Electronic Supporting Information for

Anthracene based - Lanthanide Metal Organic Frameworks: Synthesis, Photoluminescence and Radioluminescence Properties

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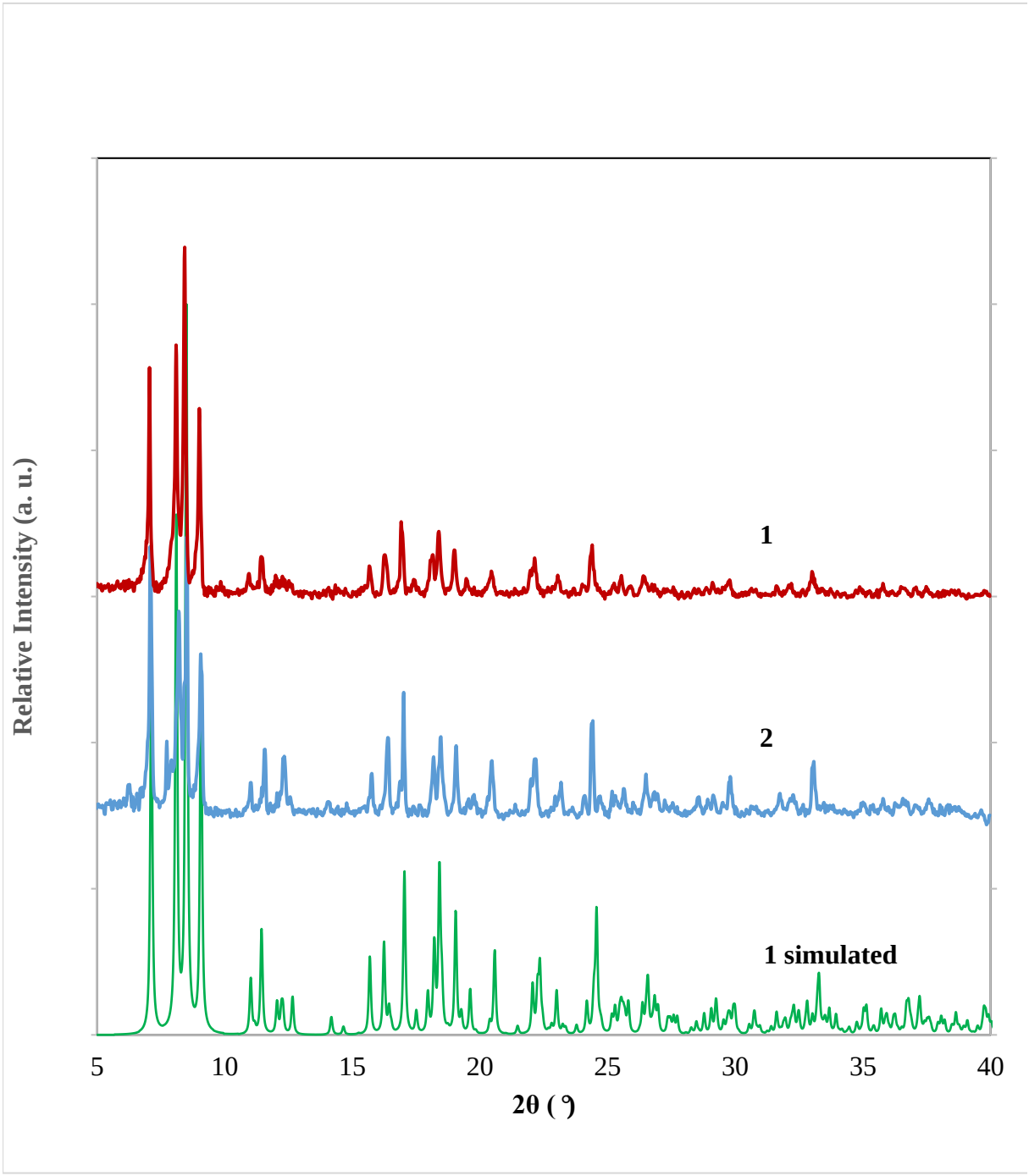


