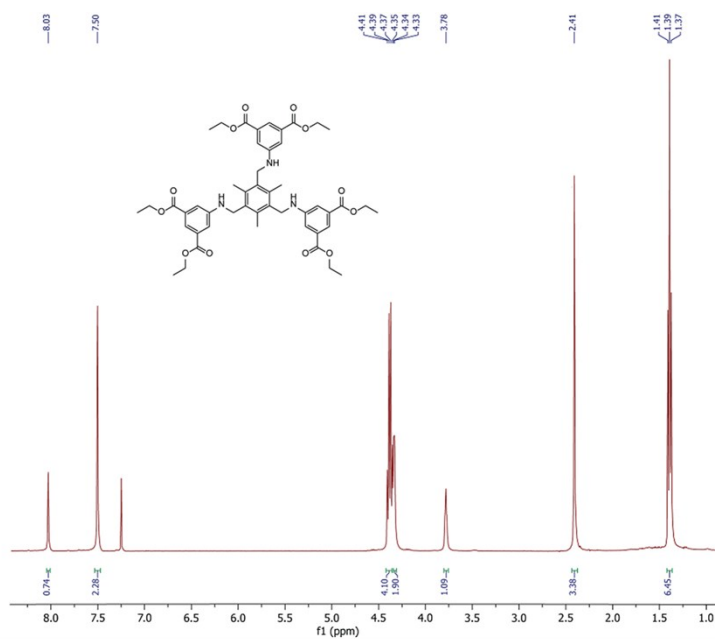
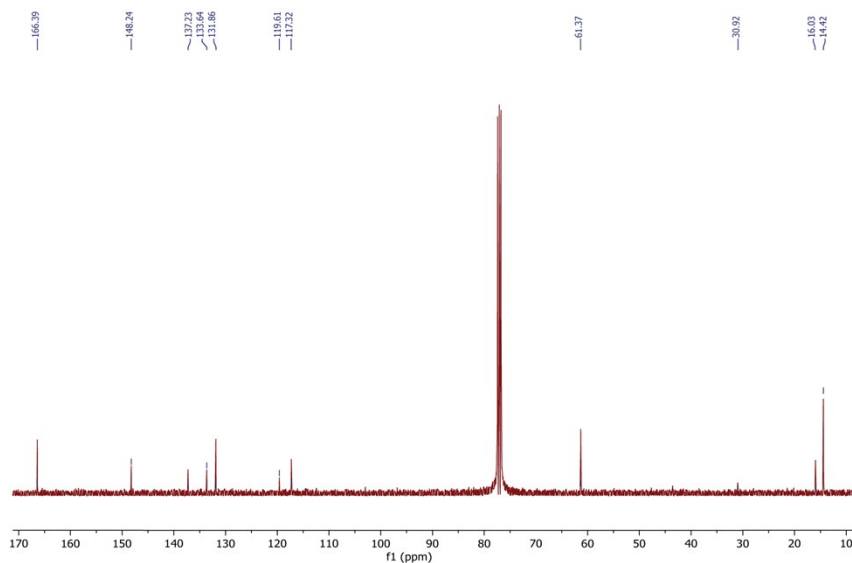


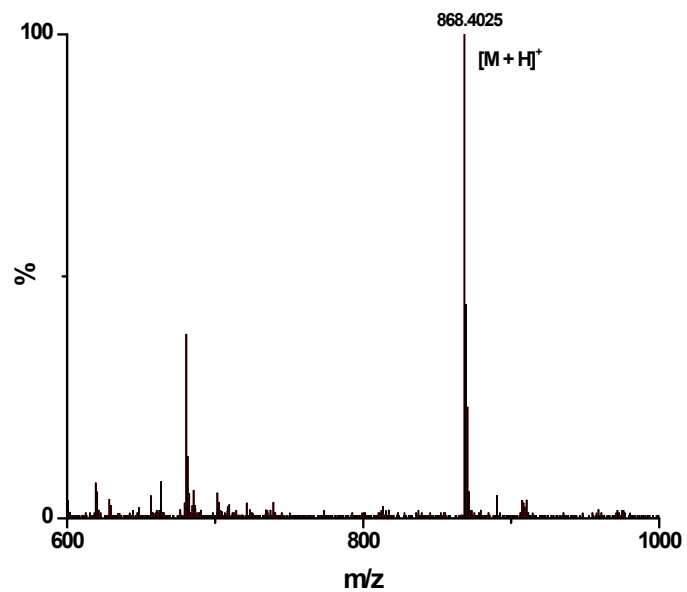
## Supporting Information



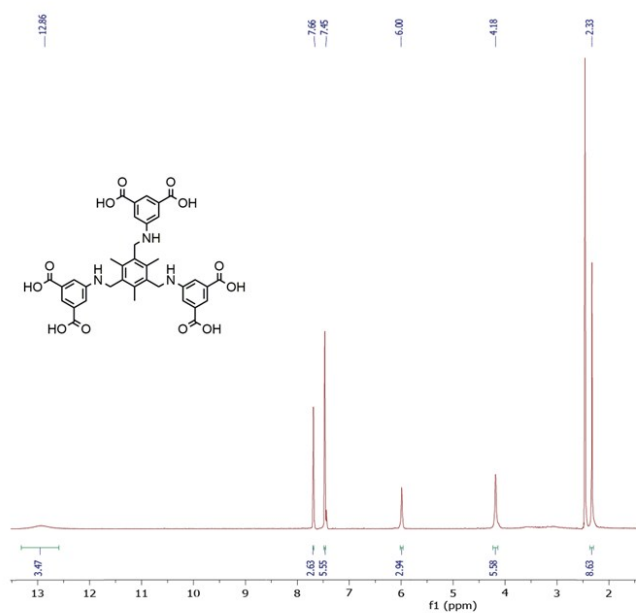
**Fig S1.** <sup>1</sup>H-NMR spectrum of hexaethyl 5,5',5''-(2,4,6-trimethyl-1,3,5-phenylene)tris(methylene)tris(azanediy) triisophthalate.



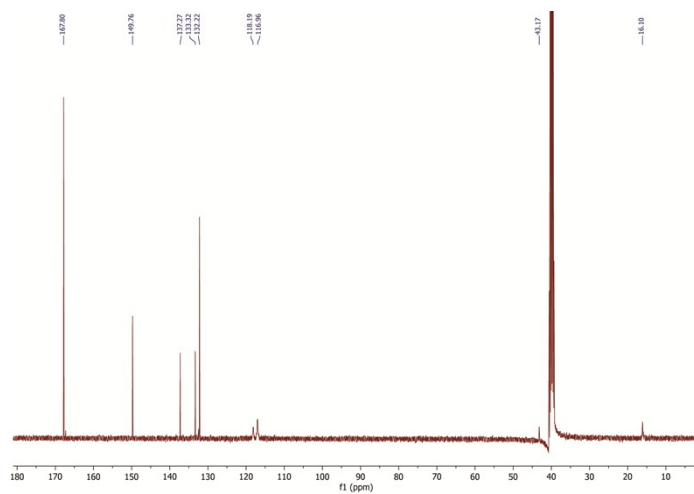
**Fig S2.** <sup>13</sup>C-NMR spectrum of hexaethyl 5,5',5''-(2,4,6-trimethyl-1,3,5-phenylene)tris(methylene)tris(azanediy) triisophthalate.



