Supramolecular Assembly of Lanthanide-2,3,5,6-Tetrafluoroterephthalic Acid Coordination Polymers via Fluorine•••Fluorine Interactions: A Platform for Luminescent Detection of Fe^{3+} and Nitroaromatic Compounds

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Table S1. Crystallographic data for compounds **1 – 14.**

	1 – La	**2 – Ce**	**3 – Pr**	**4 – Nd**	**5 – Sm**
Chemical Formula	$LaC_{12}H_6F_6O_9$	$CeC_{12}H_6F_6O_9$	$PrC_{12}H_6F_6O_9$	$NdC_{12}H_6F_6O_9$	$SmC_{12}H_6F_6O_9$
Formula Weight	547.08	548.29	549.08	552.41	558.52
Crystal System	Monoclinic	Monoclinic	Monoclinic	Monoclinic	Monoclinic
Space Group	I 2/m	I 2/m	I 2/m	I 2/m	I 2/m
a (Å)	11.8148(5)	11.7966(13)	11.7587(7)	11.7314(4)	11.6844(9)
b (Å)	11.3729(5)	11.3785(11)	11.3554(7)	11.3436(4)	11.2772(5)
c (Å)	11.8979(8)	11.9288(13)	11.9289(11)	11.9360(6)	11.8934(6)
α (°)	90	90	90	90	90
β (°)	106.398(2)	106.795(2)	106.930(11)	107.150(7)	107.051(8)
γ (°)	90	90	90	90	90
V ($Å^3$)	1533.67(14)	1532.9(3)	1523.8(2)	1517.77(12)	1498.28(16)
Z	4	4	4	4	4
T (K)	293(2)	293(2)	293(2)	293(2)	293(2)
λ (Mo Kα)	0.71073	0.71073	0.71073	0.71073	0.71073
D_{calc} (mg m^{-3})	2.369	2.376	2.393	2.417	2.476
μ (mm^{-1})	2.906	3.090	3.319	3.543	4.043
GOF on F^2	1.245	1.099	1.080	1.177	1.059
R_{int}	0.0331	0.0267	0.0301	0.0178	0.0228
R_1, wR_2 [$I > 2\sigma(I)$]	0.0203, 0.0559	0.0183, 0.0429	0.0190, 0.0433	0.0152, 0.0395	0.0214, 0.0537
R_1, wR_2 (all data)	0.0215, 0.0566	0.0188, 0.0431	0.0208, 0.0441	0.0156, 0.0397	0.0236, 0.0547
CCDC Number	1935535	1935536	1935537	1935538	1935539
	6 – Eu	**7 – Gd**	**8 – Tb**	**9 – Dy**	**10 – Ho**
Chemical Formula	$EuC_{12}H_6F_6O_9$	$GdC_{12}H_6F_6O_9$	$TbC_{12}H_6F_6O_9$	$DyC_{12}H_6F_6O_9$	$HoC_{12}H_6F_6O_9$
Formula Weight	560.13	565.42	567.09	570.67	573.10
Crystal System	Monoclinic	Monoclinic	Monoclinic	Monoclinic	Monoclinic
Space Group	I 2/m	I 2/m	I 2/m	I 2/m	I 2/m
a (Å)	11.650(4)	11.6277(8)	11.6039(12)	11.5862(12)	11.5655(7)

b (Å)	11.283(3)	11.2649(5)	11.2358(12)	11.2209(7)	11.1980(4)
c (Å)	11.966(4)	11.9648(5)	11.9986(19)	12.0224(8)	12.0457(5)
α (°)	90	90	90	90	90
β (°)	107.656(6)	107.745(6)	108.027(10)	108.174(10)	108.321(6)
γ (°)	90	90	90	90	90
V ($Å^3$)	1498.8(8)	1492.64(15)	1487.6(3)	1485.0(2)	1480.97(13)
Z	4	4	4	4	4
T (K)	293(2)	293(2)	293(2)	293(2)	293(2)
λ (Mo Kα)	0.71073	0.71073	0.71073	0.71073	0.71073
D_{calc} (mg m^{-3})	2.482	2.516	2.532	2.552	2.570
μ (mm^{-1})	4.308	4.567	4.879	5.156	5.468
GOF on F^2	1.122	1.060	1.052	1.063	1.099
R_{int}	0.0264	0.0242	0.0516	0.0180	0.0147
R_1, wR_2 [I > 2σ(I)]	0.0161, 0.0385	0.0157, 0.0379	0.0274, 0.0517	0.0136, 0.0337	0.0117, 0.0300
R_1, wR_2 (all data)	0.0172, 0.0389	0.0166, 0.0384	0.0321, 0.0534	0.0147, 0.0342	0.0121, 0.0301
CCDC Number	1935540	1935541	1935542	1935543	1935544
	11 – Er	**12 – Tm**		**13 – Yb**	**14 – Lu**
Chemical Formula	$ErC_{12}H_6F_6O_9$	$TmC_{12}H_4F_6O_9$		$YbC_{12}H_6F_6O_9$	$LuC_{12}H_6F_6O_9$
Formula Weight	575.43	575.08		581.21	583.14
Crystal System	Monoclinic	Monoclinic		Triclinic	Triclinic
Space Group	I 2/m	I 2/m		P -1	P -1
a (Å)	11.5557(7)	11.5247(3)		8.7710(7)	8.8727(16)
b (Å)	11.1689(7)	11.1200(2)		8.9368(7)	8.8936(16)
c (Å)	12.0722(11)	12.1254(3)		11.5310(9)	11.561(2)
α (°)	90	90		67.313(2)	67.613(2)
β (°)	108.475(12)	108.8680(10)		68.094(3)	67.712(3)
γ (°)	90	90		75.535(2)	75.395(2)
V ($Å^3$)	1477.8(2)	1470.43(6)		767.76(11)	774.3(2)
Z	4	4		2	2
T (K)	293(2)	293(2)		293(2)	293(2)

λ (Mo Kα)	0.71073	0.71073		0.71073	0.71073
D_{calc} (mg m^{-3})	2.586	2.598		2.497	2.501
μ (mm^{-1})	5.804	6.159		6.210	6.495
GOF on F^2	1.135	1.069		1.065	1.103
R_{int}	0.0227	0.0513		0.0369	0.0247
R_1, wR_2 [$I > 2\sigma(I)$]	0.0194, 0.0476	0.0233, 0.0471		0.0267, 0.0697	0.0267, 0.0566
R_1, wR_2 (all data)	0.0200, 0.0479	0.0259, 0.0484		0.0275, 0.0703	0.0325, 0.0582
CCDC Number	1935545	1935546		1935547	1935548

Table S2. Yields, elemental C, H analysis and main IR peaks for compounds in series **1**.

Compound	Yield based on H_2TFTA (%)	Elemental C, H Analysis (%)	Main FTIR Peaks (ATR, cm^{-1})
{[La(TFTA)$_{1.5}$(H_2O)$_2$]•H_2O}$_n$ (1)	45	Calc.: C, 26.35; H, 1.11. Found: C, 26.25; H, 0.71	3649(w), 3629(w), 3450(br,w), 1617(s), 1556(s), 1508(w), 1488(m), 1458(m), 1397(s), 1378(s), 1265(w), 1055(w), 1032(w), 992(s), 909(w), 835(w), 811(w), 753(s), 730(s), 672(w)
{[Ce(TFTA)$_{1.5}$(H_2O)$_2$]•H_2O}$_n$ (2)	38	Calc.: C, 26.29 H, 1.10. Found: C, H,	3648(w), 3629(w), 3442(br,w), 1612(s), 1554(s), 1488(m), 1458(m), 1397(s), 1378(s), 1265(w), 1028(w), 993(s), 909(w), 835(w), 811(w), 752(s), 729(s), 670(w)
{[Pr(TFTA)$_{1.5}$(H_2O)$_2$]•H_2O}$_n$ (3)	24	Calc.: C, 26.25; H, 1.10. Found: C, 26.01; H, 0.73	3755(w), 3653(w), 3451(br,w), 1613(s), 1555(s), 1487(m), 1455(m), 1396(s), 1378(s), 1265(w), 1029(w), 993(s), 909(w), 834(w), 811(w), 752(s), 730(s), 669(w)
{[Nd(TFTA)$_{1.5}$(H_2O)$_2$]•H_2O}$_n$ (4)	51	Calc.: C, 26.09; H, 1.09. Found: C, 26.09; H, 0.74	3745(w), 3647(w), 3403(br,w), 1614(s), 1555(s), 1488(m), 1456(m), 1396(s), 1379(s), 1265(w), 1030(w), 993(s), 910(w), 834(w), 811(w), 752(s), 730(s), 665(w)
{[Sm(TFTA)$_{1.5}$(H_2O)$_2$]•H_2O}$_n$ (5)		Calc.: C, 25.81; H, 1.08. Found: C, H,	3749(w), 3668(w), 3450(br,w), 1620(s), 1556(s), 1489(m), 1460(m), 1400(s), 1381(s), 1266(w), 995(s), 911(w), 835(w), 811(w), 754(s), 732(s), 672(w)
{[Eu(TFTA)$_{1.5}$(H_2O)$_2$]•H_2O}$_n$ (6)	40	Calc.: C, 25.73; H, 1.08. Found: C, 25.89 H,	3668(w), 3472(br,w), 1611(s), 1556(s), 1488(m), 1457(m), 1397(s), 1265(w), 1028(w), 994(s), 911(w), 834(w), 811(w), 753(s), 731(s), 665(w)