Fig. S1. Powder X-ray diffraction patterns of **1** and **2.**

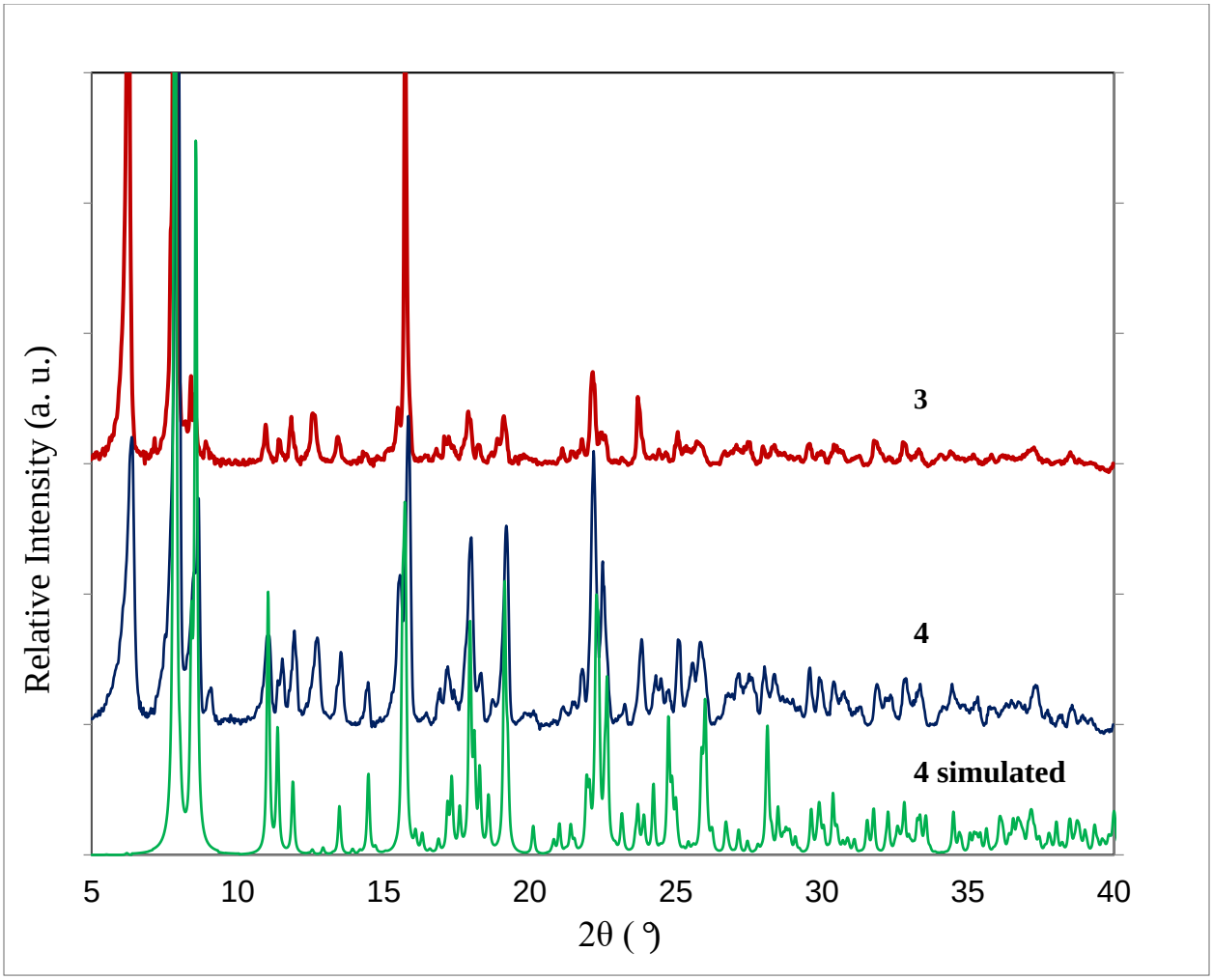


Fig. S2. Powdered X-ray diffraction pattern of simulated **3** and **4**.

