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Electronic Supporting Information

Role of structure and metal ion in the fluorescence sensing of nitro compounds for a series of lanthanide(III) 9, 10-anthracene dicarboxylate coordination polymers

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Table S1: Elemental analysis of **1-28**. With the exception of compounds 9-14 which was synthesized with DMSO, the compounds made with DMF and DMA consistently returned with lower carbon contents despite repeated attempts. This could be the trapping of water molecules during hydrolysis of these solvents during the solvothermal synthesis. Since lanthanides are hygroscopic, it might hold onto these water molecules better. Hence the formulas are fixed with water molecules.

	Experimental (%) Theo		hearetical (%)		Theoretical (after adjustment with water)									
MOF	Ехре	ппспта	1 (70)	Theo	neucai	(70)	(%)							
	С	Н	Ν	C	H	Ν	С	Н	Ν					
							Actual	Actual formula:						
1	51.04	3.99	5.14	53.6	2.5	4.96	[La ₂ (ADC) ₃ (DN	IF) ₄]·DMF·	3H ₂ O					
							51.62	2.82	4.78					
							Actual	formula:						
2	50.19	4.11	5.15	53.51	2.49	2.49	2.49 4	2.49	4.95	$[Ce_2(ADC)_3(DN)]$	IF) ₄]·DMF·:	5H ₂ O		
							50.3	3.02	4.66					
							Actual	formula:						
3	50.04	4.10	5.03	53.45	53.45	53.45	53.45 2.49		3.45 2.49	2.49	4.95	[Pr ₂ (ADC) ₃ (DM	[F) ₄]·DMF·5	5H ₂ O
							50.25	3.01	4.65					
					53.19 2.48 4.92		Actual	formula:	1					
4	49.93	4.12	5.17	53.19			[Nd ₂ (ADC) ₃ (DN	IF)4]·DMF·	5H ₂ O					
							50.03	3	4.63					
							Actual	formula:						
5	46.38	4.03	4.80	52.74	2.46 4	2.46	4.88	[Sm ₂ (ADC) ₃ (DM	[F) ₄]·DMF·1	0H ₂ O				
							46.86	3.43	4.34					
							Actual	formula:	1					
6	49.32	4.31	4.88	52.62	2.45	4.87	[Eu ₂ (ADC) ₃ (DN	IF) ₄]·DMF·:	5H ₂ O					
							49.52	2.97	4.58					
							Actual	formula:						
7	49.8	4.06	4.98	52.24	2.44	4.83	[Gd ₂ (ADC) ₃ (DN	IF) ₄]·DMF·:	5H ₂ O					
							49.18	2.95	4.55					
Q	10 51	1 10	1 01	52 12	2 12	1 87	Actual	formula:						
0	47.04	4.10	4.74	34.14	2.43	7.02	[Tb ₂ (ADC) ₃ (DN	IF) ₄]·DMF·:	5H ₂ O					

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							49.07	2.94	4.54
							Actual	formula:	
9	46.17	3.82	-	46.13	2.32	-	[Dy ₂ (ADC))3(DMSO)6]	
							-	-	-
							Actual	formula:	
10	45.88	4.23	-	45.98	2.32	-	[Ho ₂ (ADC))3(DMSO)6]	
							-	-	-
							Actual	formula:	
11	45.85	3.89	-	45.85	2.31	-	[Er ₂ (ADC))3(DMSO)6]	
							-	-	-
							Actual	formula:	
12	45.60	3.92	-	45.75	2.3	-	[Tm ₂ (ADC)3(DMSO)6]	
							-	-	-
							Actual	formula:	
13	44.93	4.00	-	45.51	2.29	-	[Yb ₂ (ADC) ₃ (I	OMSO)₀]·2H	2 0
							44.5	2.49	-
							Actual	formula:	
14	45.94	4.06	-	45.4	2.29	-	[Lu ₂ (ADC))3(DMSO)6]	
							-	-	-
							Actual	formula:	
15	53.27	4.84	5.46	55.11	3.47	5.36	[La ₂ (ADC) ₃ (]	DMA) ₆]·3H ₂	O
							53.28	3.73	5.18
							Actual	formula:	
16	50.62	4.83	5.08	55.03	3.46	5.35	$Ce_2(ADC)_3(I)$	DMA) ₃ ·8H ₂	C
							50.41	4.11	4.9
							Actual	formula:	
17	52.55	5.16	5.09	54.97	3.46	5.34	[Pr ₂ (ADC) ₃ (I	DMA) ₆]·5H ₂	0
							52	3.88	5.05
							Actual	formula:	
18	49.65	4.79	4.96	54.74	3.45	5.32	[Nd ₂ (ADC) ₃ (I	OMA) ₆]∙10H	2 0
							49.14	4.24	4.78
19	49.44	4.64	5.00	54.32	3.42	5.28	Actual	formula:	

