Electronic Supplementary Material (ESI)

An excellent thermostable dual-functionalized 3D *fsx*-type Cd(II) MOF for highly selective detection of Fe^{3+} ions and ten nitroaromatic explosives

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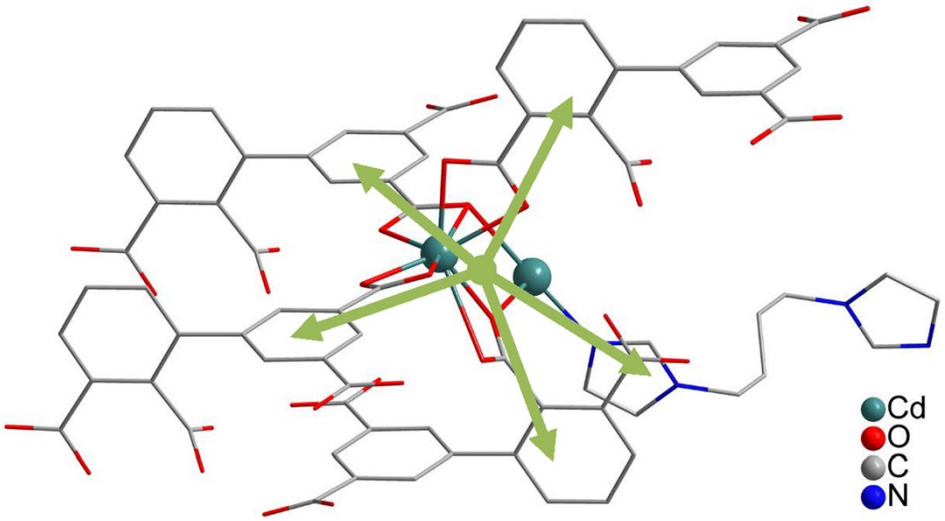
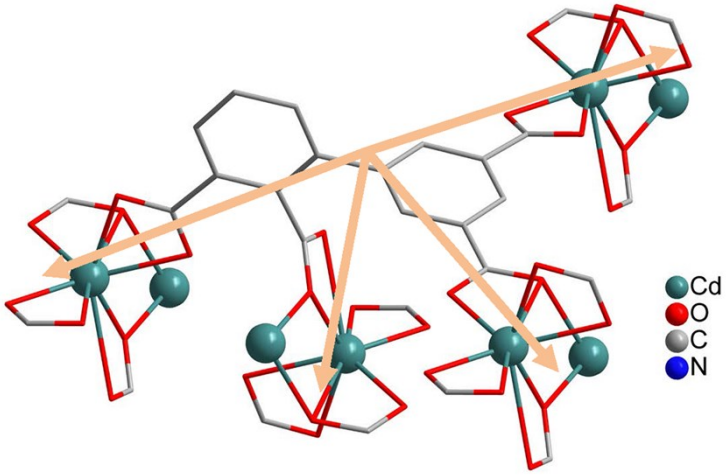


（a）



（b）

Fig. S1 Simplified nodes of metal clusters (a) and H_4L ligand (b) observed in MOF-**1**.

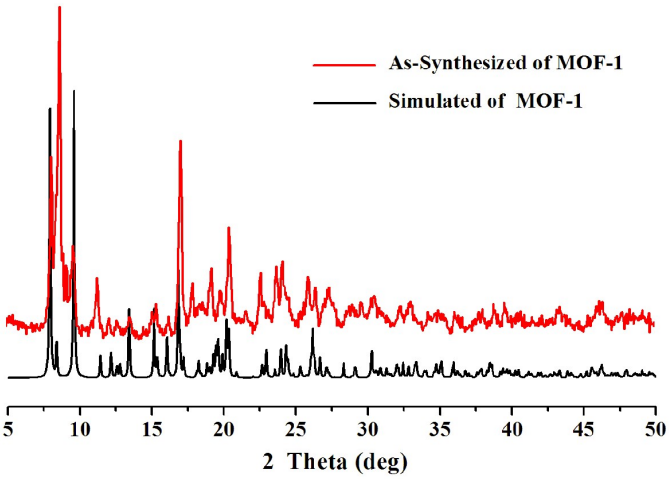
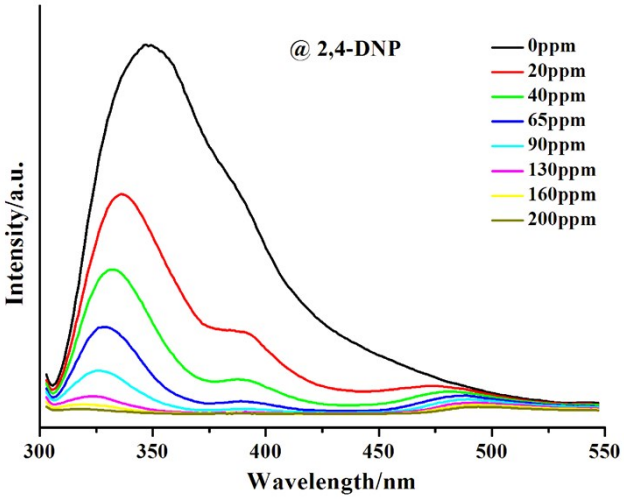


Fig. S2 PXRD patterns from the single-crystal simulated and as-synthesized powders of MOF-**1**.