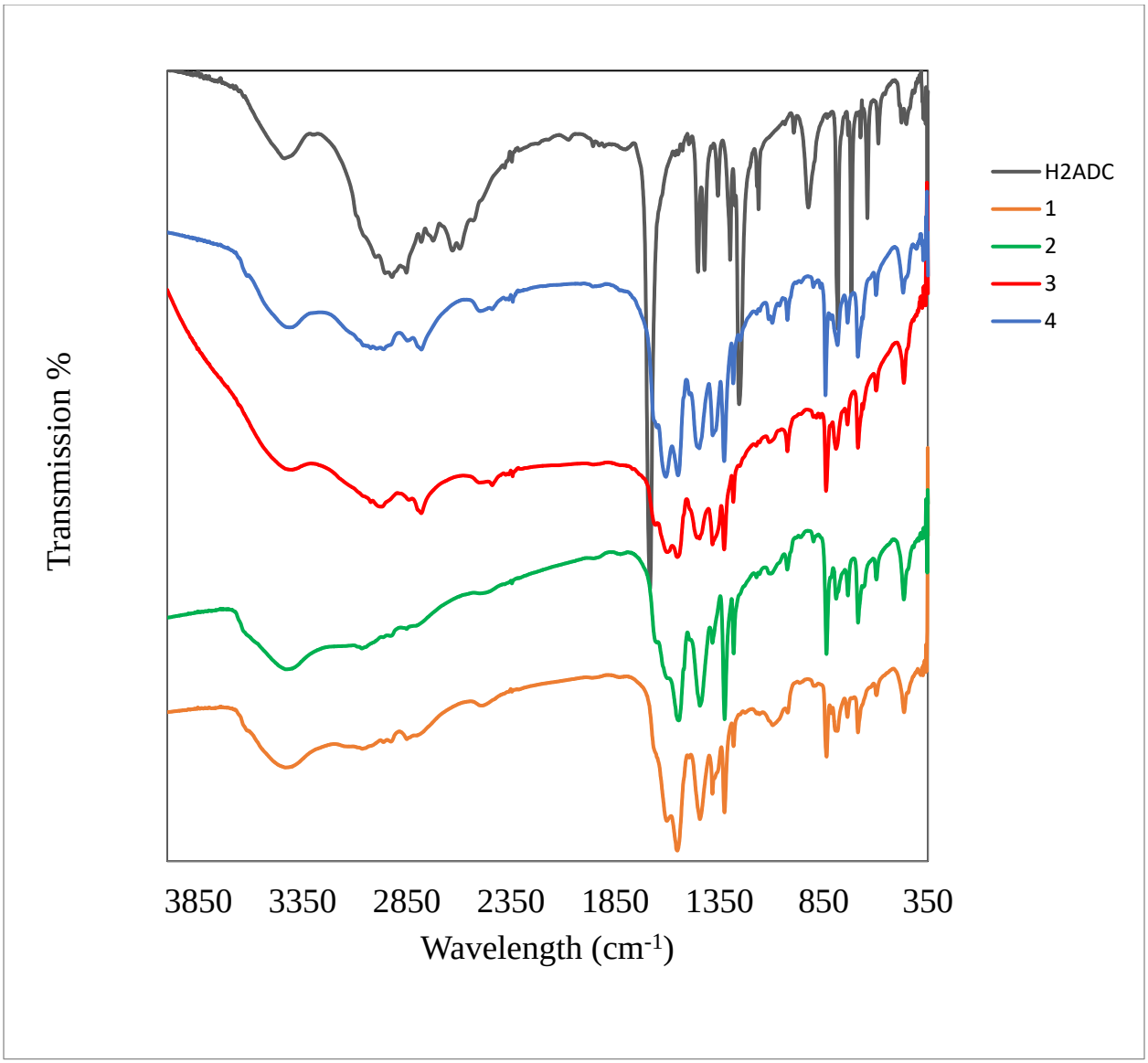


Fig. S3. FTIR spectra of **1-4** and H_2ADC

The band at 3448 cm^{-1} in all samples indicates the presence of O-H from adsorbed water on the MOFs and on H_2ADC. The 2925 cm^{-1} and 2967 cm^{-1} bands observed in H_2ADC are assigned to weak intramolecular O···H bonds between non-planar C=O with H on the aromatic ring at the 1,4,5,8 carbon positions. These bands are not observed in **1-4.** The band observed at 1687 cm^{-1} in the H_2ADC is attributed to the HO–C=O, with localized charges on the ligand's carboxylic acid functional groups. This band is not observed in **1-4,** and instead, two individual bands are observed at 1601 cm^{-1} and 1551 cm^{-1}, which are attributed to variation in stretching vibrations of the C-O bonds in the three different ligand conformations. The band at 1562 cm^{-1} in the MOF spectra is attributed to metal-oxygen bonds.