							[Sm ₂ (ADC) ₃ (DMA) ₆]·9H	20
							49.3	4.14	4.79
							Actual	formula:	1
20	51.41	4.55	5.18	54.21	3.41	5.27	[Eu ₂ (ADC	C)3(DMA)6]	
							51.31	3.83	4.99
							Actual	formula:	1
21	49.19	4.64	5.00	53.86	3.39	5.23	[Gd ₂ (ADC) ₃ (DMA) ₆]·8H	2 0
							49.42	4.03	4.8
							Actual	formula:	
22	50.85	4.55	5.48	53.74	3.38	5.22	[Tb ₂ (ADC) ₃ (DMA) ₆]·5H	2 O
							50.89	3.8	4.95
							Actual	formula:	1
23	50.09	4.67	5.31	53.51	3.37	5.2	[Dy ₂ (ADC) ₃ (J	DMA) ₆]·6H	2 O
							50.15	3.86	4.87
							Actual	formula:	1
24	52.71	4.68	5.36	53.35	3.36	5.18	[H0 ₂ (ADC) ₃ ((DMA) ₆]·H ₂	0
							52.76	3.44	5.13
							Actual	formula:	1
25	52.46	4.61	5.29	53.19	3.35	5.17	[Er ₂ (ADC) ₃ (DMA) ₆]·H ₂	0
							52.61	3.43	5.11
							Actual	formula:	1
26	52.11	4.35	5.12	53.08	3.34	5.16	[Tm ₂ (ADC) ₃	(DMA) ₆]·H ₂	$_{2}\mathbf{O}$
							52.5	3.43	5.1
							Actual	formula:	1
27	52.25	4.43	5.08	52.82	3.32	5.13	[Yb ₂ (ADC) ₃ ((DMA) ₆]·H ₂	0
							52.24	3.41	5.08
							Actual	formula:	1
28	50.36	4.40	4.60	52.69	3.32	5.12	[Lu ₂ (ADC) ₃ (DMA) ₆]·4H	2 O
							50.48	3.65	4.91

	10	11
Empirical formula	C ₁₀ H ₁₀ Er _{0.33} O ₃ S	C ₁₀ H ₁₀ Ho _{0.33} O ₃ S
Formula weight (g/mol)	265.99	265.22
Temperature (K)	100(2)	100(2)
Crystal system	Trigonal	Trigonal
Space group	<i>R</i> -3	<i>R</i> -3
Unit cell dimensions		
a (Å)	15.1961(18)	15.229(2)
b (Å)	15.1961(18)	15.229(2)
c (Å)	23.961(3)	23.906(4)
a (°)	90	90
β (°)	90	90
γ (°)	120	120
Volume (Å ³)	4791.8(13)	4801.3(16)
Z	18	18
Calculated density (g/cm ³)	1.659	1.651
Goodness-of-fit on F ²	1.098	1.097
Final R indices $[I > 2\sigma(I)]$	$R_1 = 0.0439, \ _wR_2 =$	R1 = 0.0574,
	0.1186	wR2 = 0.1321

Table S2: Crystal parameters of 10-11.



Figure S1: (a) Building unit, (b) packing, (c) topological representation of 1-8.



Figure S2: (a) Building unit, (b) packing, (c) topological representation of 9-14.



Figure S3: (a) Building unit, (b) packing, (c) topological representation of 15-28.



Figure S4: Powder XRD diffractograms of **1-8.** A representative simulated pattern from crystal data of **4**¹ (previous reported) was used to match the PXRD of the other compounds.