		0.66	
{[Gd(TFTA)$_{1.5}$(H$_2$O)$_2$]•H$_2$O}$_n$ (7)	17	Calc.: C, 25.49; H, 1.07. Found: C, H,	3670(w), 3467(br,w), 1620(s), 1559(s), 1490(m), 1459(m), 1401(s), 1382(s), 1267(w), 1032(w), 995(s), 913(w), 835(w), 812(w), 755(s), 732(s), 663(w)
{[Tb(TFTA)$_{1.5}$(H$_2$O)$_2$]•H$_2$O}$_n$ (8)	22	Calc.: C, 25.42 H, 1.07. Found: C, 25.60 H, 0.76	3668(w), 3450(br,w), 1614(s), 1556(s), 1489(m), 1458(m), 1400(s), 1382(s), 1266(w), 1032(w), 995(s), 913(w), 834(w), 811(w), 755(s), 730(s), 672(w)
{[Dy(TFTA)$_{1.5}$(H$_2$O)$_2$]•H$_2$O}$_n$ (9)	37	Calc.: C, 25.26; H, 1.06. Found: C, H,	3671(w), 3470(br,w), 1614(s), 1593(s), 1556(s), 1490(m), 1457(m), 1401(s), 1383(s), 1267(w), 1092(w), 1032(w), 996(s), 913(w), 834(w), 811(w), 756(s), 731(s), 663(w)
{[Ho(TFTA)$_{1.5}$(H$_2$O)$_2$]•H$_2$O}$_n$ (10)	80	Calc.: C, 25.15 H, 1.06. Found: C, H,	3670(w), 3416(br,w), 1615(s), 1593(s), 1556(s), 1489(m), 1457(m), 1401(s), 1382(s), 1266(w), 1092(w), 1032(w), 995(s), 913(w), 834(w), 811(w), 755(s), 731(s), 663(w)
{[Er(TFTA)$_{1.5}$(H$_2$O)$_2$]•H$_2$O}$_n$ (11)	39	Calc.: C, 25.05; H, 1.05. Found: C, 24.62 H, 0.58	3671(w), 3472(br,w), 1619(s), 1594(s), 1559(s), 1489(m), 1459(m), 1402(s), 1382(s), 1267(w), 1136(w), 1034(w), 996(s), 914(w), 834(w), 812(w), 755(s), 732(s), 698(w)
{[Tm(TFTA)$_{1.5}$(H$_2$O)$_2$]•H$_2$O}$_n$ (12)	19	Calc.: C, 24.97; H, 1.05. Found: C, H	3670(w), 3450(br,w), 1615(s), 1593(s), 1557(s), 1490(m), 1458(m), 1404(s), 1267(w), 1137(w), 1034(w), 996(s), 915(w), 834(w), 812(w), 756(s), 731(s), 698(w)

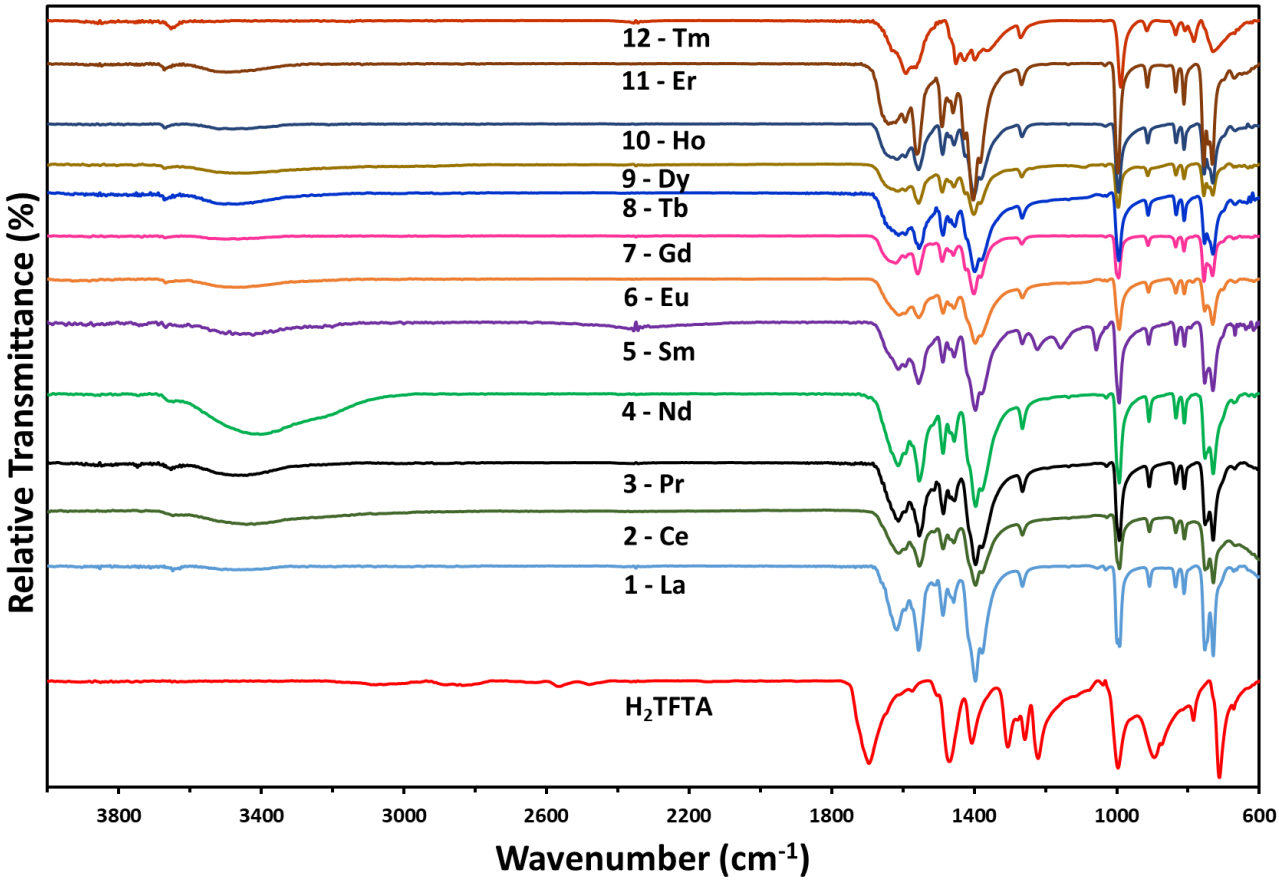

Figure S1. FTIR spectra of 2,3,5,6-tetrafluoroterephthalic acid (H_2TFTA) and compounds in series **1**.