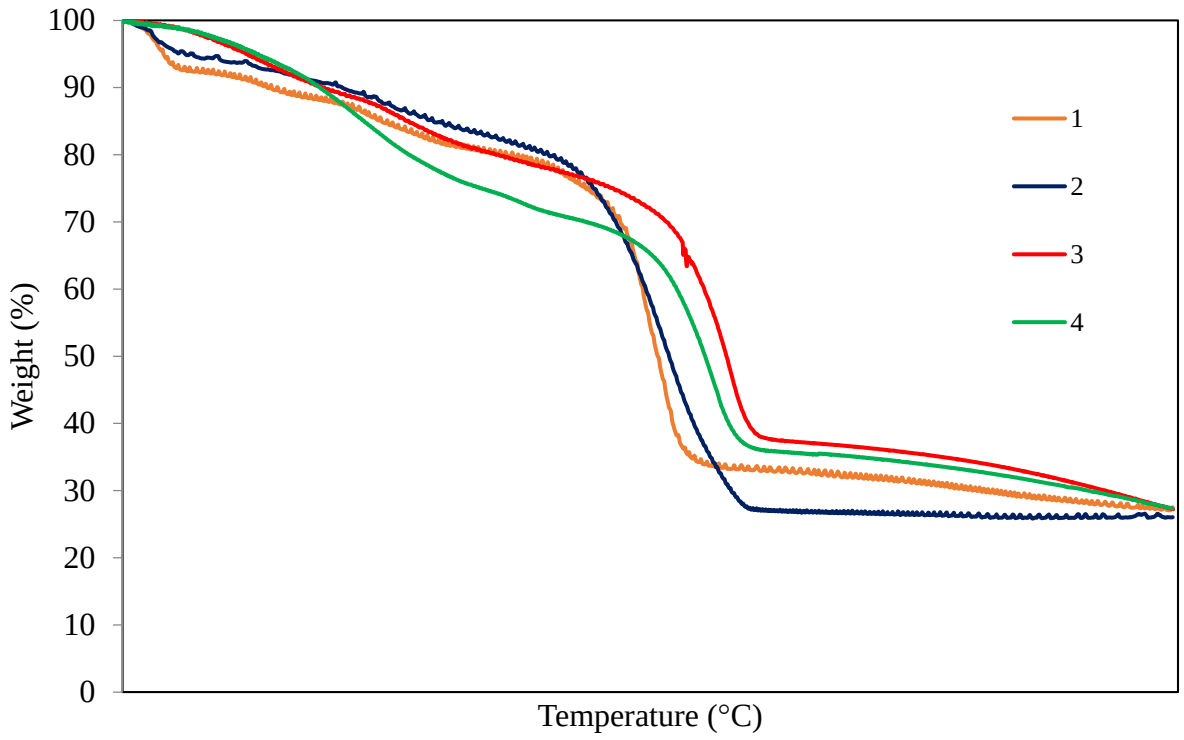


Fig. S4. TGA curves of **1-4**.

The TGA curves of **1** and **2** small weight loss events at approximately 100 ℃ representing the loss of H_2O and $CHCl_3$ molecules (~10 %). Steady weight loss up to 200 ℃ is attributed to loss of DMF. Weight loss event around 460 ℃ is attributed to the loss of ADC units and residue of about 30% is attributed to lanthanide oxides. The TGA curves of **3** and **4** show small weight loss events at approximately 100 ℃, which also represent the loss of H_2O and $CHCl_3$ molecules (~10 %). Steady loss up until 200 ℃ is attributed to loss of DMF. Weight loss around 460 ℃ is attributed to the loss of ADC units. Residue of amount to about ~ 20 % is attributed to lanthanide oxides.