Figure S5: Powder XRD diffractograms of **9-14**. A representative simulated pattern from crystal data of **10** was used to match the PXRD of the other compounds.



Figure S6: Powder XRD diffractograms of **15-28**. A representative simulated pattern from crystal data of **18**¹ (previous reported) was used to match the PXRD of the other compounds.



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Figure S7: TGA overlay of compounds a) 1-8, b) 9-14, c) 15-28.











Figure S8: Solid State photoluminescence of 1-28.



PL quenching experiments

An example of the quenching graph. The same colours representing the amount of analyte added are used for all the quenching curves. The legends are hence not shown for clarity.



4-Nitroaniline	and a standard a stand	
2,4- Dinitrophenylhydrazin e		

Figure S9: PL quenching of 6-8 with various analytes.



Figure S10: PL quenching of 20-22 with various analytes.

Analyte	Eu exfoliated (6)	Gd exfoliated (7)	Tb exfoliated (8)
4-Nitrophenyl phenyl ether			
4 Nitrobenzyl chloride		Research for the second	
1-Chloro-4- nitrobenzene	Transformer Transf		and a state of the
1-lodo-3-nitrobenzene			a source for the sour
2,4 Dinitrophenol	100000 0 00000 0 00000 0 00000 0 000000 0 0000000 0 00000000	Horizon Harrison Harr	Not of the second secon
2,5 Dinitrophenol	Transformer Transf		
2-nitrophenol	tomore of other states of the	HERE AND	and a state of the
2,4 Dinitroaniline			Anomaly and a state of the stat
4-Nitroaniline	internet int	and a second sec	Transa anno ta ta t
2,4- Dinitrophenylhydrazin e	HIGHER BOTTON BO	Without have been and the set of	

Figure S11: PL quenching of exfoliated 6-8 with various analytes.



Figure S12: K_{sv} values of the CP when 2,4-dinitrophenylhydrazine, 4-nitroaniline, 2,4-dinitroaniline, 2-nitrophenol, 2,5-dinitrophenol and 2,4-dinitrophenol used for the sensing. (a) K_{sv} values of CP 6, 20 and exfoliated 6; (b) K_{sv} values of CP 7, 21 and exfoliated 7; (c) K_{sv} values of CP 8, 22 and exfoliated 8.

Stern-Volmer plot

Analyte	Eu (6)	Gd (7)	Tb (8)
4-Nitrophenyl phenyl ether	R2=0.89 Slope = 1.37	R ² =0.97 Slope = 2.092	R2=0.99 Slope = 3.442
4 Nitrobenzyl chloride	$\frac{R^2=0.43}{Slope} = 0.127$	$R^{2} = 0.99$ Slope = 0.357 $\frac{1}{50}$ 0.0 0.5 1.0 1.5 2.0 2.5 mM	$\frac{1}{5}$ $R^{2}=0.99$ Slope = 0.546 $R^{2}=0.99$ Slope = 0.253 $0.0 0.5 1.0 1.5 2.0 2.5$ mM
1-Chloro-4-			
nitrobenzene	R ² =0.92 Slope = 0.436	Ferrit R2=0.96 Slope = 0.378 0.0 0.5 10 15 20 2.5 mM	R ² =0.99 Slope = 0.453
1-lodo-3-nitrobenzene			
	R ² =0.98 Slope = 0.185	R ² =0.99 Slope = 0.472	R ² =0.99 Slope = 0.536
2,4 Dinitrophenol	7	8-	7-
	$R^{2=0.99}$ Slope = 1.824 $r_{0.0}^{4}$ $r_{0.5}^{4}$ $r_{0.0}^{4}$ $r_{0.5}$ $r_{0.$	$R^2=0.99$ Slope = 4.106 10^{-1} mM	$R^{2}=0.99$ Slope = 3.737 mM
2,5 Dinitrophenol	13-]	· · · · · · · · · · · · · · · · · · ·	4
	$R^{2}=0.99$ Slope = 6.623 $R^{2}=0.99$ M	$R^{2}=0.99$ $Slope = 15.038$ MM	R ² =0.99 Slope = 9.585 00 0.5 1.0 1.5 2.0 2.5 mM
2-nitrophenol	$R^2=0.99$ Slope = 7.648 $B_{0,0}^{40}$ Slope = 7.648 $B_{0,0}^{40}$ $B_{0,0}^{40}$ $B_{1,0}^{4$	$rac{1}{5}$	$\sum_{i=0}^{50} \frac{R^2=0.99}{Slope} = 13.082$



Figure S13: Stern-Volmer plot of 6-8 with various analytes.