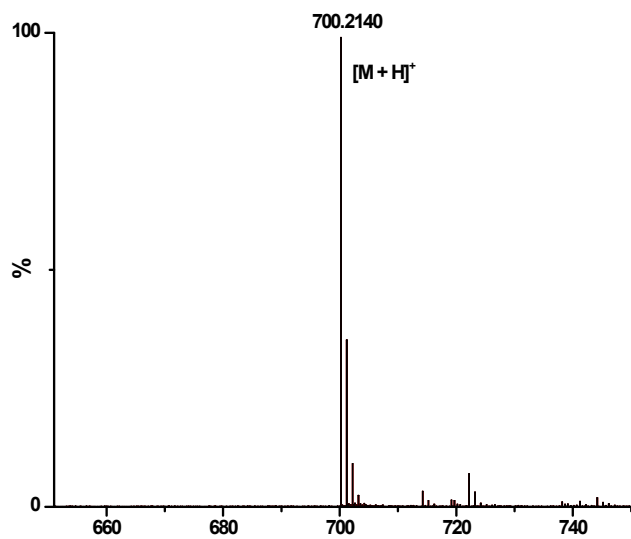
**Fig S3.** ESI-MS of hexaethyl 5,5',5''-(2,4,6-trimethyl-1,3,5-phenylene)tris(methylene)tris(azanediy) triisophthalate.



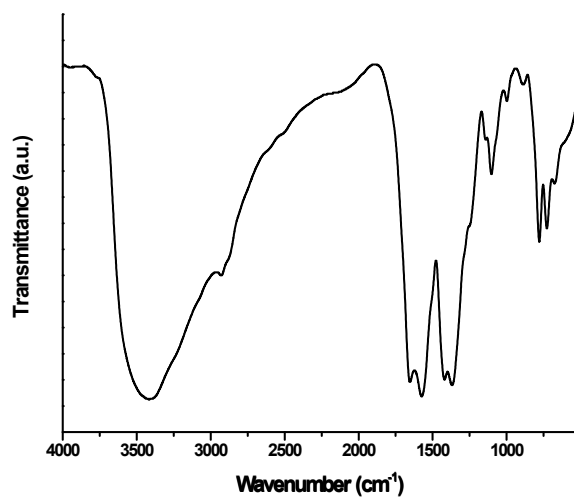
**Fig S4.**  $^1\text{H-NMR}$  spectrum of  $\text{H}_6\text{L}$  ligand.



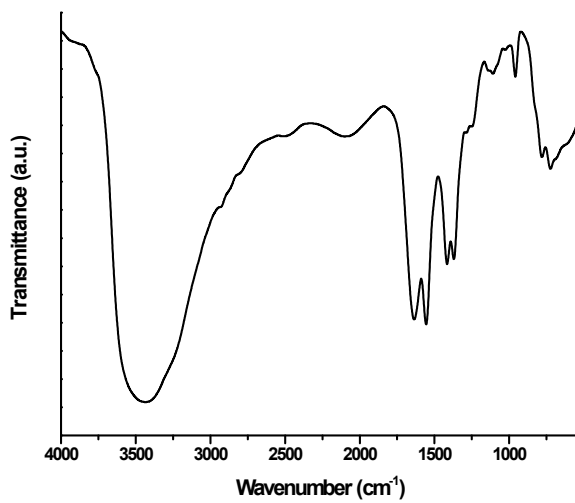
**Fig S5.** <sup>13</sup>C-NMR spectrum of H<sub>6</sub>L ligand.



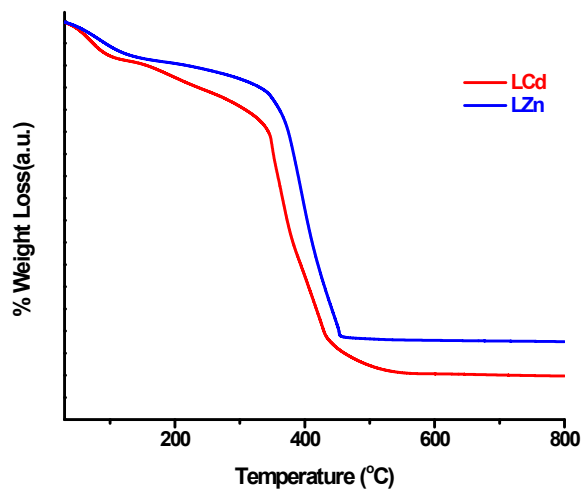
**Fig S6.** ESI-MS of H<sub>6</sub>L ligand.



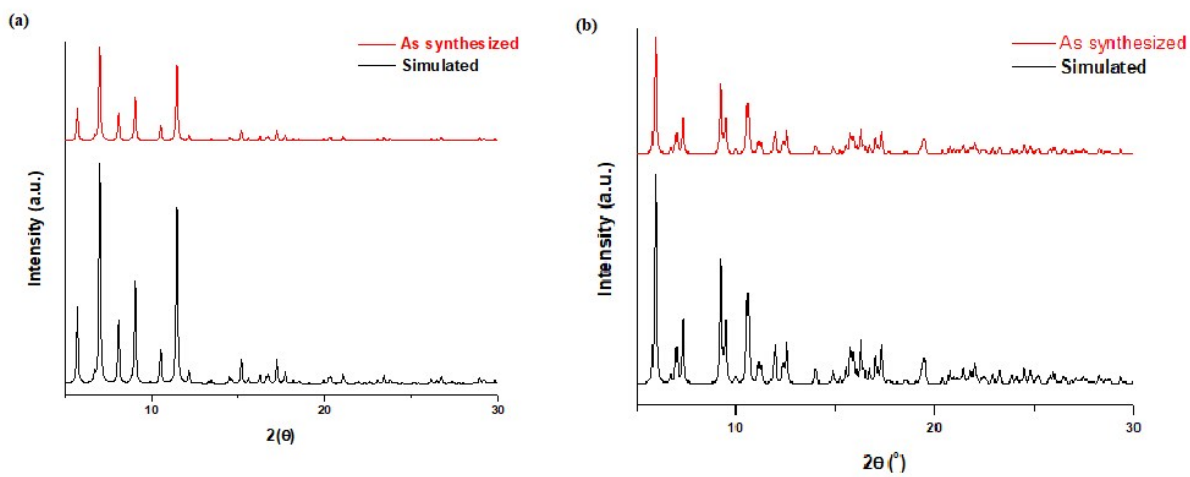
**Fig S7.** FT-IR spectrum of LZn.



**Fig S8.** FT-IR spectrum of LCd.



**Fig S9.** Thermogravimetric analysis curve of LZn and LCd.



**Fig S10.** Powder X-ray diffraction patterns of LZn (a) and LCd (b): as synthesized (red) and simulated (black).

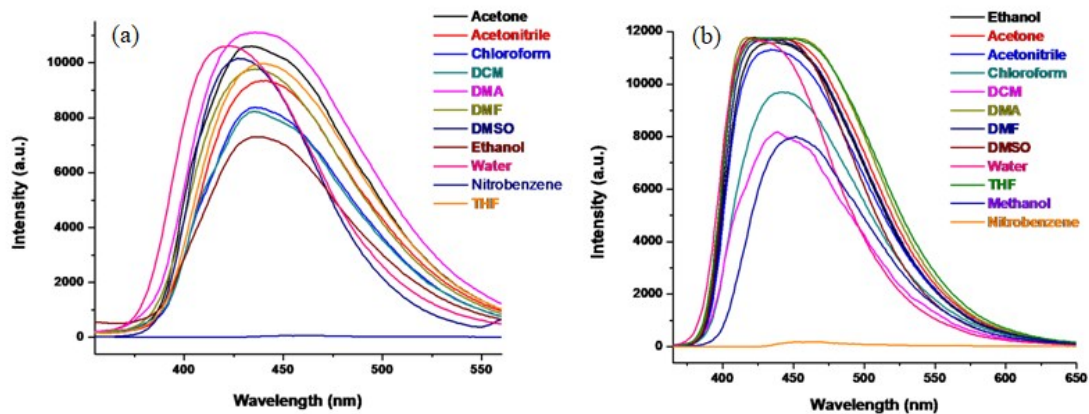


Fig S11. Emission spectra of LCd (a) and LZn (b) MOFs in different solvents.

