RE...RE distances (Å) for the isostructural [RE(3fur)₃(H₂O)₂]_n **1RE** series.

	La1 (1La)	Ce1 (1Ce)	Pr1 (1Pr)	Nd1 (1Nd)	Gd1 (1Gd)	Dy1 (1Dy)	Ho1 (1Ho)	Y1 (1Y)
RE1 = RE1#1	5.1559(18)	5.1374(18)	5.1306(18)	5.1246(18)	5.0823(18)	5.0582(18)	5.0451(18)	5.0528(18)
O1#4	2.410(2)	2.385(2)	2.3624(18)	2.3487(15)	2.2968(19)	2.267(2)	2.252(4)	2.2535(14)
O1	2.410(2)	2.385(2)	2.3624(18)	2.3487(15)	2.2968(19)	2.267(2)	2.252(4)	2.2535(14)
O2#1	2.459(2)	2.4306(19)	2.4139(16)	2.3991(13)	2.3443(17)	2.308(2)	2.294(4)	2.2969(12)
O2#3	2.459(2)	2.4306(19)	2.4139(16)	2.3991(13)	2.3443(17)	2.308(2)	2.294(4)	2.2969(12)
O5#4	2.538(2)	2.513(2)	2.5010(17)	2.4848(14)	2.4464(18)	2.436(2)	2.422(4)	2.4196(14)
O5	2.538(2)	2.513(2)	2.5009(17)	2.4848(14)	2.4464(18)	2.436(2)	2.422(4)	2.4197(14)
O4#4	2.640(2)	2.621 (19)	2.6026(17)	2.5830(14)	2.5276(18)	2.506(2)	2.494(4)	2.4908(13)
O4	2.640(2))	2.621 (19)	2.6026(17)	2.5830(14)	2.5276(18)	2.506(2)	2.494(4)	2.4908(13)

Table S3. Selected bond angles (°) for the isostructural [RE(3fur)₃(H₂O)₂]_n **1RE** series.

	(1La)	(1Ce)	(1Pr)	(1Nd)	(1Gd)	(1Dy)	(1Ho)	(1Y)
O4-Nd-O4#4	126.59(10)	126.72(9)	126.91(7)	127.16(6)	127.28(9)	127.46(10)	127.36(18)	127.62(6)
Nd1#1-Nd1-Nd1#3	167.764(13)	167.565(13)	167.485(13)	167.339(5)	166.961(13)	166.873(13)	166.706(13)	166.725(13)

Table S4. Hydrogen bonds for [Nd(3fur)₃(H₂O)₂]_n (**1Nd**) [d/Å and </°].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O4#1-H4A#1...O5#4	0.8534(14)	2.1716(15)	2.954(2)	152.32(10)
O4#3-H4A#3...O5	0.8534(14)	2.1716(15)	2.954(2)	152.32(10)

Table S5. Selected bond lengths and Na...RE distances (Å) for the isostructural [NaRE(3fur)₄]_n **2RE** series.

	Ho1 (2Ho)	Y1 (2Y)	Er1 (2Er)	Yb1 (2Yb)	Lu1 (2Lu)
Na1	3.403(2)	3.4031(15)	3.401(3)	3.3841(16)	3.381(2)
O1	2.392(4)	2.384(3)	2.372(5)	2.360(3)	2.351(4)
O1#1	2.392(4)	2.384(3)	2.372(5)	2.360(3)	2.351(4)
O2	2.453(4)	2.457(3)	2.449(6)	2.432(3)	2.428(4)
O2#1	2.453(4)	2.457(3)	2.449(6)	2.432(3)	2.428(4)
O4	2.238(4)	2.239(3)	2.221(5)	2.208(3)	2.196(4)
O4#1	2.238(4)	2.238(3)	2.222(5)	2.208(3)	2.196(4)
O5#2	2.357(3)	2.356(2)	2.340(5)	2.321(3)	2.313(4)
O5#3	2.357(3)	2.356(2)	2.340(5)	2.321(3)	2.313(4)

	Ho2 (2Ho)	Y2 (2Y)	Er2 (2Er)	Yb2 (2Yb)	Lu2 (2Lu)
Na1	3.398(2)	3.4005(15)	3.392(3)	3.3705(16)	3.374(2)
O7	2.356(3)	2.355(2)	2.340(5)	2.317(3)	2.312(4)
O7#4	2.355(3)	2.355(2)	2.340(5)	2.317(3)	2.311(4)
O8	2.510(4)	2.507(3)	2.509(6)	2.495(3)	2.492(4)
O8#4	2.510(4)	2.507(3)	2.509(6)	2.495(3)	2.492(4)
O10	2.212(4)	2.213(3)	2.207(5)	2.180(3)	2.170(4)
O10#4	2.212(4)	2.213(3)	2.207(5)	2.180(3)	2.170(4)
O11#5	2.391(4)	2.390(3)	2.367(5)	2.349(3)	2.341(4)
O11#6	2.391(4)	2.390(3)	2.367(5)	2.349(3)	2.341(4)