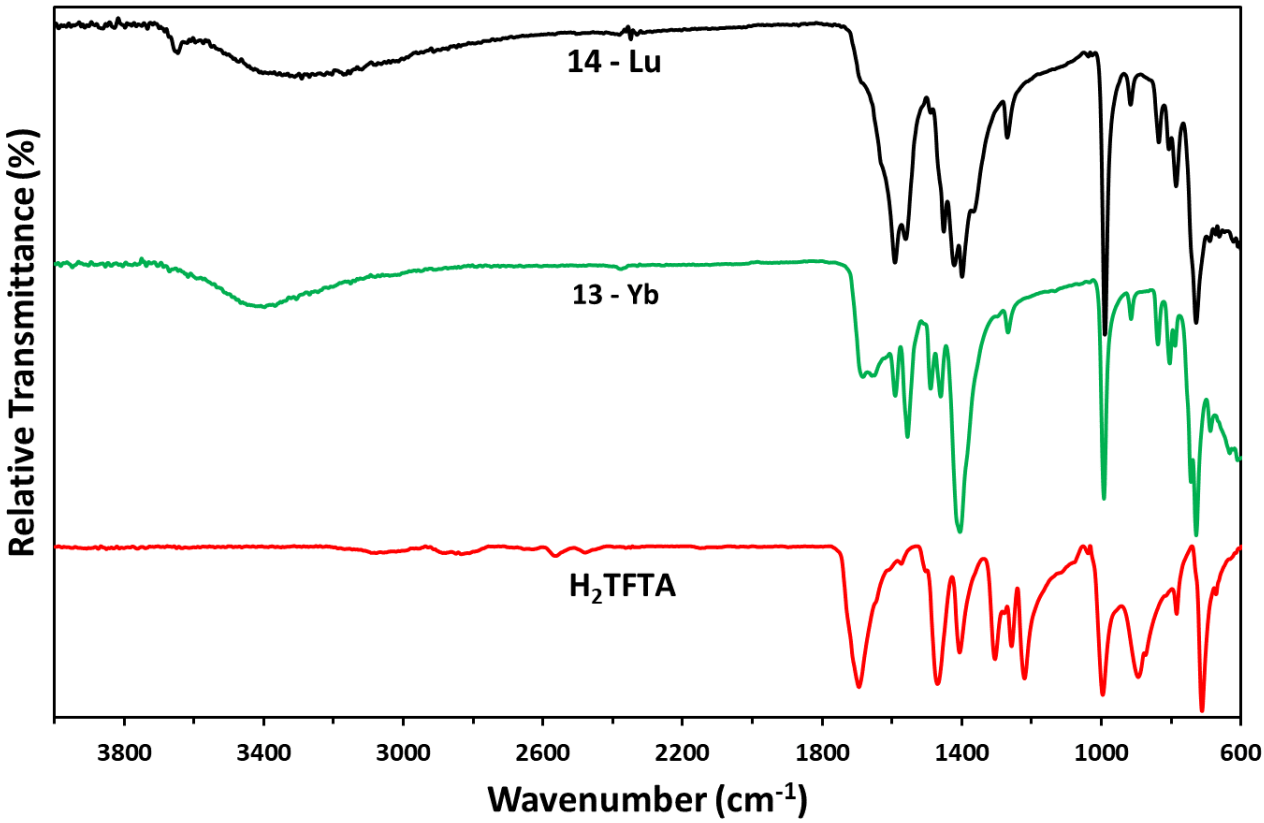

Figure S2. FTIR scans of 2,3,5,6-tetrafluoroterephthalic acid (H_2TFTA) and compounds in series **2**.

Table S3. Yields, elemental C, H analysis and main FTIR peaks for compounds in series **2**.

Compound	Yield based on H_2TFTA (%)	Elemental C, H Analysis (%)	Main FT-IR Peaks (ATR, cm^{-1})
{[Yb(TFTA)$_{1.5}$(H$_2$O)$_2$]•H$_2$O}$_n$ (13)	33	Calc.: C, 24.80; H, 1.04. Found: C, H,	3414(br,w), 1684(m), 1659(m), 1592(m), 1556(s), 1490(m), 1461(m), 1406(s), 1268(w), 1135(w), 993(s), 916(w), 839(w), 805(w), 790(w), 744(s), 729(s), 688(w), 633(w)
{[Lu(TFTA)$_{1.5}$(H$_2$O)$_2$]•H$_2$O}$_n$ (14)	26	Calc.: C, 24.72; H, 1.04. Found: C, H,	3647(w), 3305(br,w), 1592(s), 1561(s), 1490(w), 1453(s), 1422(s), 1400(s), 1270(w), 990(s), 917(w), 836(w), 807(w), 787(w), 729(s), 690(w), 663(w)

Table S4. Selected bond lengths (Å) and angles (°) for Compounds **1 – 14**.

Compound 1				Compound 2			
La1-O4	2.4558(19)	La1-O2	2.488(2)	Ce1-O2	2.470(2)	Ce1-O4	2.4403(17)
La1-O3	2.5723(18)	La1-OW1	2.557(2)	Ce1-O3	2.5569(17)	Ce1-OW1	2.537(2)
O4-La1-O2	72.21(5)	O4-La1-OWI	146.74(8)	O4#1-Ce1-O4	132.45(9)	O2-Ce1-O3	79.09(7)
O3-La1-OW1	105.11(8)	O2-La1-O1	119.48(8)	O4#1-Ce1-O3	125.04(7)	O4-Ce1-OW1	146.56(8)
Symmetry transformations used to generate equivalent atoms: #1: x,-y,z; #2: -x+1,-y,-z; #3: x+1,y,z; #4: x+1,-y,z; #5: -x+1,y,-z; #6: x-1,y,z; #7: x,-y-1,z				Symmetry transformations used to generate equivalent atoms: #1: x,-y,z; #2: x+1,-y,z; #3: x+1,y,z; #4: x-1,y,z; #5: -x+1,-y,-z; #6: -x+1,y,-z; #7: x,-y-1,z			
Compound 3				Compound 4			
Pr1-O4	2.4233(17)	Pr1-O2	2.444(2)	Nd1-O3	2.4122(12)	Nd1-O1	2.5830(19)
Pr1-OW1	2.519(2)	Pr1-O2#2	2.702(2)	Nd1-OW1	2.5063(14)	Nd1-O2#2	2.6889(17)
O4-Pr1-O4#1	132.79(9)	O4-Pr1-O2	72.89(5)	O3-Nd1-O2	73.14(3)	O2-Nd1-OW1	141.15(4)
O2-Pr1-OW1	141.02(6)	OW1-Pr1-O3	104.79(7)	OW1-Nd1-OW3	145.71(5)	O3-Nd1-O4#1	125.72(5)
Symmetry transformations used to generate equivalent atoms: #1: x,-y,z; #2: -x+1,-y,-z; #3: -x+1,y,-z; #4: x,-y-1,z; #5: x+1,y,z; #6: x+1,-y,z; #7 x-1,y,z				Symmetry transformations used to generate equivalent atoms: #1: x,-y,z; #2: -x+1,-y,-z+1; #3: x+1,-y,z; #4: x+1,y,z; #5: -x+1,y,-z+1; #6: x-1,y,z; #7: x,-y-1,z			
Compound 5				Compound 6			
Sm1-O3	2.381(2)	Sm1-O1	2.549(3)	Eu1-O3	2.3725(18)	Eu1-O1	2.535(3)
Sm1-OW1	2.472(2)	Sm1-O2	2.685(3)	Eu1-OW1	2.463(2)	Eu1-O2#2	2.668(2)
O3-Sm1-O3#1	133.63(11)	OW1-Sm1-O1	75.27(9)	O2-Eu1-OW1#1	141.30(6)	OW1-Eu1-O4#1	104.73(7)
O3-Sm1-O4#1	126.46(8)	O3-Sm1-OW1	144.75(9)	O3-Eu1-O2	73.79(5)	O3-Eu1-O3#1	133.77(9)
Symmetry transformations used to generate equivalent atoms: #1: x,-y,z; #2: -x,-y,-z; #3: -x,y,-z; #4: x+1,y,z; #5: x+1,-y,z; #6: x-1,y,z; #7: x,-y-1,z				Symmetry transformations used to generate equivalent atoms: #1: x,-y+1,z; #2: -x,-y+1,-z; #3: x-1,y,z; #4: x-1,-y+1,z; #5: -x,y,-z; #6: x+1,y,z; #7: x,-y,z			
Compound 7				Compound 8			
Gd1-O4	2.3637(16)	Gd1-O3	2.4705(16)	Tb1-O3	2.345(3)	Tb1-O1	2.501(4)
Gd1-OW1	2.4476(18)	Gd1-O2#2	2.663(2)	Tb1-OW1	2.435(3)	Tb-O2#2	2.666(4)
O4-Gd1-O2	73.97(4)	O2-Gd1-O1	121.77(8)	O3-Tb1-O2	74.03(7)	O2-Tb1-OW1#1	141.49(9)
O2-Gd1-O3	79.33(7)	O4-Gd1-OW1	144.65(7)	O3-Tb1-O4	127.04(10)	OW1#1-Tb1-O4	104.59(11)
Symmetry transformations used to generate equivalent atoms: #1: x,-y,z; #2: -x+1,-y,-z+2; #3: x,-y+1,z; #4: -x+1,y,-z+2; #5: x+1,y,z; #6: x-1,y,z				Symmetry transformations used to generate equivalent atoms: #1: x,-y+1,z; #2: -x,-y+1,-z; #3: -x,y,-z; #4: x,-y,z; #5: x+1,y,z; #6: x-1,y,z			
Compound 9				Compound 10			
Dy1-O4	2.3351(14)	Dy1-O2	2.340(2)	Ho1-O4	2.3239(12)	Ho1-O2	2.3292(18)
Dy1-OW1	2.4207(16)	Dy1-O2#2	2.668(2)	Ho1-OW1	2.4095(14)	Ho1-O2#2	2.6733(18)
O4#1-Dy1-O4	133.99(7)	O2-Dy1-OW1	141.39(5)	O4-Ho1-O4#1	133.92(6)	O2-Ho1-OW1#1	141.50(4)