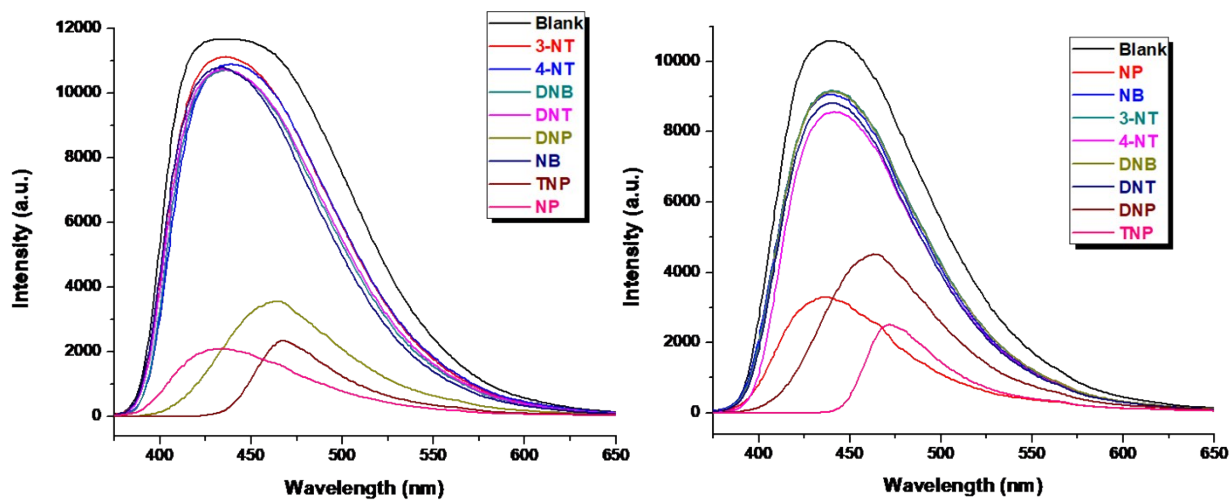


Fig S12. Emission spectra of LZn (a) and LCd (b) in different nitroaromatic compounds.

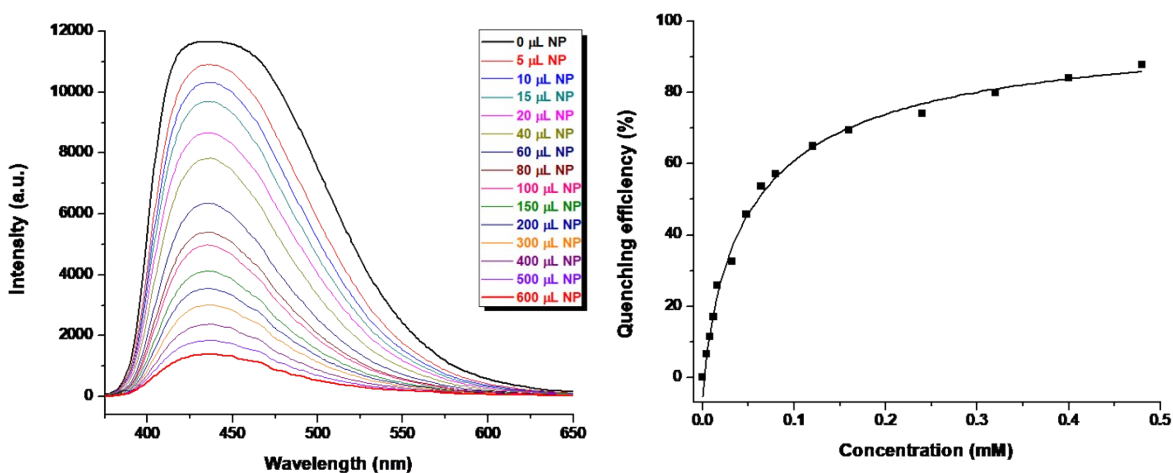


Fig S13. Fluorescence titration of the dispersed LZn in EtOH by gradual addition of 2 mM solution of nitrophenol (NP) in EtOH and the corresponding quenching efficiency.

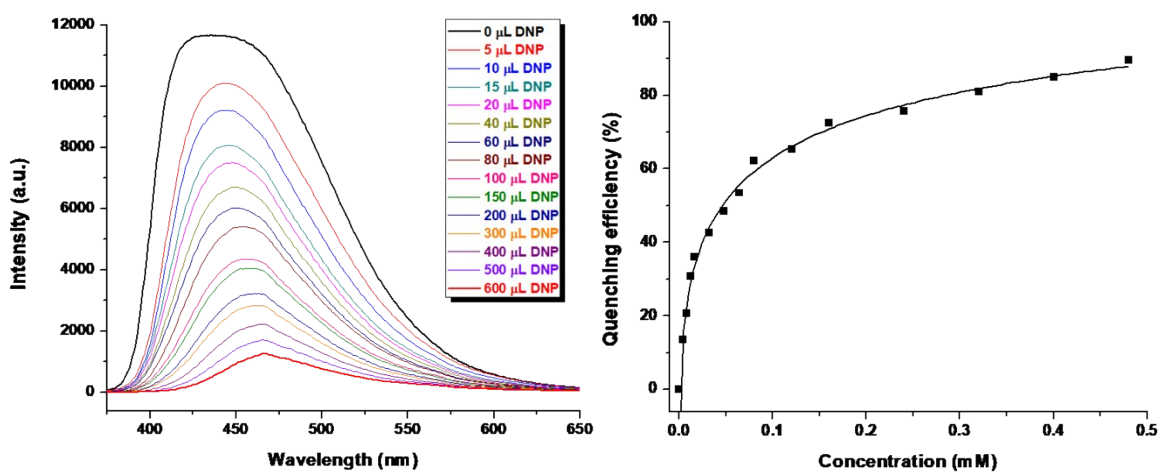
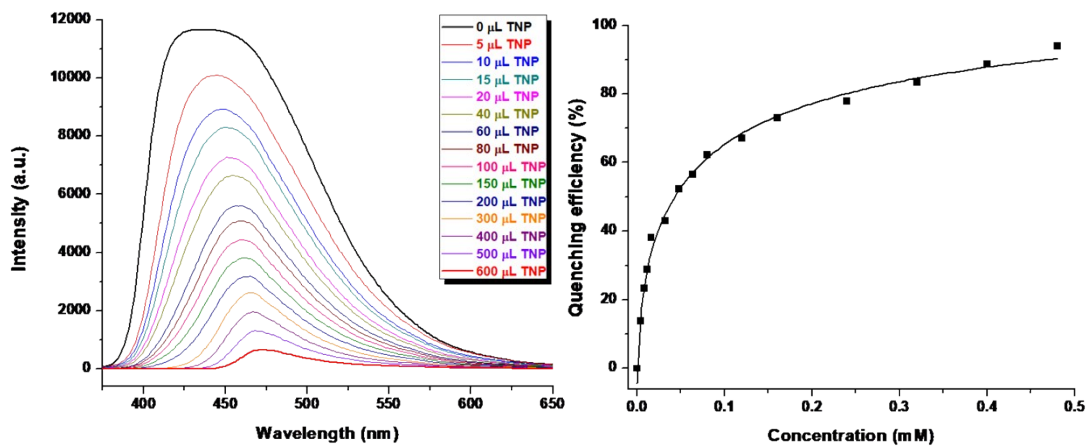
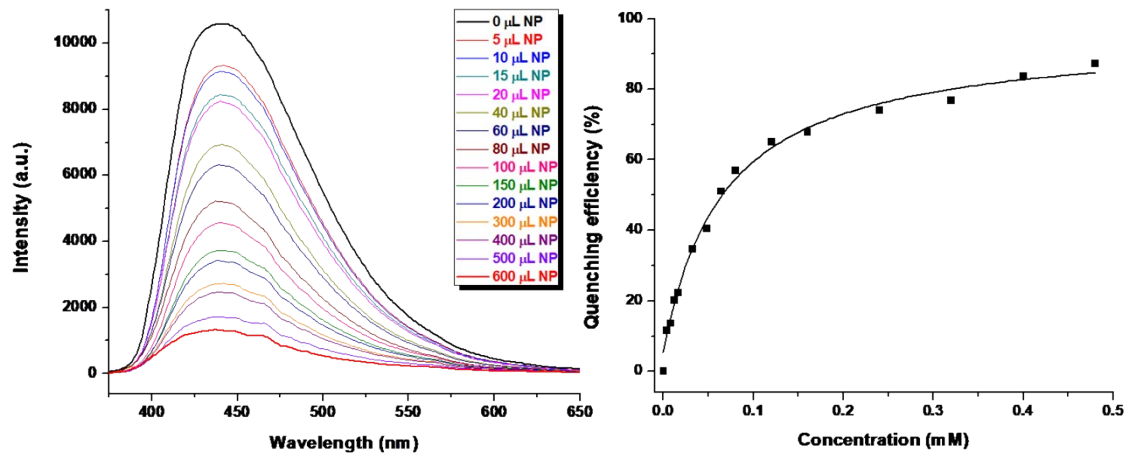