	Na1 (2Ho)	Na1 (2Y)	Na1 (2Er)	Na1 (2Yb)	Na1 (2Lu)
O1	2.323(4)	2.320(3)	2.327(6)	2.317(3)	2.310(5)
O2#1	2.347(4)	2.348(3)	2.347(6)	2.338(4)	2.334(5)
O5#2	2.418(4)	2.420(3)	2.429(6)	2.428(4)	2.430(5)
O7	2.344(5)	2.340(3)	2.344(7)	2.332(4)	2.333(5)

O8#4	2.388(4)	2.387(3)	2.389(6)	2.369(4)	2.374(5)
O11#6	2.367(4)	2.373(3)	2.368(6)	2.367(4)	2.368(5)

Table S6. Selected bond angles (°) for the isostructural $[\text{NaRE}(\text{3fur})_4]_n$ **2RE** series.

	(2Ho)	(2Y)	(2Er)	(2Yb)	(2Lu)
C1-Yb1-C1#1	85.3(2)	85.18(15)	85.2(3)	85.81(9)	85.7(2)
C11-Yb2-C11#4	82.3(2)	82.48(15)	82.7(3)	82.54(18)	83.1(2)
Yb1-Na1-Yb2	174.29(7)	174.32(5)	174.549(10)	175.26(7)	175.50(8)

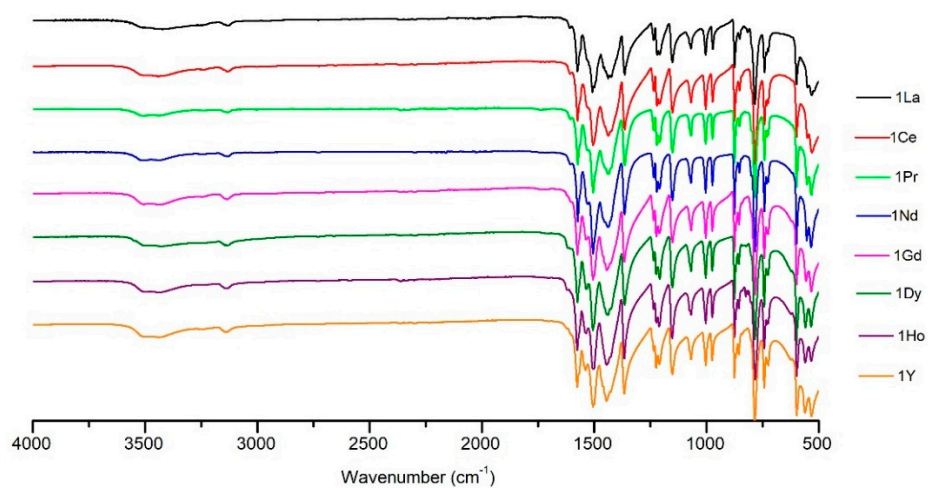


Figure S1. IR spectra of $[\text{RE}(\text{3fur})_3(\text{H}_2\text{O})_2]_n$ **1RE** series