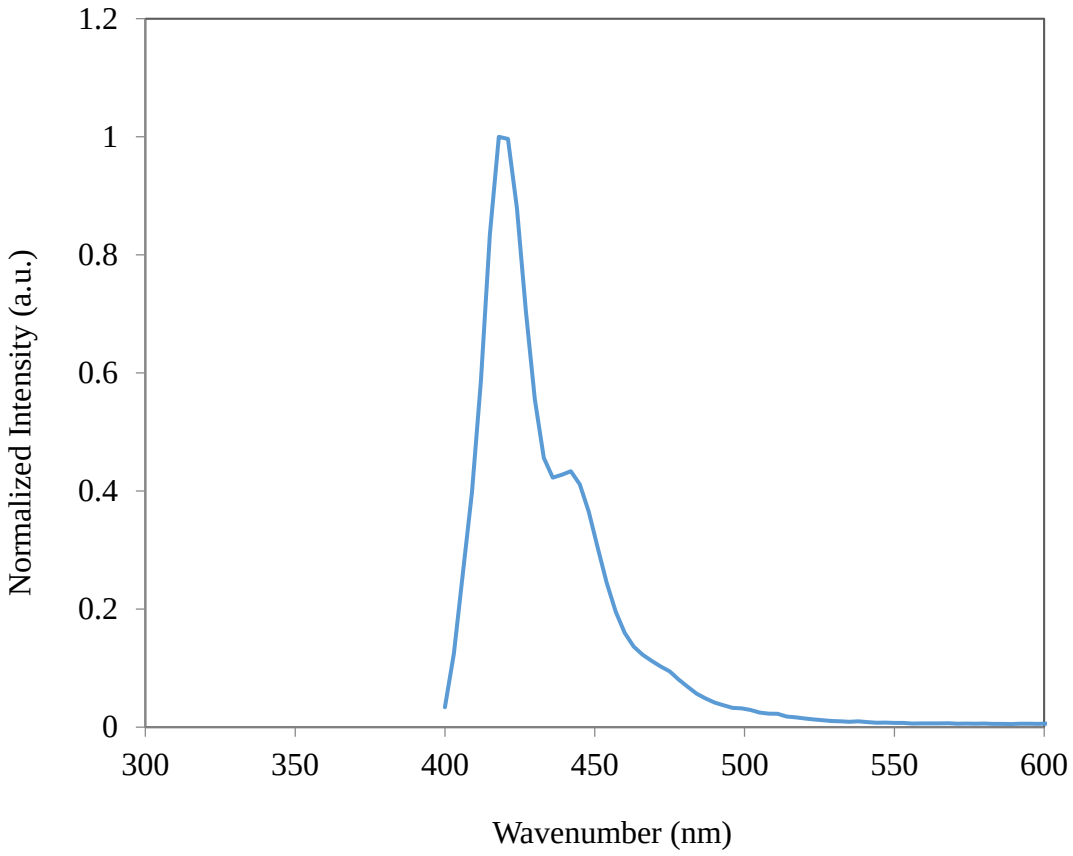
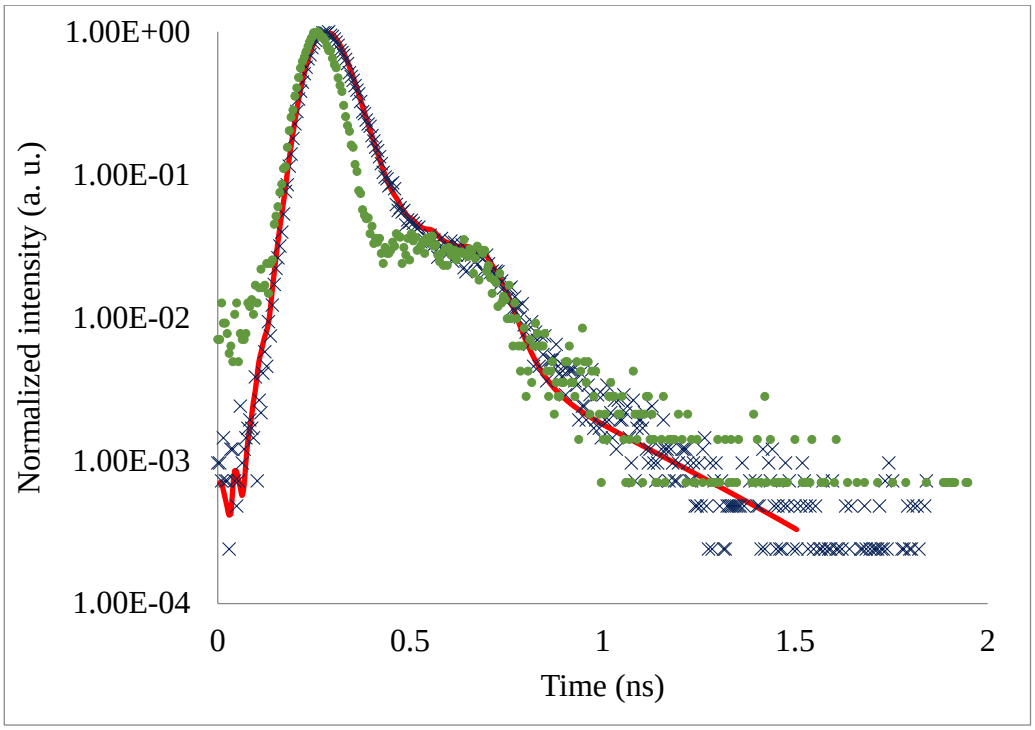
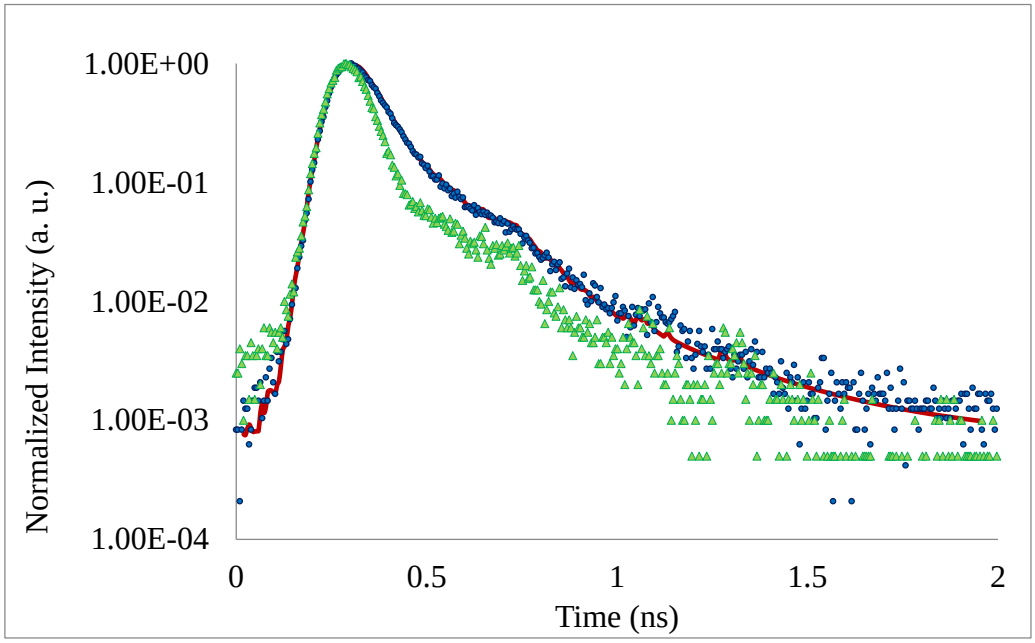