Fig S14. Fluorescence titration of the dispersed LZn in EtOH by gradual addition of 2 mM solution of dinitrophenol (DNP) in EtOH and the corresponding quenching efficiency.

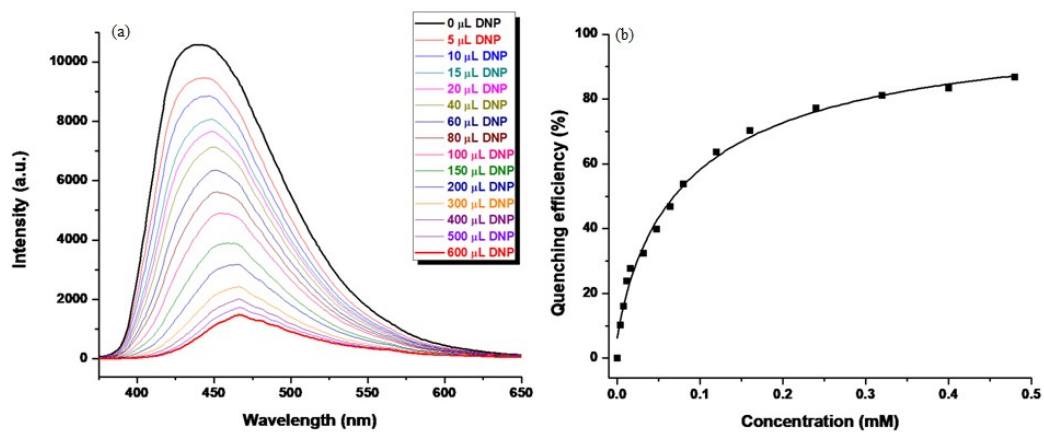


**Fig S15.** Fluorescence titration of the dispersed LZn in EtOH by gradual addition of 2 mM solution of trinitrophenol (TNP) in EtOH and the corresponding quenching efficiency.

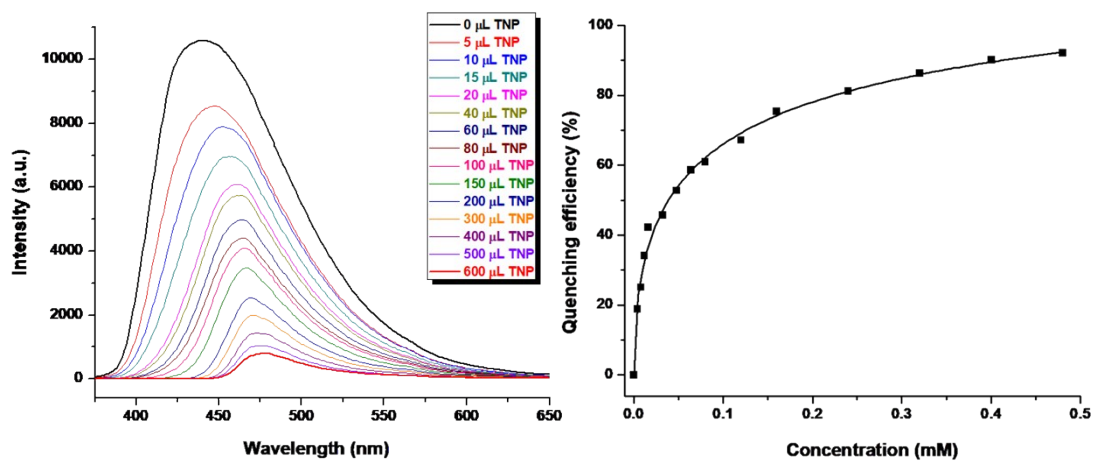


**Fig S16.** Fluorescence titration of the dispersed LCd in EtOH by gradual addition of 2 mM solution of nitrophenol (NP) in EtOH and the corresponding quenching efficiency.

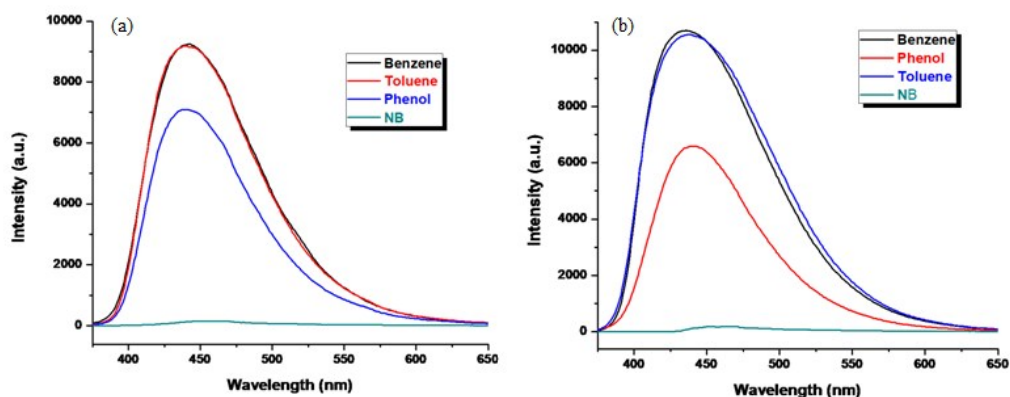




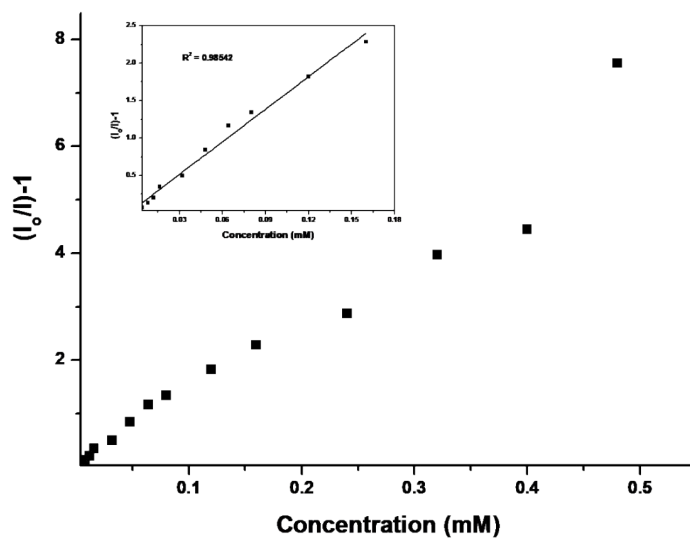
**Fig S17.** Fluorescence titration of the dispersed LCD in EtOH by gradual addition of 2 mM solution of dinitrophenol (DNP) in EtOH and the corresponding quenching efficiency.