O2-Dy1-O3	79.16(6)	OW1-Dy1-O3	104.62(6)	O4-Ho1-O2	74.42(4)	OW1-Ho1-O3#1	104.67(5)
Symmetry transformations used to generate equivalent atoms: #1: x,-y+1,z; #2: -x+1,-y+1,-z; #3: x+1,-y+1,z; #4: x+1,y,z; #5: -x+1,y,-z; #6: x-1,y,z; #7: x,-y,z				Symmetry transformations used to generate equivalent atoms: #1: x,-y,z; #2: -x+1,-y,-z+2; #3: x-1,y,z; #4: -x+1,y,-z+2; #5: x+1,y,z; #6: x,-y+1,z			
Compound 11				Compound 12			
Er1-O4	2.3116(17)	Er1-OW1	2.399(2)	Tm1-O1	2.422(4)	Tm1-O4	2.410(3)
Er1-O3	2.4284(19)	Er1-O2#2	2.689(3)	Tm1-O3	2.297(3)	Tm1-OW1	2.385(3)
O4-Er1-OW1	143.90(7)	O4#1-Er1-O3	128.09(7)	O2-Tm1-O3	74.62(8)	O3-Tm1-O3#2	133.16(14)
O4-Er1-O2	74.54(5)	OW1-Er1-O3	104.72(8)	O3-Tm1-OW1	143.92(11)	O3-Tm1-O4#2	128.43(10)
Symmetry transformations used to generate equivalent atoms: #1: x,-y,z; #2: -x+2,-y,-z+1; #3: -x+1,-y,-z+1; #4: -x+2,y,-z+1; #5: x,-y+1,z				Symmetry transformations used to generate equivalent atoms: #1: -x+1,-y+1,-z+1; #2: x,-y+1,z; #3: x-1,y,z; #4: x+1,y,z; #5: x+1,-y+1,z; #6: -x+1,y,-z+1; #7: x,-y,z			
Compound 13				Compound 14			
Yb1-O3	2.349(3)	Yb1-O4	2.414(3)	Lu1-O1	2.247(4)	Lu1-O4	2.389(4)
Yb1-O6	2.283(3)	Yb1-OW1	2.366(3)	Lu1-OW1	2.348(4)	Lu1-O6	2.284(4)
O1-Yb1-O6	75.17(14)	O6-Yb1-O5	122.19(13)	O1-Lu1-O6	74.53(15)	O6-Lu1-O5	121.85(14)
O6-Yb1-OW2	141.20(13)	O1-Yb1-O3	132.72(13)	O2#2-Lu1-OW2	144.77(16)	O5-Lu1-OW1	76.39(15)
Symmetry transformations used to generate equivalent atoms: #1: -x+1,-y+2,-z+1; #2: -x+2,-y+1,-z+1; #3: x,y,z+1; #4: x,y,z-1				Symmetry transformations used to generate equivalent atoms: #1: -x+1,-y+2,-z+1; #2: -x+2,-y+1,-z+1; #3: x,y,z+1; #4: x,y,z-1			

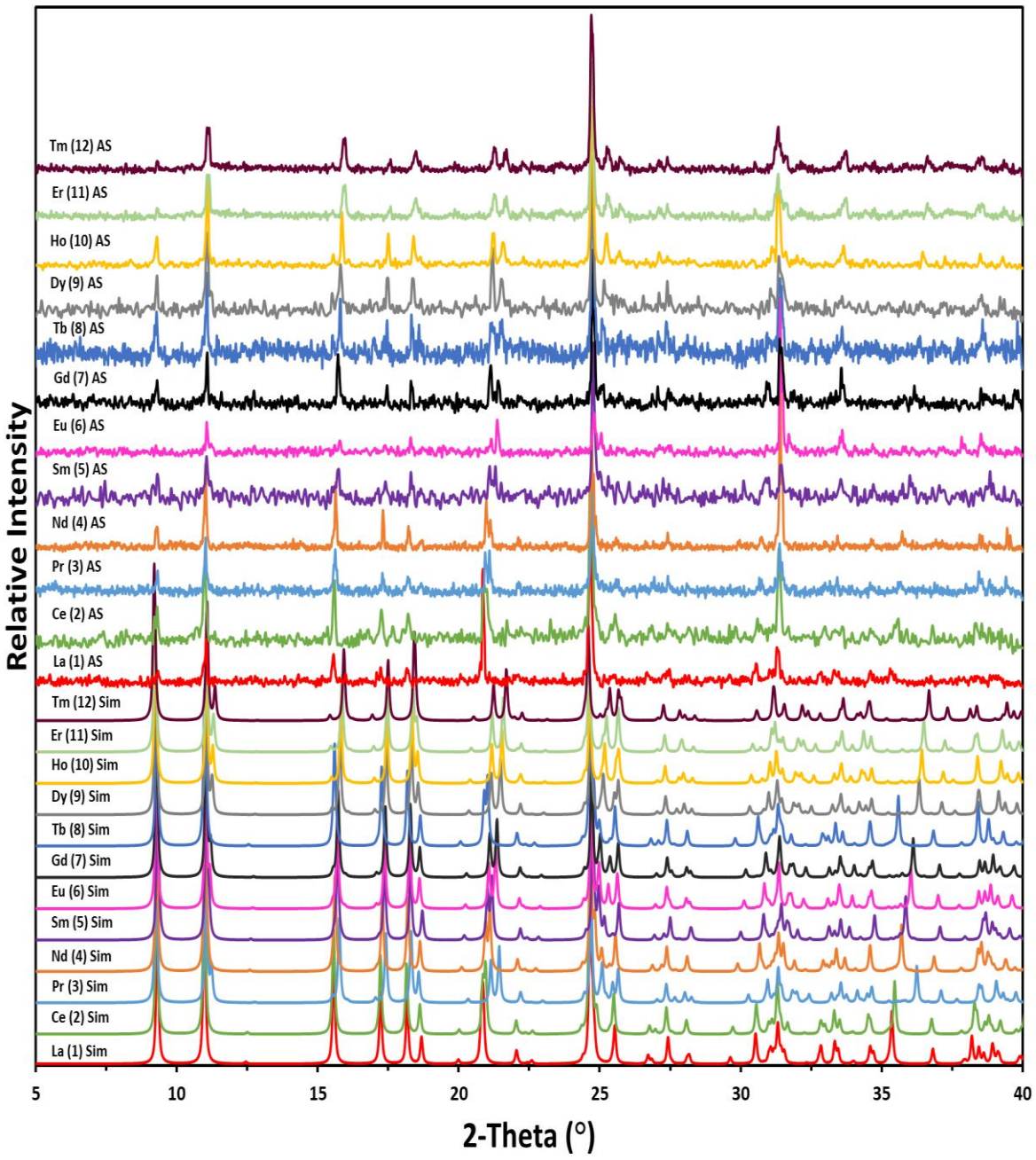

Figure S3. Simulated (Sim) and as-synthesized (AS) PXRD patterns for compounds **1 – 12**.