Fig. S5. Photoluminescence emission spectrum of 0.1 M aqueous solution of Na_2ADC.



a) **3** (Er)



b) **4** (Tm)

Fig. S6. Photoluminescence decay curves of structures **3** and **4**.

Table S1. Selected bond lengths (Å) and angles (°) for **1-4.**

1		2		3		4	
Eu1-O1	2.572(2)	Tb1 -O1	2.543(2)	Er1-O10	2.236(3)	Tm1-O10	2.228(2)
Eu1-O1	2.448(2)	Tb1 -O1	2.414(2)	Er1-O1W	2.304(4)	Tm1-O14	2.291(2)
Eu1-O2	2.538(2)	Tb1 -O2	2.513(2)	Er1-O14	2.307(3)	Tm1-O1W	2.292(3)
Eu1-O3	2.360(1)	Tb1 -O3	2.322(1)	Er1-O7	2.310(3)	Tm1-O7	2.293(3)
Eu1-O4	2.468(2)	Tb1 -O4	2.437(2)	Er1-O4	2.335(4)	Tm1-O4	2.322(3)
Eu1-O5	2.483(1)	Tb1 -O5	2.456(2)	Er1-O1	2.350(4)	Tm1-O1	2.334(3)
Eu1-O6	2.465(1)	Tb1 -O6	2.437(2)	Er1-O3	2.449(4)	Tm1-O3	2.441(3)
EuI-O7	2.408 (1)	Tb1 -O7	2.380(2)	Er1-O2	2.509(4)	Tm1-O2	2.512(3)
Eu1-O8	2.447(2)	Tb1 -O8	2.421(2)	Er2-O13	2.229(4)	Tm2-O13	2.219(3)
				Er2-O8	2.236(3)	Tm2-O8	2.224(2)
O5-Eu1-O1	93.42(5)	O1 -Tb1- O2	51.45(5)	Er2-O9	2.279(3)	Tm2-O9	2.257(2)
O6-Eu1-O8	80.10(6)	O1 -Tb1- O3	75.57(6)	Er2-O11	2.291(3)	Tm2-O11	2.276(2)
O8-Eu1-O3	76.83(6)	O1 -Tb1- O6	139.36(6)	Er2-06	2.322(3)	Tm2-O6	2.314(3)
05-Eu1-O8	76.43(5)	O1 -Tb1- O8	119.54(6)	Er2-O2W	2.335(4)	Tm2-O2W	2.328(3)
O1-Eu1-O3	76.00(5)	O1 -Tb1- O5	141.95(6)	Er2-O5	2.400(4)	Tm2-O5	2.393(3)
O4-Eu1-06	73.72(5)	O1 -Tb1- O7	75.02(6)				
O2-Eu1-O3	73.23(5)	O1 -Tb1- O4	71.64(6)	O1 -Er1- O14	76.9(1)	O1 -Tm1- O10	129.50(9)
O1-Eu1-O1	73.00(5)	O2 -Tb1- O3	73.41(6)	O1 -Er1- O1W	144.7(1)	O1 -Tm1- O14	102.0(1)
O1-Eu1-O4	71.77(5)	O2 -Tb1- O4	106.25(6)	O1 -Er1- O7	78.8(1)	O1 -Tm1- O1W	131.9(1)
O1-Eu1-O4	71.64(5)	O2 -Tb1- O5	71.18(6)	O10 -Er1- O1	129.6(1)	O1 -Tm1- O2	74.4(1)
O5-Eu1-O2	71.49(5)	O2 -Tb1- O6	121.65(6)	O10 -Er1- O14	153.4(1)	O1 -Tm1- O7	143.13(9)
O1-Eu1-O3	70.70(5)	O2 -Tb1- O7	137.84(6)	O10 -Er1- O1W	79.1(1)	O10 -Tm1- O1W	79.0(1)
O4-Eu1-O5	70.49(5)	O2 -Tb1- O8	69.38(6)	O10 -Er1- O4	89.8(2)	O10 -Tm1- O2	78.39(9)