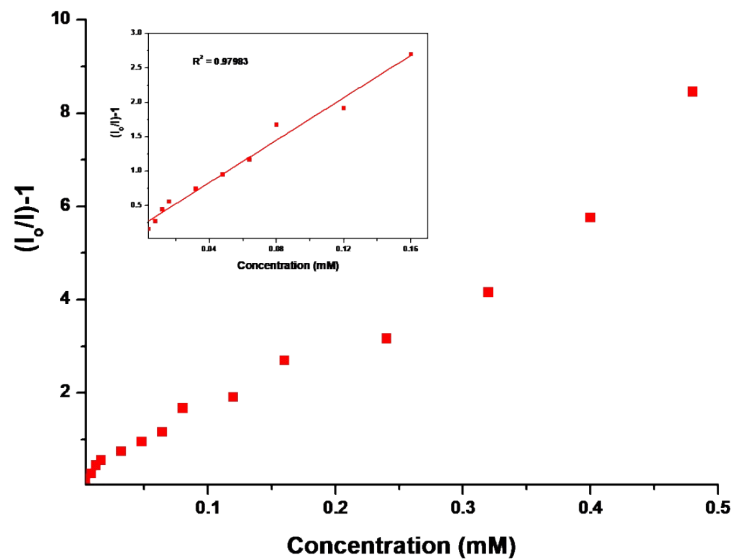
**Fig S18.** Fluorescence titration of the dispersed LCD in EtOH by gradual addition of 2 mM solution of trinitrophenol (TNP) in EtOH and the corresponding quenching efficiency.



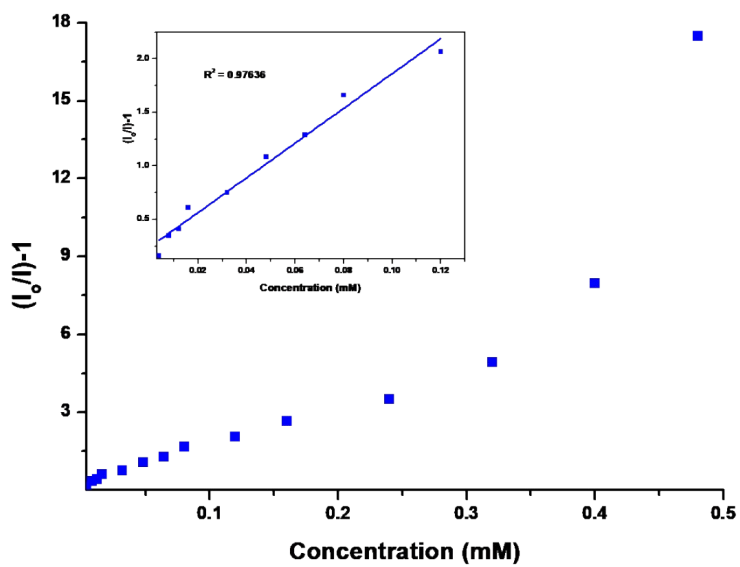
**Fig S19.** Emission spectra of LCd (a) and LZn (b) in different solvents.



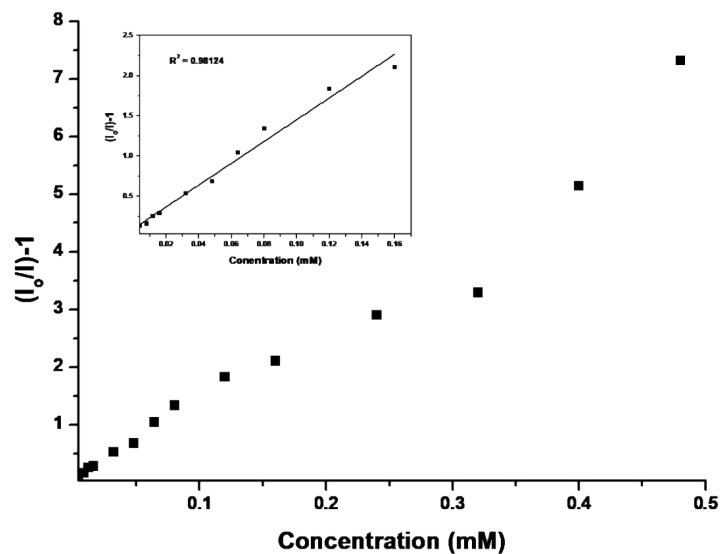
**Fig S20.** Stern–Volmer plot for the fluorescence quenching of LZn upon addition of NP. Inset: The Stern–Volmer plot at low NP concentrations.



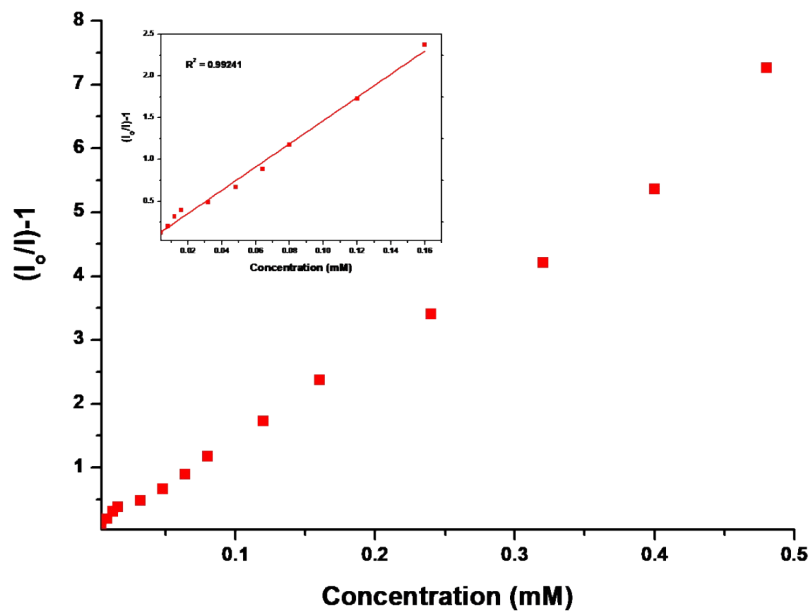
**Fig S21.** Stern–Volmer plot for the fluorescence quenching of LZn upon addition of DNP. Inset: The Stern–Volmer plot at low DNP concentrations.



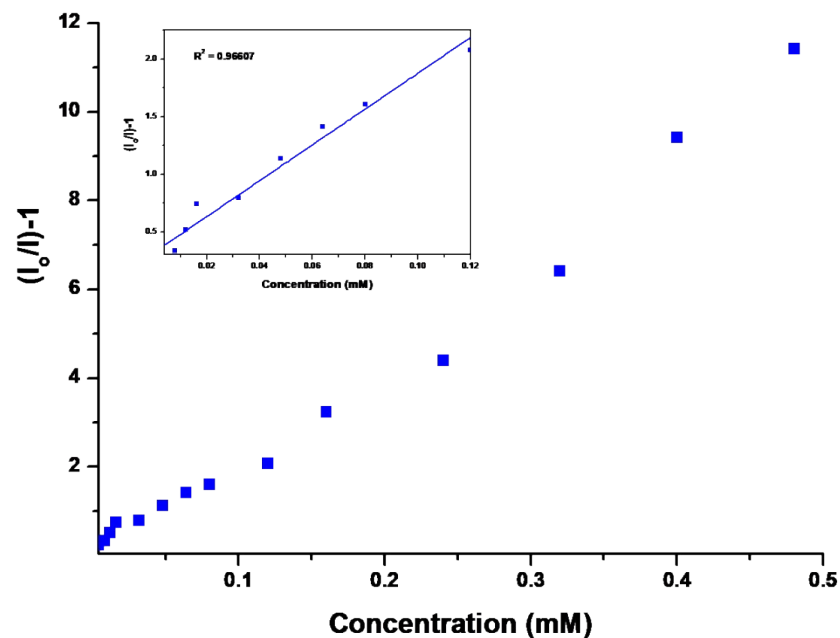
**Fig S22.** Stern–Volmer plot for the fluorescence quenching of LZn upon addition of TNP. Inset: The Stern–Volmer plot at low TNP concentrations.