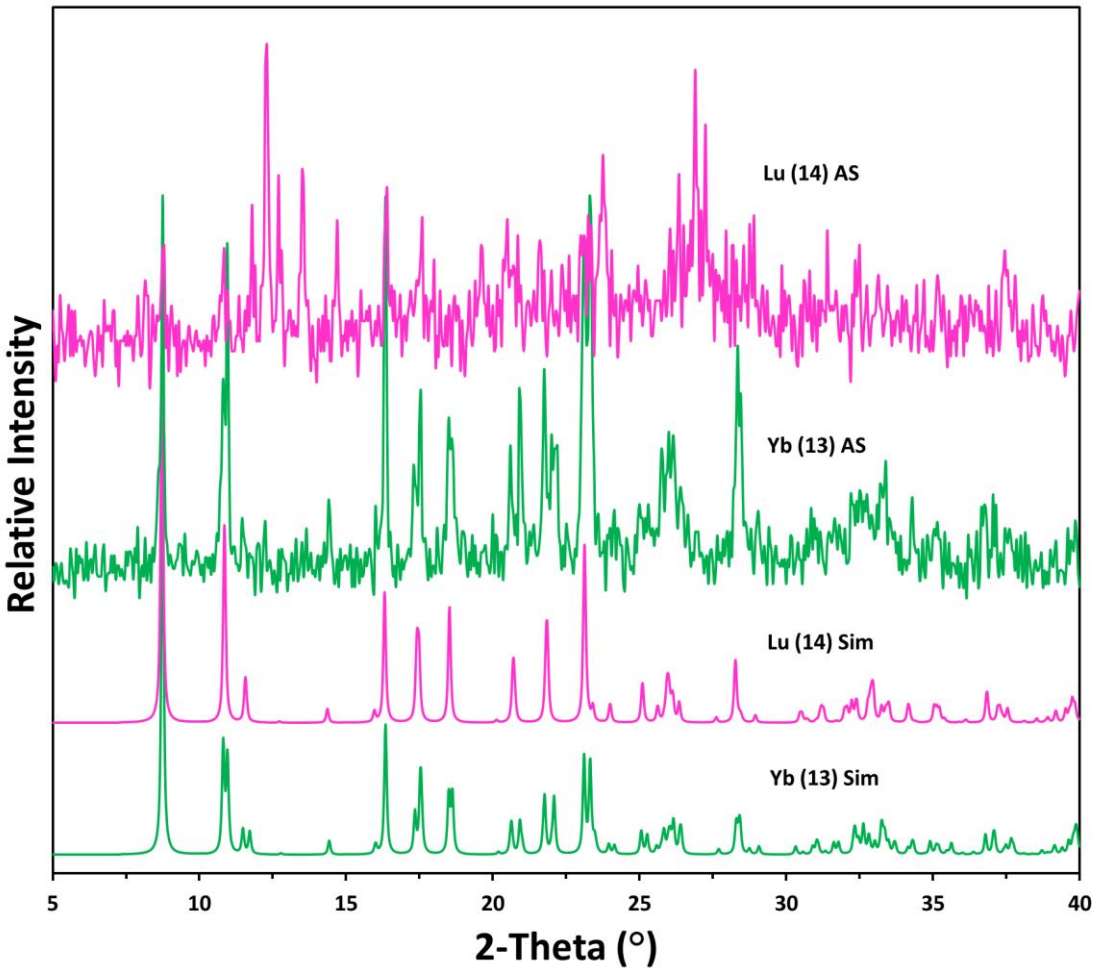

Figure S4. Simulated (Sim) and as-synthesized (AS) PXRD patterns for compounds **13** and **14**.

Table S5. Structures in which F•••F interactions were identified in research article.

CSD Code	Reference	F•••F distance (Å)	∠C–F•••F (θ_1; θ_2) °	Type of F•••F interaction
ADUQUL	[1]	2.924	148.56; 116.47	II
		2.846	160.65; 130.25	II
ATEKIV	[2]	2.866	100.02; 100.02	I
AVIRAZ	[3]	2.646	146.85; 146.85	I
		2.782	175.18; 175.18	I
		2.796	146.62; 122.12	Quasi type I/type II
		2.833	158.64; 121.20	II
		2.837	98.96; 98.96	I
		2.850	122.34; 101.76	Quasi type I/type II
		2.862	138.66; 91.80	II
		2.901	138.49; 95.86	II
AVIRED	[3]	2.814	175.49; 116.90	II
		2.855	148.22; 99.62	II
		2.856	164.26; 152.82	I
		2.860	150.61; 139.73	I
		2.883	170.44; 98.14	II
AVIRIH	[3]	2.753	167.55; 163.61	I
		2.816	175.28; 116.81	II
		2.838	149.76; 100.31	II
		2.859	149.74; 137.60	I
		2.923	114.19; 114.19	I
AVIRON	[3]	2.809	175.73; 117.05	II
		2.838	148.51; 99.42	II
		2.842	150.49; 139.47	I
		2.851	164.65; 151.87	I
		2.901	170.13; 98.60	II
AVIRUT	[3]	2.836	149.89; 131.20	Quasi type I/type II
AWIWIM	[4]	2.880	130.46; 117.59	I
AWIXEJ01	[4]	2.855	124.66; 110.11	I
BAPMEN	[5]	2.934	172.54; 107.76	II
BAPMOX	[5]	2.860	86.00; 86.00	I
		2.877	122.17; 85.41	II

BEKDUR	[6]	2.824	123.14; 123.14	I
BEKDUR01	[7]	2.815	123.48; 123.48 between interstitial CF_3SO_3	I
BEMSAO01	[8]	2.918	108.74; 108.74	I
BEMSAO02	[8]	2.856	109.56; 109.56	I
BEMSAO04	[8]	2.858	111.82; 110.12	I
BODJUA	[9]	2.729	160.93; 160.93 between interstitial CF_3SO_3	I
CEPKUG	[10]	2.939	109.30; 104.87	I
CEYDUG	[11]	2.576	162.60; 162.60	I
CUVWOG	[12]	2.873	93.74; 93.74	I
CUVXEX	[12]	2.768 2.916	168.72; 106.37 136.43; 99.55	II II
CUVXIB	[12]	2.929	137.59; 137.59	I
CUWXIC	[13]	2.857	122.94; 118.32	I
DAPPER	[14]	2.667	126.23; 126.23	I
DULFIA	[15]	2.780	137.69; 137.69	I
DULFIA01	[16]	2.774	138.52; 138.52	I
GIVBAR	[17]	2.719	134.96; 134.96	I
HADMAD01	[18]	2.693	157.93; 144.20	I
HAFPOV	[19]	2.935	102.35; 102.13	I
HALLOX	[20]	2.737 2.938	138.02; 119.14 102.78; 93.84	Quasi type I/type II I
HIJWUU*	[21]	2.847 2.934	150.46; 135.39 137.76; 116.18	Quasi type I/type II Quasi type I/type II
HIVJEB	[22]	2.894	98.83; 98.83	I
HIZJEG	[23]	2.936	119.91; 115.75	I
HOLRIL	[24]	2.795	137.69; 128.09	I
IXACOZ*	[25]	2.843 2.935	175.77; 143.86 174.60; 127.49	II II
KEVVIQ	[26]	2.875 2.895	125.96; 122.02 109.93; 109.93	I I
KIDCOR	[27]	2.549	155.99; 155.99	I

KIPJIE	[28]	2.793	152.29; 104.90	II
		2.835	117.30; 117.30	I
LOWLIU	[29]	2.741	157.34; 95.44	II
		2.817	166.80; 86.87	II
		2.858	127.74; 122.21	I
		2.879	139.07; 95.48	II
MIYZIF	[30]	2.830	115.75; 115.75	I
MULQIT*	[31]	2.648	158.79; 123.54	II
MULQOZ*	[31]	2.719	140.91; 111.91	Quasi type I/type II
		2.863	139.29; 119.25	Quasi type I/type II
MULRAM	[31]	2.904	116.59; 116.59	I
NUWCAK	[32]	2.786	141.03; 141.03	I
		2.876	128.92; 128.92	I
NUWHUK	[33]	2.864	123.03; 123.03	I
		2.867	148.94; 148.94	I
NUWJAS	[33]	2.939	122.78; 122.78	I
NUWJEW	[33]	2.799	110.27; 110.27	I
		2.837	167.00; 132.22	II
OCULIK	[34]	2.937	79.13; 79.13	I
OJEDEN	[35]	2.779	144.04; 144.04	I
PUSQOK	[36]	2.730	161.92; 117.97	II
PUSREB	[36]	2.829	125.08; 112.26	I
		2.860*	120.19; 113.33	I
PUSRIF	[36]	2.616	154.68; 154.68	I
PUSROL	[36]	2.706	126.08; 111.07	Quasi type I/type II
PUSSAY	[36]	2.781	128.33; 128.33	I
PUSSIG	[36]	2.904*	140.36; 120.51	Quasi type I/type II
PUSSOM	[36]	2.829	150.97; 150.97	I
PUSSUS	[36]	2.873	168.21; 167.24	I
PUSTAZ	[36]	2.844	134.49; 122.16	I
QAQGUL	[37]	2.870	152.29; 152.29	I
QAQHEW	[37]	2.790	118.99; 96.88	Quasi type I/type II
		2.902	151.08; 105.80	II
		2.931	148.32; 90.26	II
SAZROD	[38]	2.872*	139.59; 112.58	Quasi type I/type II

SAZRUJ	[38]	2.557* 2.719*	143.26; 143.26 131.00; 96.33	I II
SIWBUX	[39]	2.544	148.73; 148.73	I
SIWCAE	[39]	2.860	150.27; 150.27	I
TEZSEZ	[40]	2.743	167.74; 128.48	II
TOZDUJ	[41]	2.863*	155.48; 111.26	II
TOZFAR	[41]	2.914	118.19; 99.29	Quasi type I/type II
TUGGUY	[42]	2.780	131.81; 117.64	I
URESIV	[43]	2.743* 2.743* 2.794*	150.68; 141.36 134.16; 124.86 102.62; 102.62	I I I
VEZPAT	[44]	2.877	135.11; 117.13	Quasi type I/type II
VUNXEI	[45]	2.912 2.939	160.84; 120.42 158.26; 105.05	II II
WIFBAP	[46]	2.884	103.84; 103.84	I
WILKAF	[47]	2.787	115.59; 115.59	I
XALPIJ	[48]	2.744 2.908	128.14; 128.14 158.01; 158.01	I I
XALPOP	[48]	2.555 2.662 2.712	132.16; 132.16 176.45; 155.78 161.90; 161.90	I I I
XIRZIK	[49]	2.880	142.73; 119.85	Quasi type I/type II
XIRZOQ	[49]	2.903	141.52; 118.27	Quasi type I/type II
XIRZUW	[49]	2.924	140.11; 114.72	Quasi type I/type II
YEMNUA	[50]	2.725	154.61; 152.85	I

* - Disordered atoms are involved in F•••F interaction

Table S6. F•••F interactions in series **1** and **2**.