O6-Eu1-O5	53.12(5)	O3 -Tb1- O6	144.92(6)	O10 -Er1- O7	95.7(1)	O10 -Tm1- O3	88.44(9)
O1-Eu1-O2	50.98(5)	O3 -Tb1- O8	77.14(6)	O14 -Er1- O1W	75.3(1)	O10 -Tm1- O4	89.1(1)
O8-Eu1-O4	145.91(5)	O3 -Tb1- O4	136.23(6)	O14 -Er1- O2	130.0(1)	O10 -Tm1- O7	96.32(9)
O1-Eu1-O5	142.09(5)	O3 -Tb1- O7	75.18(6)	O14 -Er1- O3	78.4(1)	O14 -Tm1- O10	86.10(9)
O1-Eu1-O8	141.23(5)	O3 -Tb1- O5	141.14(6)	O14 -Er1- O4	101.7(1)	O14 -Tm1- O3	77.15(9)
O6-Eu1-O1	138.47(5)	O3 -Tb1- O6	144.92(6)	O14 -Er1- O7	86.3(1)	O14 -Tm1- O4	130.36(9)
O2-Eu1-O6	121.49(5)	O4 -Tb1- O5	70.34(6)	O1W -Er1- O2	143.5(1)	O1W -Tm1- O1	77.15(9)
O8-Eu1-O1	119.05(5)	O4 -Tb1- O6	73.80(6)	O1W -Er1- O3	78.7(1)	O1W -Tm1- O10	78.01(9)
O1-Eu1-O2	118.68(5)	O4 -Tb1- O7	115.88(6)	O1W -Er1- O4	132.0(1)	O1W -Tm1- O2	130.36(9)
O6-Eu1-01	116.48(5)	O5 -Tb1- O6	53.57(6)	O2 -Er1- O1	53.6(1)	O1W -Tm1- O3	131.9(1)
O2-Eu1-O4	106.65(5)	O5 -Tb1- O7	124.05(6)	O2 -Er1- O10	76.1(1)	O1W -Tm1- O4	143.13(9)
		O5 -Tb1- O8	75.89(6)	O2 -Er1- O7	78.1(1)	O1W -Tm1- O7	78.87(9)
		O6 -Tb1- O7	74.11(6)	O3 -Er1- O1	116.3(1)	O2 -Tm1- O10	75.90(9)
		O6 -Tb1- O8	79.70(6)	O3 -Er1- O10	89.4(1)	O2 -Tm1- O14	116.65(9)
		O6 -Tb1- O8	79.70(6)	O3 -Er1- O2	127.0(1)	O2 -Tm1- O1W	78.87(9)
		O7 -Tb1- O8	76.78(6)	O3 -Er1- O4	54.5(1)	O2 -Tm1- O4	53.78(9)
				O4 -Er1- O2	74.5(1)	O3 -Tm1- O1	54.6(1)
				O7 -Er1- O1W	78.1(1)	O3 -Tm1- O7	79.05(9)
				O7 -Er1- O3	154.8(1)	O4 -Tm1- O1	53.78(9)
				O7 -Er1- O4	149.8(1)	O4 -Tm1- O3	126.83(9)
				O11 -Er2- O13	113.2(1)	O4 -Tm1- O7	78.39(9)
				O11 -Er2- O2W	86.7(1)	O7 -Tm1- O1	150.0(1)
				O11 -Er2- O5	79.5(1)	O7 -Tm1- O10	76.6(1)
				O11 -Er2- O8	160.5(1)	O7 -Tm1- O14	54.6(1)
				O13 -Er2- O2W	146.4(1)	O7 -Tm1- O1W	78.01(9)
				O13 -Er2- O5	129.9(1)	O7 -Tm1- O2	75.5(1)
				O2W -Er2- O6	134.0(1)	O11 -Tm2- O2W	160.7(1)
				O2W -Er2- O8	83.5(1)	O11 -Tm2- O5	83.4(1)
				O2W -Er2- O9	80.1(1)	O11 -Tm2- O5	78.40(9)