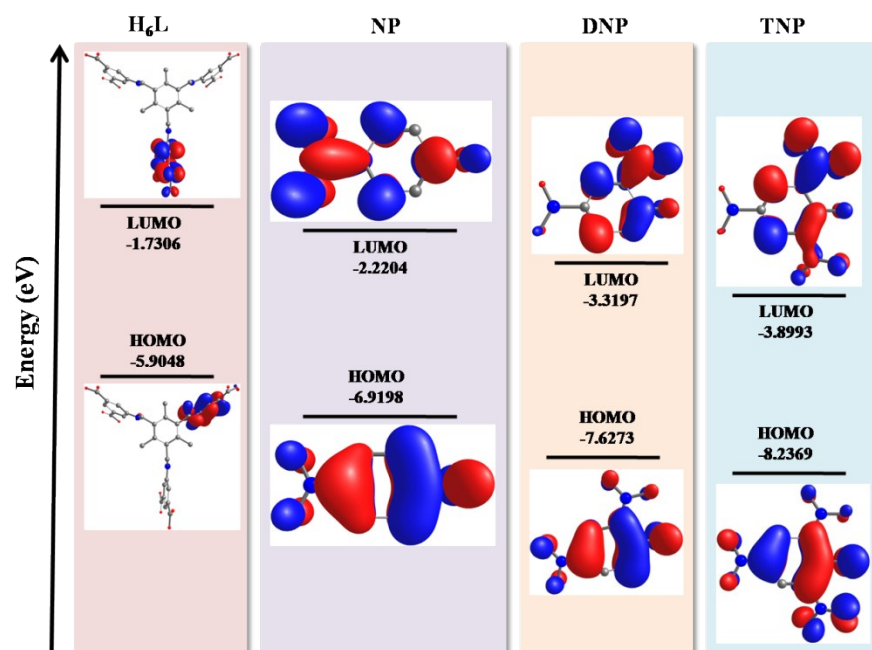
**Fig S23.** Stern–Volmer plot for the fluorescence quenching of LCd upon addition of NP. Inset: The Stern–Volmer plot at low NP concentrations.



**Fig S24.** Stern–Volmer plot for the fluorescence quenching of LCd upon addition of DNP. Inset: The Stern–Volmer plot at low DNP concentrations.



**Fig S25.** Stern–Volmer plot for the fluorescence quenching of LCd upon addition of TNP. Inset: The Stern–Volmer plot at low TNP concentrations.



**Fig S26.** Comparison of HOMO and LUMO energies of ligand (H<sub>6</sub>L), nitrophenol (NP), dinitrophenol (DNP) and trinitrophenol (TNP).

**Table S1. Crystal data and structure refinement for LZn and LCd**

Identification code	LZn	LCd
Empirical formula	C <sub>72</sub> H <sub>72</sub> N <sub>6</sub> O <sub>31</sub> Zn <sub>7</sub>	C <sub>109</sub> H <sub>147</sub> Cd <sub>4</sub> N <sub>19</sub> Na <sub>2</sub> O <sub>35</sub>
Formula weight	1975.09	2779.03
Temperature	296(2) K	296(2) K
Wavelength	0.71073 Å	0.71073 Å
Crystal system	Cubic	Monoclinic
Space group	F m -3 m	P 21/c
Unit cell dimensions	a = 43.6114(18) Å    α = 90° b = 43.6114(18) Å    β = 90° c = 43.6114(18) Å    γ = 90°	a = 16.8360(14) Å    α = 90° b = 24.094(2) Å    β = 117.791(3)° c = 17.7653(15) Å    γ = 90°
Volume	82947(10) Å <sup>3</sup>	6375.3(9) Å <sup>3</sup>
Z	16	2
Density (calculated)	0.638 Mg/m <sup>3</sup>	1.448 Mg/m <sup>3</sup>
Absorption coefficient	0.830 mm <sup>-1</sup>	0.747 mm <sup>-1</sup>
F(000)	16352	2856
Crystal size	0.18 x 0.17 x 0.16 mm <sup>3</sup>	0.21 x 0.15 x 0.11 mm <sup>3</sup>
Theta range for data collection	2.642 to 25.267°.	0.845 to 25.266°.
Index ranges	-52 ≤ h ≤ 52, -52 ≤ k ≤ 52, - 52 ≤ l ≤ 52	-19 ≤ h ≤ 20, -28 ≤ k ≤ 28, - 21 ≤ l ≤ 19
Reflections collected	290540	70069
Independent reflections	3648 [R(int) = 0.1901]	11620 [R(int) = 0.1076]
Completeness to theta = 25.242°	99.2 %	99.8 %
Absorption correction	Semi-empirical from equivalents	Semi-empirical from equivalents
Max. and min. transmission	0.7457 and 0.6050	0.7457 and 0.5911
Refinement method	Full-matrix least-squares on F <sup>2</sup>	Full-matrix least-squares on F <sup>2</sup>
Data / restraints / parameters	3648 / 6 / 127	11620 / 948 / 804
Goodness-of-fit on F <sup>2</sup>	1.688	1.045
Final R indices [I > 2σ(I)]	R1 = 0.1448, wR2 = 0.3452	R1 = 0.0692, wR2 = 0.1884
R indices (all data)	R1 = 0.2533, wR2 = 0.4833	R1 = 0.1197, wR2 = 0.2217
Extinction coefficient	n/a	n/a
Largest diff. peak and hole	4.599 and -0.837 e.Å <sup>-3</sup>	2.449 and -1.457 e.Å <sup>-3</sup>

**Table S2. Bond lengths [Å] and angles [°] for LZn**

Bond lengths			
O(1)-Zn(1)	2.049(7)	O(4)-Zn(4)	1.923(10)
O(2)-Zn(2)	1.988(9)	O(3W)-Zn(3)	2.17(2)
O(1W)-Zn(1)	2.007(16)	O(4W)-Zn(4)	2.167(14)
O(3)-Zn(3)	1.903(9)	Zn(1)-Zn(2)	2.971(3)
O(2W)-Zn(2)	1.926(17)		