Series 1	F1•••F3 distance (Å)	Sum of vdW radii (%)	type of X•••X interaction	F1•••F1 distance (Å)	Sum of vdW radii (%)	type of X•••X interaction
1 – La(III)	2.596(3)	88.3	I	2.896(3)	98.5	I
2 – Ce(III)	2.591(2)	88.1	I	2.898(3)	98.6	I
3 – Pr(III)	2.584(3)	87.9	I	2.893(3)	98.4	I
4 – Nd(III)	2.5694(19)	87.4	I	2.896(3)	98.5	I
5 – Sm(III)	2.540(3)	86.4	I	2.884(5)	98.1	I
6 – Eu(III)	2.544(3)	86.5	I	2.896(3)	98.5	I
7 – Gd(III)	2.533(2)	86.2	I	2.900(3)	98.6	I
8 – Tb(III)	2.528(3)	86.0	I	2.913(5)	99.1	I
9 – Dy(III)	2.517(2)	85.6	I	2.911(3)	99.0	I
10 – Ho(III)	2.510(2)	85.4	I	2.918(3)	99.3	I
11 – Er(III)	2.501(3)	85.1	I	2.929(3)	99.6	I
12 – Tm(III)	2.4951(1)	84.9	I	2.9385(1)	99.9	I
Series 2	F2•••F5(A) distance (Å)	Sum of vdW radii (%)	F1•••F4(A) distance (Å)	Sum of vdW radii (%)	F2•••F6(A) distance (Å)	Sum of vdW radii (%)
13 – Yb(III)	2.850(8)	96.9	2.635	89.6	2.730(9)	92.9
14 – Lu(III)	2.907(9)	98.9	2.604	88.6	2.743(9)	93.3

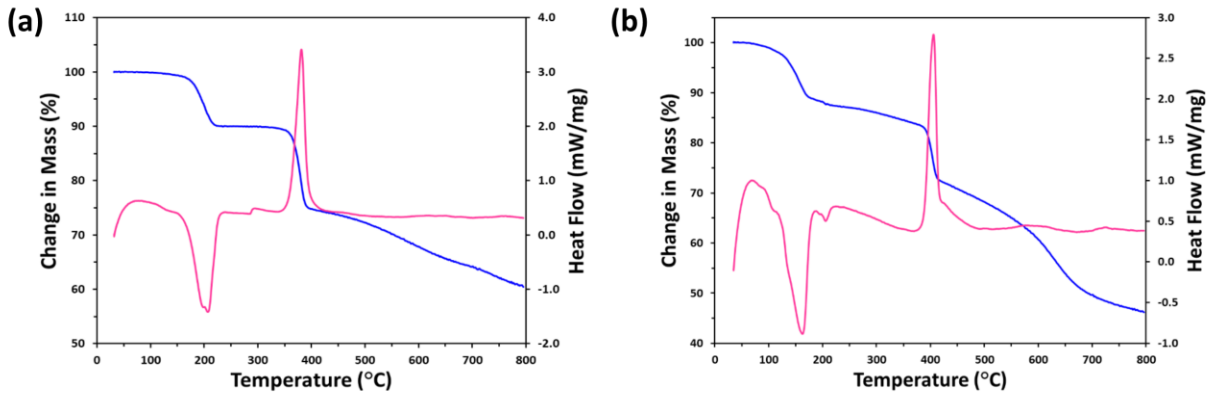

Figure S5. TGA (blue) – DSC (pink) scans of compounds (a) **5** (Sm-TFTA) and (b) **13** (Yb-TFTA) under helium atmosphere.