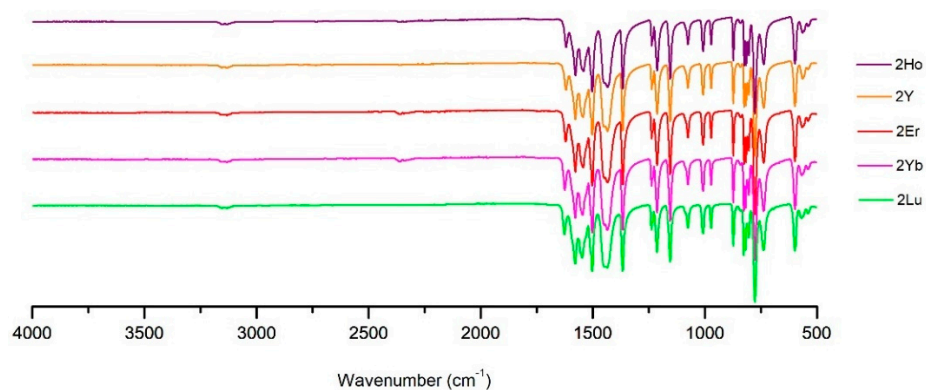


Figure S2. IR spectra of $[\text{NaRE}(\text{3fur})_4]_n$ **2RE** series

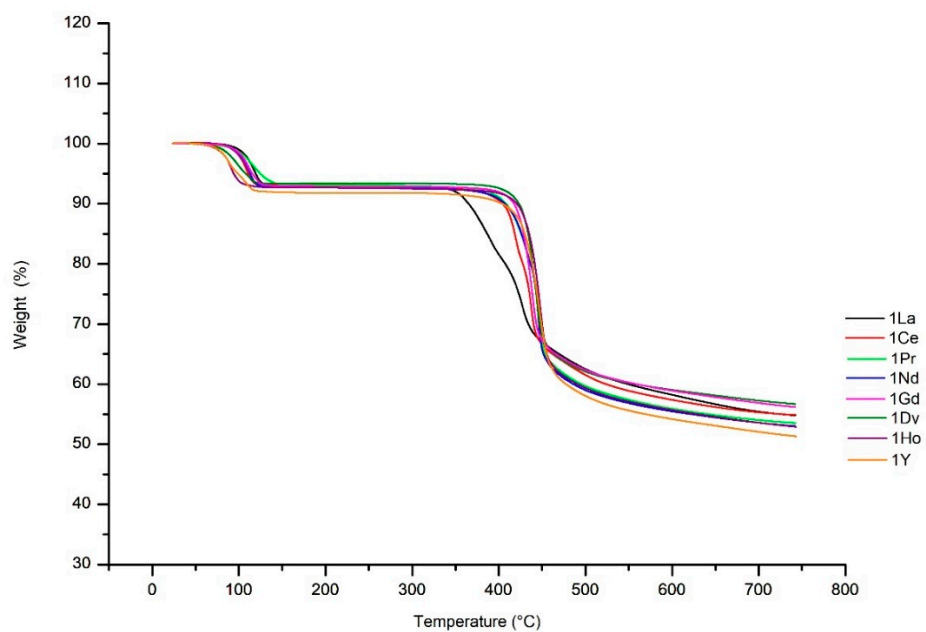


Figure S3. TGA plots of the $[\text{RE}(\text{3fur})_3(\text{H}_2\text{O})_2]_n$ 1RE series