Bond Angles			
C(1)-O(1)-Zn(1)	126.6(9)	O(2)#9-Zn(2)-O(2)	87.93(11)
C(1)-O(2)-Zn(2)	130.8(9)	O(2W)-Zn(2)-Zn(1)	180.0
Zn(1)-O(1W)-H(01K)	130.6	O(2)#7-Zn(2)-Zn(1)	79.0(3)
C(8)-O(3)-Zn(3)	130.6(9)	O(1)-Zn(1)-O(1)#8	88.31(9)
Zn(2)-O(2W)-H(01A)	128.7	O(1)#7-Zn(1)-O(1)#8	88.31(9)
C(8)-O(4)-Zn(4)	137.9(10)	O(1W)-Zn(1)-O(1)#9	99.9(3)
Zn(3)-O(3W)-H	129.8	O(1)-Zn(1)-O(1)#9	88.31(9)
Zn(3)-O(3W)-H#4	129.759(7)	O(1)#7-Zn(1)-O(1)#9	88.31(9)
Zn(3)-O(3W)-H#5	129.759(5)	O(1)#8-Zn(1)-O(1)#9	160.2(5)
Zn(4)-O(4W)-H(01E)	128.1	O(1W)-Zn(1)-Zn(2)	180.0
O(1W)-Zn(1)-O(1)	99.9(3)	O(1)-Zn(1)-Zn(2)	80.1(3)
O(1W)-Zn(1)-O(1)#7	99.9(3)	O(2)#8-Zn(2)-Zn(1)	79.0(3)
O(1)-Zn(1)-O(1)#7	160.2(5)	O(2)#9-Zn(2)-Zn(1)	79.0(3)
O(1W)-Zn(1)-O(1)#8	99.9(3)	O(2)-Zn(2)-Zn(1)	79.0(3)
O(1)#7-Zn(1)-Zn(2)	80.1(3)	O(3)#4-Zn(3)-O(3)#10	114.8(2)
O(1)#8-Zn(1)-Zn(2)	80.1(3)	O(3)#4-Zn(3)-O(3)	114.8(2)
O(1)#9-Zn(1)-Zn(2)	80.1(3)	O(3)#10-Zn(3)-O(3)	114.8(2)
O(2W)-Zn(2)-O(2)#7	101.0(3)	O(3)#4-Zn(3)-O(3W)	103.4(3)
O(2W)-Zn(2)-O(2)#8	101.0(3)	O(3)#10-Zn(3)-O(3W)	103.4(3)
O(2)#7-Zn(2)-O(2)#8	87.93(11)	O(3)-Zn(3)-O(3W)	103.4(3)
O(2W)-Zn(2)-O(2)#9	101.0(3)	O(4)-Zn(4)-O(4)#4	110.2(3)
O(2)#7-Zn(2)-O(2)#9	87.93(11)	O(4)-Zn(4)-O(4)#10	110.2(3)
O(2)#8-Zn(2)-O(2)#9	158.1(6)	O(4)#4-Zn(4)-O(4)#10	110.2(3)
O(2W)-Zn(2)-O(2)	101.0(3)	O(4)-Zn(4)-O(4W)	108.7(3)
O(2)#7-Zn(2)-O(2)	158.1(6)	O(4)#4-Zn(4)-O(4W)	108.7(3)

O(2)#8-Zn(2)-O(2)	87.93(11)	O(4)#10-Zn(4)-O(4W)	108.7(3)
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Symmetry transformations used to generate equivalent atoms:

#1 y,z,x #2 x,z,y #3 z,y,x #4 x,-z+1/2,-y+1/2

#5 z,-x+1/2,-y+1/2 #6 z,x,y #7 -x,y,-z #8 -x,y,z

#9 x,y,-z #10 -y+1/2,-x+1/2,z

**Table S3. Bond lengths [Å] and angles [°] for LCd**

Bond lengths			
Cd(1)-O(3)	2.234(5)	Cd(2)-O(7)#5	2.349(5)
Cd(1)-O(10)#1	2.299(5)	Cd(2)-O(8)#5	2.361(5)
Cd(1)-O(6)#2	2.361(5)	Cd(2)-O(1)#4	2.424(5)
Cd(1)-O(1S)	2.362(6)	Cd(2)-C(27)#5	2.701(7)
Cd(1)-O(5)#2	2.399(5)	Cd(2)-C(17)#4	2.714(7)
Cd(1)-O(9)#1	2.461(6)	Cd(2)-Na(1)#5	3.411(3)
Cd(1)-O(4S)#3	2.507(6)	Na(1)-O(1)#1	2.394(6)
Cd(1)-C(26)#2	2.716(7)	Na(1)-O(8)	2.403(6)
Cd(1)-C(35)#1	2.724(7)	Na(1)-O(5)#6	2.413(6)
Cd(1)-Na(1)#3	3.503(3)	Na(1)-O(11)#7	2.474(6)
Cd(2)-O(12)	2.147(5)	Na(1)-O(4S)	2.497(7)
Cd(2)-O(2)#4	2.313(5)	Na(1)-O(1S)#3	2.565(7)
Cd(2)-O(2S)	2.319(6)		

Bond Angles			
O(3)-Cd(1)-O(10)#1	104.3(2)	C(26)#2-Cd(1)-C(35)#1	131.9(2)
O(3)-Cd(1)-O(6)#2	99.6(2)	O(3)-Cd(1)-Na(1)#3	117.87(15)
O(10)#1-Cd(1)-O(6)#2	128.3(2)	O(10)#1-Cd(1)-Na(1)#3	116.60(17)
O(3)-Cd(1)-O(1S)	88.2(2)	O(6)#2-Cd(1)-Na(1)#3	89.98(14)
O(10)#1-Cd(1)-O(1S)	93.4(2)	O(1S)-Cd(1)-Na(1)#3	47.07(16)
O(6)#2-Cd(1)-O(1S)	132.8(2)	O(5)#2-Cd(1)-Na(1)#3	43.44(13)
O(3)-Cd(1)-O(5)#2	95.68(19)	O(9)#1-Cd(1)-Na(1)#3	151.01(17)
O(10)#1-Cd(1)-O(5)#2	157.9(2)	O(4S)#3-Cd(1)-Na(1)#3	45.46(15)
O(6)#2-Cd(1)-O(5)#2	55.31(17)	C(26)#2-Cd(1)-Na(1)#3	66.45(17)



O(1S)-Cd(1)-O(5)#2	77.7(2)	C(35)#1-Cd(1)-Na(1)#3	137.95(18)
O(3)-Cd(1)-O(9)#1	90.8(2)	O(12)-Cd(2)-O(2)#4	112.8(2)
O(10)#1-Cd(1)-O(9)#1	54.21(19)	O(12)-Cd(2)-O(2S)	89.1(2)
O(6)#2-Cd(1)-O(9)#1	80.63(18)	O(2)#4-Cd(2)-O(2S)	94.2(2)
O(1S)-Cd(1)-O(9)#1	146.16(19)	O(12)-Cd(2)-O(7)#5	152.5(2)
O(5)#2-Cd(1)-O(9)#1	135.94(17)	O(2)#4-Cd(2)-O(7)#5	93.95(19)
O(3)-Cd(1)-O(4S)#3	161.4(2)	O(2S)-Cd(2)-O(7)#5	82.3(2)
O(10)#1-Cd(1)-O(4S)#3	81.9(2)	O(12)-Cd(2)-O(8)#5	109.1(2)
O(6)#2-Cd(1)-O(4S)#3	89.6(2)	O(2)#4-Cd(2)-O(8)#5	124.76(19)
O(1S)-Cd(1)-O(4S)#3	73.7(2)	O(2S)-Cd(2)-O(8)#5	121.0(2)
O(5)#2-Cd(1)-O(4S)#3	76.27(19)	O(7)#5-Cd(2)-O(8)#5	55.66(17)
O(9)#1-Cd(1)-O(4S)#3	106.7(2)	O(12)-Cd(2)-O(1)#4	106.8(2)
O(3)-Cd(1)-C(26)#2	97.1(2)	O(2)#4-Cd(2)-O(1)#4	55.19(17)
O(10)#1-Cd(1)-C(26)#2	152.0(2)	O(2S)-Cd(2)-O(1)#4	148.9(2)
O(6)#2-Cd(1)-C(26)#2	27.82(19)	O(7)#5-Cd(2)-O(1)#4	93.4(2)
O(1S)-Cd(1)-C(26)#2	105.3(2)	O(8)#5-Cd(2)-O(1)#4	79.54(19)
O(5)#2-Cd(1)-C(26)#2	27.56(19)	O(12)-Cd(2)-C(27)#5	133.6(2)
O(9)#1-Cd(1)-C(26)#2	108.4(2)	O(2)#4-Cd(2)-C(27)#5	110.79(19)
O(4S)#3-Cd(1)-C(26)#2	83.5(2)	O(2S)-Cd(2)-C(27)#5	103.0(2)
O(3)-Cd(1)-C(35)#1	98.7(2)	O(7)#5-Cd(2)-C(27)#5	28.04(19)
O(10)#1-Cd(1)-C(35)#1	27.4(2)	O(8)#5-Cd(2)-C(27)#5	27.63(19)
O(6)#2-Cd(1)-C(35)#1	104.4(2)	O(1)#4-Cd(2)-C(27)#5	85.4(2)
O(1S)-Cd(1)-C(35)#1	120.3(2)	O(12)-Cd(2)-C(17)#4	114.7(2)
O(5)#2-Cd(1)-C(35)#1	157.1(2)	O(2)#4-Cd(2)-C(17)#4	28.17(19)
O(9)#1-Cd(1)-C(35)#1	26.8(2)	O(2S)-Cd(2)-C(17)#4	121.8(2)
O(4S)#3-Cd(1)-C(35)#1	94.5(2)	O(7)#5-Cd(2)-C(17)#4	91.8(2)
O(8)#5-Cd(2)-C(17)#4	101.0(2)	O(11)#7-Na(1)-Cd(1)#3	125.97(17)
O(1)#4-Cd(2)-C(17)#4	27.20(18)	O(4S)-Na(1)-Cd(1)#3	45.70(15)
C(27)#5-Cd(2)-C(17)#4	96.6(2)	O(1S)#3-Na(1)-Cd(1)#3	42.40(14)
O(12)-Cd(2)-Na(1)#5	91.40(16)	Cd(2)#7-Na(1)-Cd(1)#3	174.49(9)
O(2)#4-Cd(2)-Na(1)#5	99.74(14)	C(17)-O(1)-Na(1)#8	174.2(5)
O(2S)-Cd(2)-Na(1)#5	164.6(2)	C(17)-O(1)-Cd(2)#9	89.5(4)
O(7)#5-Cd(2)-Na(1)#5	90.25(15)	Na(1)#8-O(1)-Cd(2)#9	90.16(19)
O(8)#5-Cd(2)-Na(1)#5	44.77(14)	C(17)-O(2)-Cd(2)#9	93.6(4)
O(1)#4-Cd(2)-Na(1)#5	44.55(13)	C(18)-O(3)-Cd(1)	136.0(5)