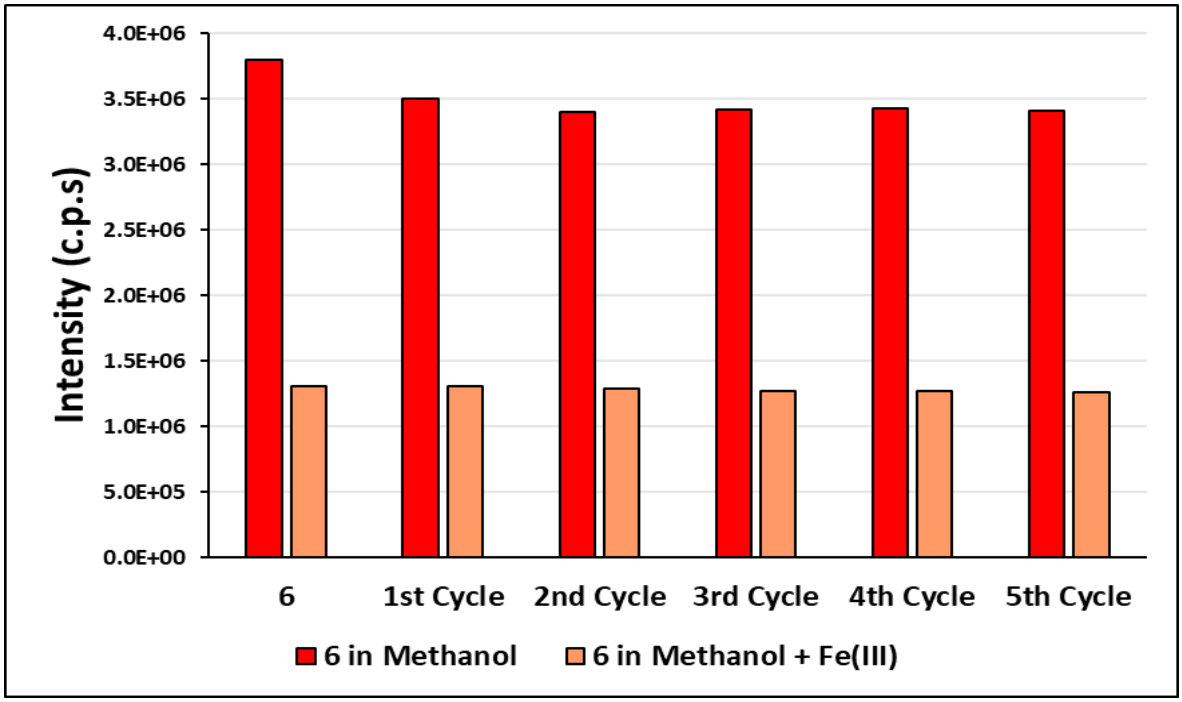

Figure S6. Recyclability toward Fe^{3+} sensing

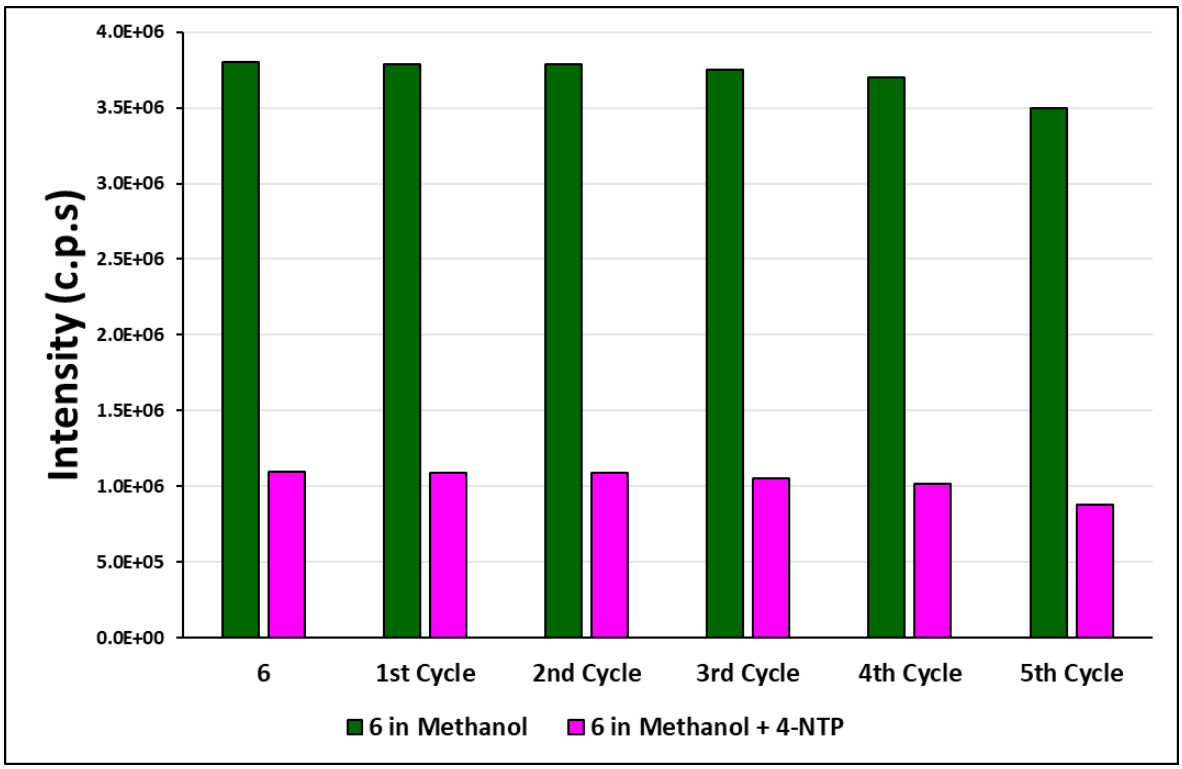

Figure S7. Recyclability toward 4-NTP sensing

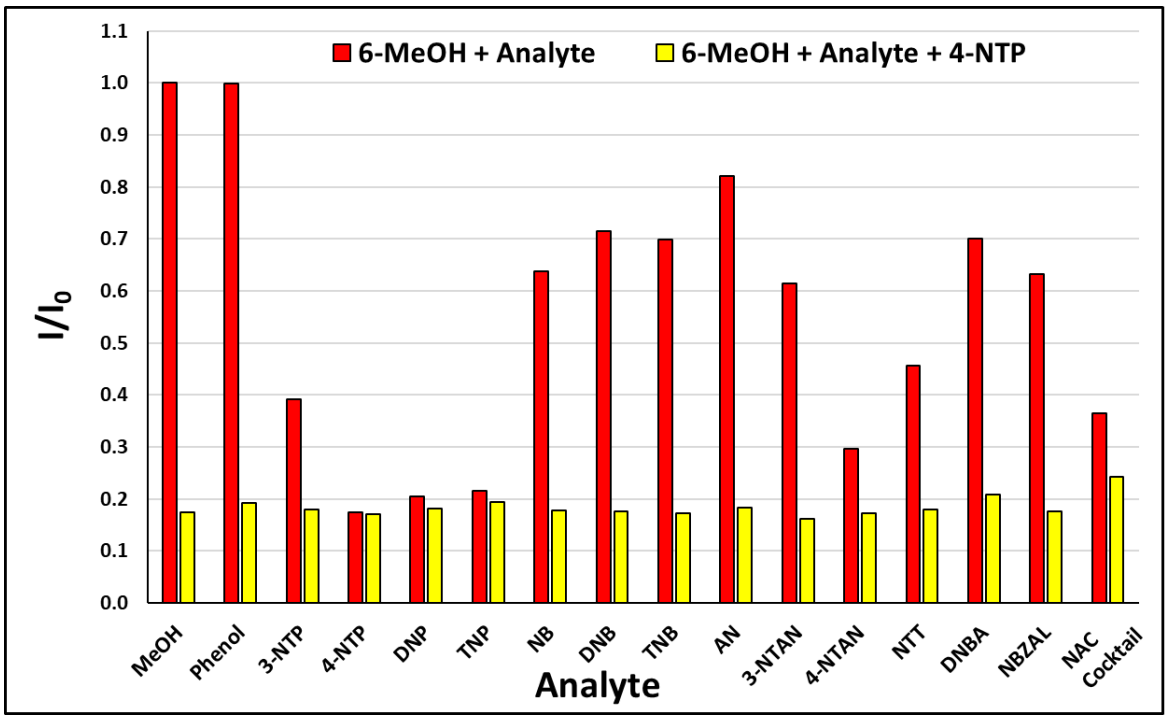

Figure S8. Relative fluorescence of **6**-MeOH in the presence of varying NAC solutions (red) and NACs mixed with 4-NTP upon 317 nm excitation (yellow).

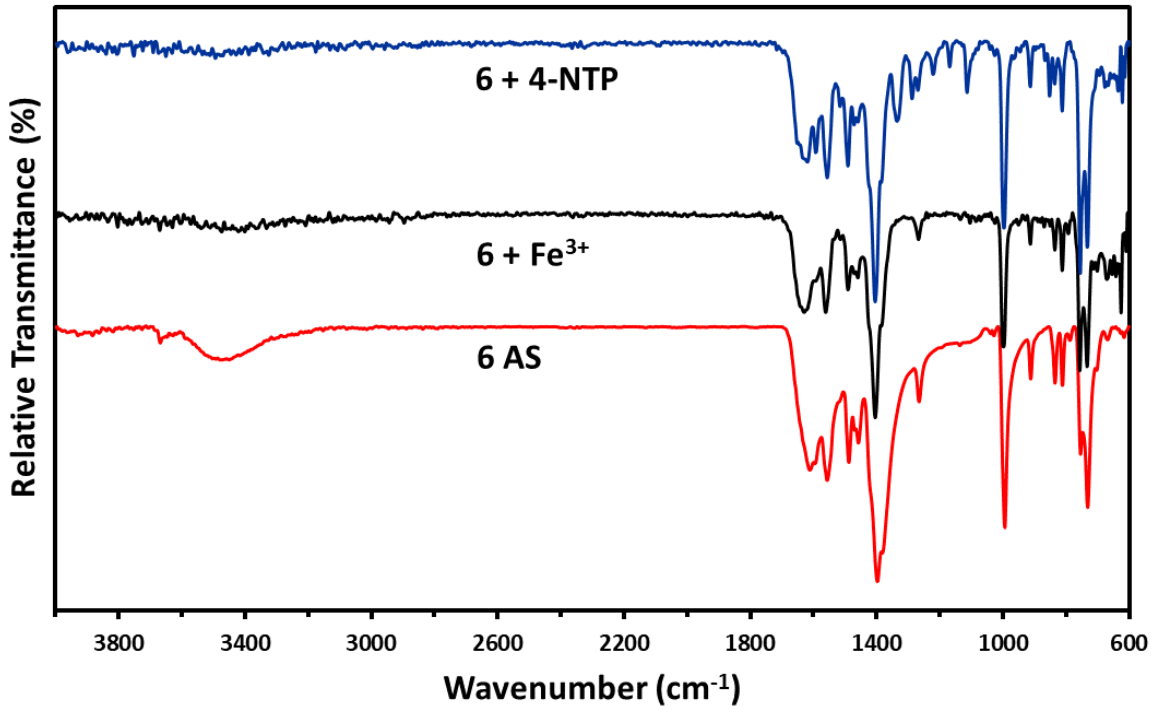

Figure S9. FTIR spectra of as-synthesized (AS) $\{[Eu_2(TFTA)_3(H_2O)_4]\bullet 2H_2O\}_n$ **(6)** upon interaction with $FeCl_3$ and 4-NTP, respectively.