O5 -Er2- O2W	78.7(1)	O11 -Tm2- O9	112.8(1)
O5 -Er2- O6	55.4(1)	O13 -Tm2- O11	86.3(1)
O6 -Er2- O11	82.3(1)	O13 -Tm2- O11	160.7(1)
O6 -Er2- O13	77.6(1)	O13 -Tm2- O2W	83.9(1)
O6 -Er2- O8	92.5(1)	O13 -Tm2- O5	77.0(1)
O8 -Er2- O11	160.5(1)	O13 -Tm2- O6	83.9(1)
O8 -Er2- O13	83.7(1)	O13 -Tm2- O8	130.0(1)
O8 -Er2- O5	82.1(1)	O2W -Tm2- O11	76.6(1)
O9 -Er2- O11	76.2(1)	O2W -Tm2- O13	83.9(1)
O9 -Er2- O13	78.9(1)	O2W -Tm2- O5	134.0(1)
O9 -Er2- O5	148.4(1)	O2W -Tm2- O6	139.3(1)
O9 -Er2- O6	138.4(1)	O5 -Tm2- O13	82.28(9)
O9 -Er2- O8	118.3(1)	O5 -Tm2- O2W	148.56(9)
		O5 -Tm2- O6	79.53(9)
		O5 -Tm2- O9	139.3(1)
		O6 -Tm2- O11	78.8(1)
		O6 -Tm2- O11	134.0(1)
		O6 -Tm2- O2W	82.28(9)
		O6 -Tm2- O5	55.69(9)
		O6 -Tm2- O8	86.3(1)
		O6 -Tm2- O9	77.0(1)
		O8 -Tm2- O11	79.53(9)
		O8 -Tm2- O2W	78.40(9)
		O8 -Tm2- O5	83.4(1)
		O8 -Tm2- O9	83.9(1)
		O9 -Tm2- O13	79.9(1)
		O9 -Tm2- O13	117.70(9)
		O9 -Tm2- O2W	146.9(1)
		O9 -Tm2- O5	130.0(1)
		O9 -Tm2- O8	148.56(9)

(**1**) [1]+X,-1+Y,+Z; [2]+X,1+Y,+Z; [3]-X,1-Y,2-Z; [4]1-X,-Y,1-Z; [5]-X,1-Y,1-Z; [6]1-X,-Y,2-Z; (**2**)[1]2-X,1-Y,1-Z; [2]1-X,-Y,1-Z; [3]1-X,2-Y,-Z; [4]-X,-Y,-Z; (**3**) [1]+X,-1+Y,+Z; [2]+X,1+Y,+Z; [3]-X,1-Y,2-Z; [4]1-X,-Y,1-Z; [5]-X,1-Y,1-Z; [6]1-X,-Y,2-Z; (**4**) [1]+X,-1+Y,+Z; [2]+X,1+Y,+Z; [3]-X,1-Y,2-Z; [4]1-X,-Y,1-Z; [5]-X,1-Y,1-Z; [6]1-X,-Y,2-Z

Table S2. Photoluminescence lifetimes of **2-4** and H_2ADC.

Sample ID	**τ1 (ns)**	**τ2 (ns)**	**Avg τ₀ (ns)**	**α_1**	**α_2**	**A**	**χ^2**
TbADC (**2**)	0.20	0.46	0.31	0.57	0.43	0.89	1.023
ErADC (**3**)	0.04	0.32	0.04	1.00	0.00	0.017	1.55
TmADC **(4)**	0.05	0.32	0.05	0.99	0.01	2.46	1.39
H_2ADC	4.91	16.18	9.59	0.58	0.42	2.192	1.061

Decay curves were fitted by the equation, $I(t) = \alpha_1 \exp\left(-t/\tau_1\right) + \alpha_2 \exp\left(-t/\tau_2\right)$, where *I* is the intensity, α is the pre-exponential factor, *t* is the time, τ_1 and τ_2 are lifetimes. The excitation wavelength was 372 nm.