C(27)#5-Cd(2)-Na(1)#5	65.97(17)	C(26)-O(5)-Cd(1)#10	90.4(4)
C(17)#4-Cd(2)-Na(1)#5	71.65(16)	C(26)-O(5)-Na(1)#6	140.0(5)
O(1)#1-Na(1)-O(8)	79.3(2)	Cd(1)#10-O(5)-Na(1)#6	93.44(17)
O(1)#1-Na(1)-O(5)#6	102.9(2)	C(26)-O(6)-Cd(1)#10	91.8(4)
O(8)-Na(1)-O(5)#6	106.7(2)	C(27)-O(7)-Cd(2)#7	91.6(4)
O(1)#1-Na(1)-O(11)#7	86.6(2)	C(27)-O(8)-Cd(2)#7	91.5(4)
O(8)-Na(1)-O(11)#7	80.3(2)	C(27)-O(8)-Na(1)	132.7(5)
O(5)#6-Na(1)-O(11)#7	169.0(2)	Cd(2)#7-O(8)-Na(1)	91.46(19)
O(1)#1-Na(1)-O(4S)	178.8(2)	C(35)-O(9)-Cd(1)#8	88.6(5)
O(8)-Na(1)-O(4S)	101.6(2)	C(35)-O(10)-Cd(1)#8	95.4(4)
O(5)#6-Na(1)-O(4S)	76.2(2)	O(1)-C(17)-Cd(2)#9	63.3(4)
O(11)#7-Na(1)-O(4S)	94.2(2)	O(2)-C(17)-Cd(2)#9	58.3(4)
O(1)#1-Na(1)-O(1S)#3	108.5(2)	C(13)-C(17)-Cd(2)#9	168.2(5)
O(8)-Na(1)-O(1S)#3	172.0(2)	O(9)-C(35)-Cd(1)#8	64.6(4)
O(5)#6-Na(1)-O(1S)#3	73.7(2)	O(10)-C(35)-Cd(1)#8	57.2(4)
O(11)#7-Na(1)-O(1S)#3	98.2(2)	C(31)-C(35)-Cd(1)#8	174.4(6)
O(4S)-Na(1)-O(1S)#3	70.5(2)	C(41S)-O(4S)-Na(1)	128.4(7)
O(1)#1-Na(1)-Cd(2)#7	45.29(14)	C(41S)-O(4S)-Cd(1)#3	120.6(7)
O(8)-Na(1)-Cd(2)#7	43.77(14)	Na(1)-O(4S)-Cd(1)#3	88.8(2)
O(5)#6-Na(1)-Cd(2)#7	131.53(15)	O(1S)#3-Na(1)-Cd(2)#7	141.58(17)
O(11)#7-Na(1)-Cd(2)#7	59.33(16)	O(1)#1-Na(1)-Cd(1)#3	133.13(17)
O(4S)-Na(1)-Cd(2)#7	135.88(19)	O(8)-Na(1)-Cd(1)#3	132.91(17)
O(5)#6-Na(1)-Cd(1)#3	43.12(12)		

Symmetry transformations used to generate equivalent atoms:

#1  $-x+1, y+1/2, -z-1/2$  #2  $x, y, z+1$  #3  $-x+1, -y+2, -z$

#4  $x+1, y, z$  #5  $-x+2, y-1/2, -z-1/2$  #6  $-x+1, -y+2, -z-1$

#7  $-x+2, y+1/2, -z-1/2$  #8  $-x+1, y-1/2, -z-1/2$  #9  $x-1, y, z$

#10  $x, y, z-1$

**Table S4. Quenching Constants ( $K_{SV}$ ) for the NP, DNP and TNP**

NACs	LZn	LCd
NP	$1.45 \times 10^4$	$1.35 \times 10^4$
DNP	$1.54 \times 10^4$	$1.39 \times 10^4$
TNP	$1.62 \times 10^4$	$1.56 \times 10^4$

**Table S5. Standard deviation and detection limit calculation for NP, DNP and TNP**

	LZn	LCd
1	1167.932	1061.354
2	1168.324	1061.455
3	1168.555	1060.998
4	1168.001	1061.254
5	1167.969	1060.967
Standard deviation( $\sigma$ )	0.2723	0.2160
LOD (NP)	$5.63 \times 10^{-5}$	$4.80 \times 10^{-5}$
LOD (DNP)	$5.30 \times 10^{-5}$	$4.66 \times 10^{-5}$
LOD (TNP)	$5.04 \times 10^{-5}$	$4.15 \times 10^{-5}$

**Table S6. Comparison of adsorption activity of LZn and LCd with reported complexes**

	CO <sub>2</sub> adsorption	Temperature (K) and pressure (bar)	Reference
LZn	1.1	273 and 1	This work
LCd	0.85	273 and 1	This work
[Cu <sub>24</sub> (TPBTM <sup>6-</sup> ) <sub>8</sub> (H <sub>2</sub> O) <sub>24</sub> ]	23.53	298 and 20	1
PCN-61	21.4	298 and 20	1
PCN-61	22.1	298 and 20	1
PCN-61	22.1	298 and 20	1
MOF-205	0.49	273 and 1	2
MOF-205-NH <sub>2</sub>	0.57	273 and 1	2
MOF-205-NO <sub>2</sub>	0.55	273 and 1	2
MOF-205-OBn	0.78	273 and 1	2
Cu-TDPAT	10.13	273 and 1	3
{[Sr(BDPO) <sub>0.5</sub> (H <sub>2</sub> O)] 2H <sub>2</sub> O} <sub>n</sub>	4.4	273 and 1	4
[Co <sub>3</sub> (tzba) <sub>2</sub> (bpy) <sub>3</sub> (F) <sub>2</sub> ] <sub>2</sub> ·DMF·C <sub>2</sub> H <sub>5</sub> OH·2H <sub>2</sub> O	3.8	273 and 1	5

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