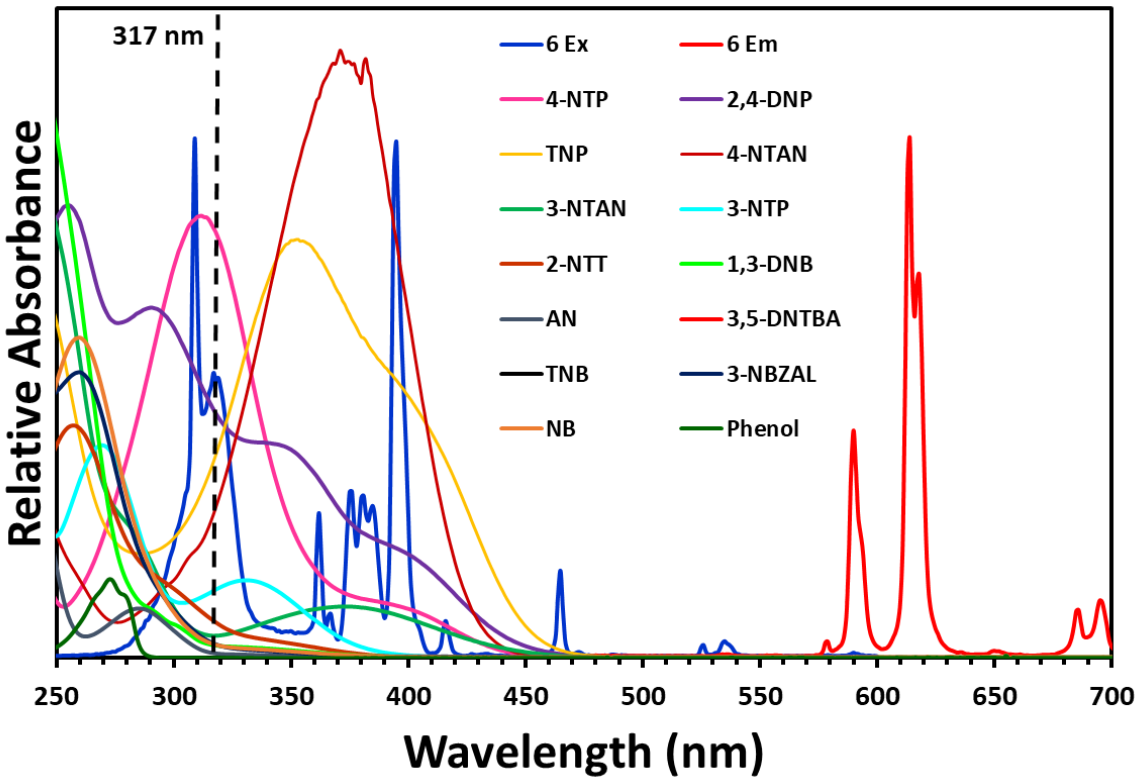

Figure S10. UV-Vis spectra of methanol solutions containing NACs and solid-state excitation and emission spectrum of **6** (λ_{em} = 617 nm; λ_{ex} = 317 nm).

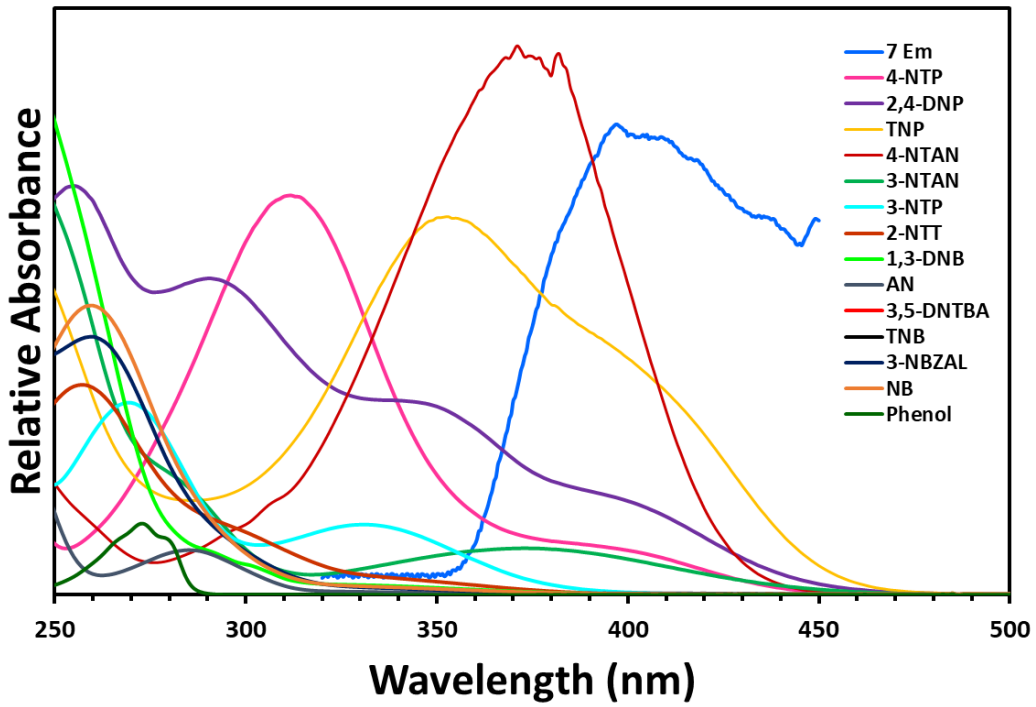

Figure S11. Absorbance spectra of nitroaromatic analytes and emission spectrum of $\{[Gd(TFTA)_{1.5}(H_2O)_2]\bullet H_2O\}_n$ (7). 7 Em is from the lowest triplet state of the ligand (ligand phosphorescence).

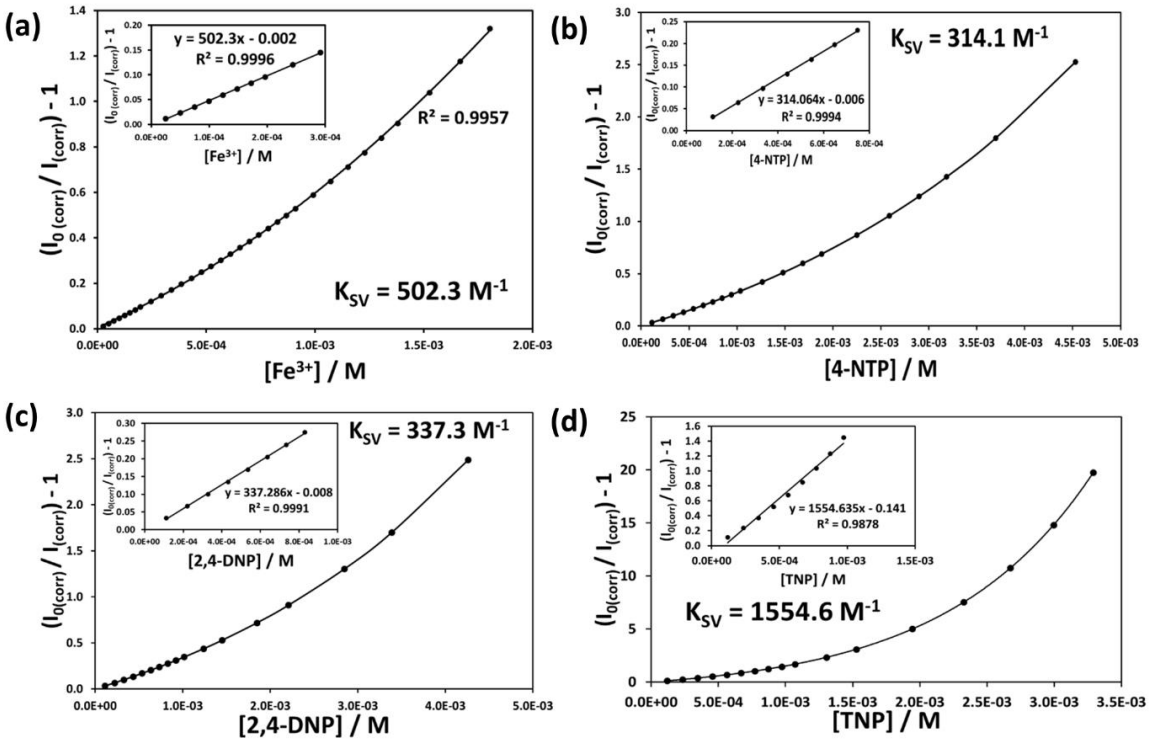

Figure S12. Corrected S–V plots for (a) Fe^{3+} (b) 4-NTP (c) 2,4-DNP (d) TNP in $\{[Eu_2(TBrTA)_3(H_2O)_8]\bullet 2H_2O\}_n$.[51]

Table S7. HOMO and LUMO energies of TFTA ligand, TBrTA ligand and nitroaromatic compounds.

Ligand or NAC	HOMO (eV)	LUMO (eV)	Band Gap (eV)
TFTA	-0.30541	-0.12486	0.18055
TBrTA	-0.27272	-0.08087	0.19185
4-NTP	-0.26811	-0.10088	0.16723
DNP	-0.29421	-0.13908	0.15513
TNP	-0.31585	-0.15948	0.15637
4-NTAN	-0.22945	-0.07167	0.15778
3-NTP	-0.26267	-0.10690	0.15577
2-NTT	-0.27798	-0.10242	0.17556
3-NTAN	-0.23743	-0.10126	0.13617
NBZAL	-0.28957	-0.12224	0.16733
NB	-0.29021	-0.10737	0.18284
TNB	-0.34394	-0.15203	0.19191
DNBA	-0.32266	-0.14775	0.17491
DNB	-0.32098	-0.13238	0.18860
AN	-0.21002	-0.01111	0.19891
Phenol	-0.23252	-0.01870	0.21382

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