	Eu (20)	Gd (21)	Tb (22)
Analyte			
4-Nitrophenyl phenyl ether	$\mathbf{F}_{0,0}^{7} = 0.98$ Slope = 1.434 Slope = 1.434 M	R ² =0.97 Slope = 1.343	R ² =0.98 Slope = 1.08
4 Nitrobenzyl chloride	R ² =0.99 Slope = 2.016 mM	$R^{2=0.99}$ Slope = 0.177 $\frac{1}{0.0}$ $\frac{1}{0.5}$ $\frac{1}{1.0}$ $\frac{1}{1.5}$ $\frac{2}{2.0}$ $\frac{2}{2.5}$ mM	$\frac{R^{2}=0.99}{Slope} = 0.173$
1-Chloro-4-			
nitrobenzene	$R^{2}=0.99$ Slope = 0.691 $\frac{1}{0.0}$ $\frac{1}{0.5}$ $\frac{1}{1.0}$ $\frac{1}{1.5}$ $\frac{2}{2.0}$ $\frac{2}{2.5}$ mM	R2=0.99 Slope = 0.198	R ² =0.97 Slope = 0.215 0.0 0.5 1.0 1.5 2.0 2.5 mM
1-lodo-3-nitrobenzene	$\sum_{i=1}^{1} \frac{1}{10000000000000000000000000000000000$	R ² =0.99 Slope = 0.248 	R ² =0.98 Slope = 0.25



Figure S14: Stern-Volmer plot of 20-22 with various analytes.

Analyte	Eu exfoliated (6)	Gd exfoliated (7)	Tb exfoliated (8)
4-Nitrophenyl phenyl ether	$R^{2}=0.99$ Slope = 0.952	R ² =0.99 Slope = 0.557	$\mathbf{R}^{2}=0.98$ $\mathbf{R}^{2}=0.97$ Slope = 0.33 Slope = 0.665 $\mathbf{R}^{2}=0.97$ M
4 Nitrobenzyl chloride	Slope = 0 Slope = 0	R ² =0.99 Slope = 0.113	$F_{0,0}^{2} = 0.99$ Slope = 0.116 0.0 0.5 100 15 2.0 2.5



Figure S15: Stern-Volmer plot of exfoliated 6-8 with various analytes.

Metal ion	Compound 1-14	Compound 15-28
La	source recommendations recomme	Provide the second seco
Ce	70000 g conserved sources s conserved s	and a single sin
Pr	assesse asses assesse assesse assesse assesse asses as asses as asses asses as asses as asses asses asses asses asses asses as asses as asses asses as asses as asses as asses as as as asses as as as as as as as as asses as as as as as as as as as as as as as	
Nd	Research and the second	
Sm	Values 0 0 0 0 0 0 0 0 0 0 0 0 0	With the second
Dy	Transformer Transf	transformed by the second seco
Но	success economic second	teorore teo
Er	USBROAD TO THE TAXABLE STATES TO THE TAXABLE	Teamon te
Tm	Kusses But manual roome a da	Valence Building assesse abilding build
Yb	700000 g 40000 g 4000 g	Laster Comme Comme Joseph Jose
Lu	ticasson transme tr	Another and a set of the set of t

Figure S16: PL quenching of 1-28 with various Brady's reagent.





Figure S17: Stern-Volmer plot of 1-28 with various Brady's reagent.





Figure S18: PL emission of the analytes.



Figure S19: Stoke's shift of the CPs with various analytes added. Values of the CP when 2,4-dinitrophenylhydrazine, 4-nitroaniline, 2,4-dinitroaniline, 2-nitrophenol, 2,5-dinitrophenol and 2,4-dinitrophenol used for the sensing.