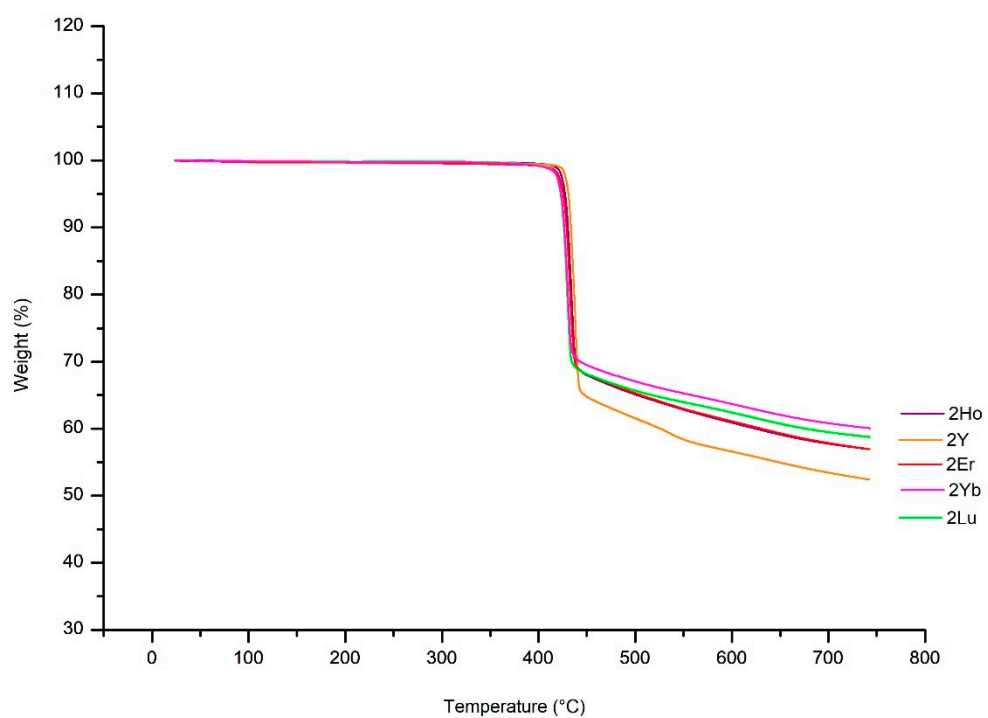


Figure S4. TGA plots of the $[\text{NaRE}(\text{3fur})_4]_n$ 2RE series

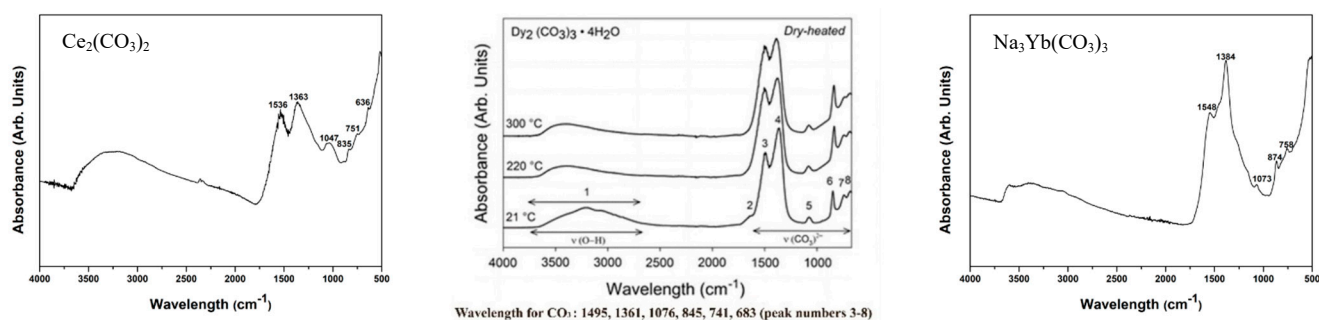


Figure S5. IR spectra of $\text{Ce}_2(\text{CO}_3)_2$ (Left) from thermal decomposition of **1Ce**, reported $\text{Dy}_2(\text{CO}_3)_3 \cdot 4\text{H}_2\text{O}$ (middle) [32] and $\text{Na}_3\text{Yb}(\text{CO}_3)_3$ (right) from thermal decomposition of **2Yb**

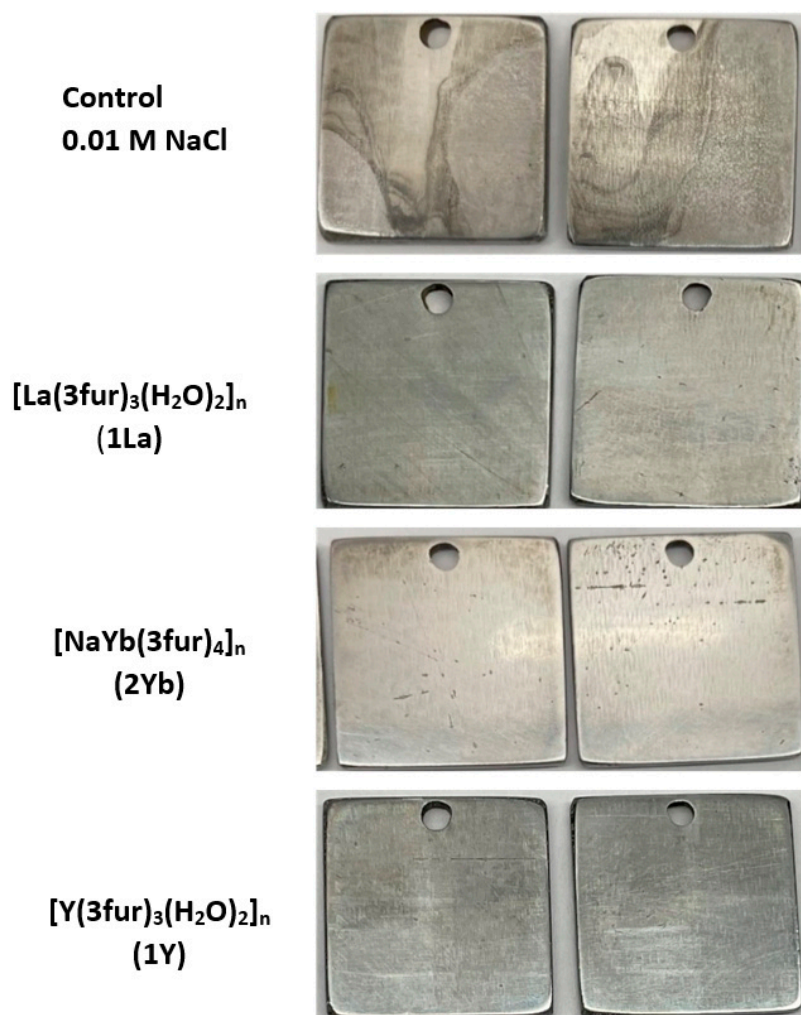


Figure S6. Mild steel coupons immersed in control and the three best inhibited solutions for 168 h (Left – Trial 1; right – Trial 2.)