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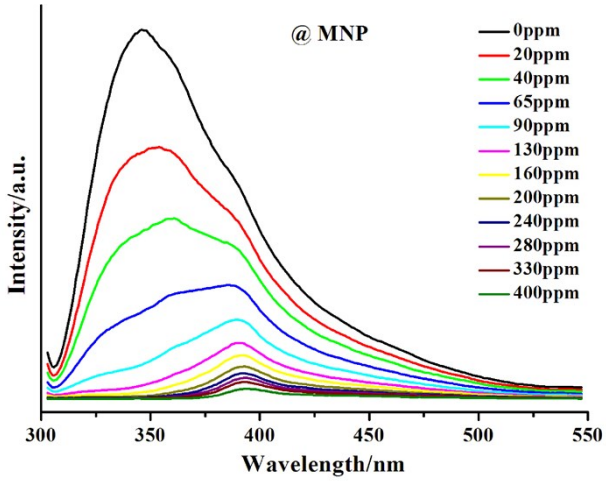

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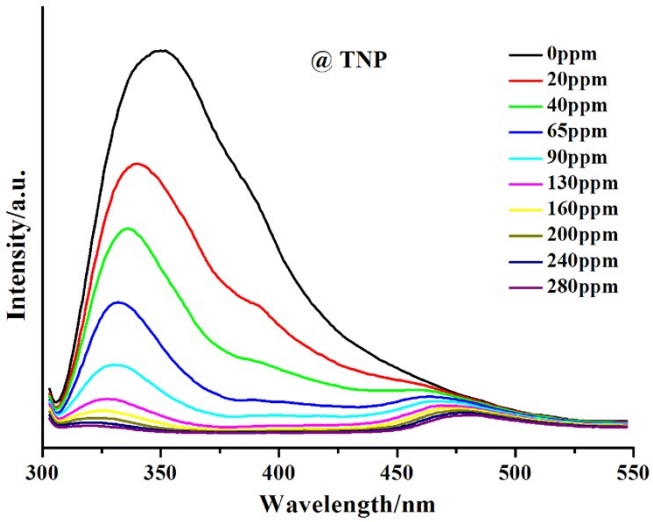
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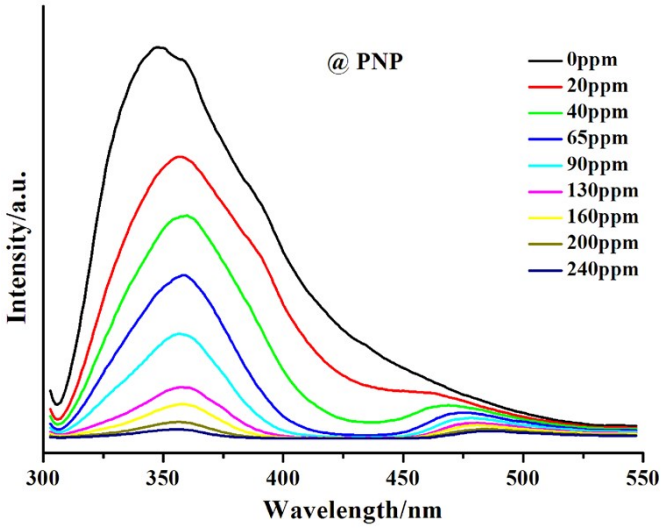
0ppm
20ppm
40ppm
65ppm
90ppm
130ppm
160ppm
200ppm
240ppm
280ppm
Intensity/a.u.
300
350
400
450
500
550
Wavelength/nm

（c）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40ppm
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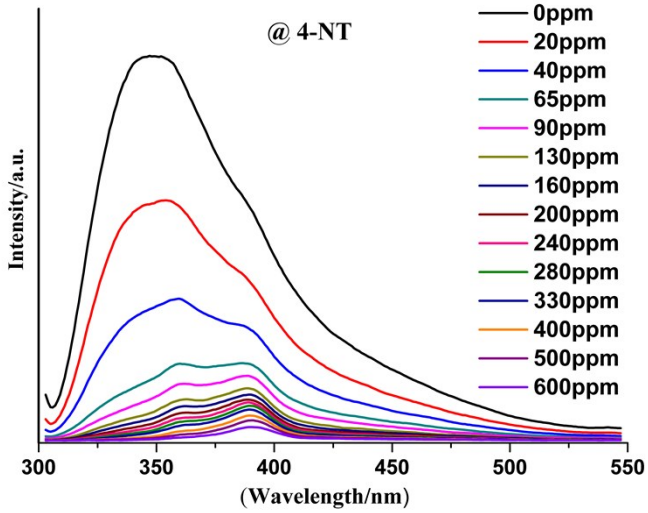
160ppm
200ppm
240ppm
Intensity/a.u.
300
350
400
450
500
550
Wavelength/nm

（d）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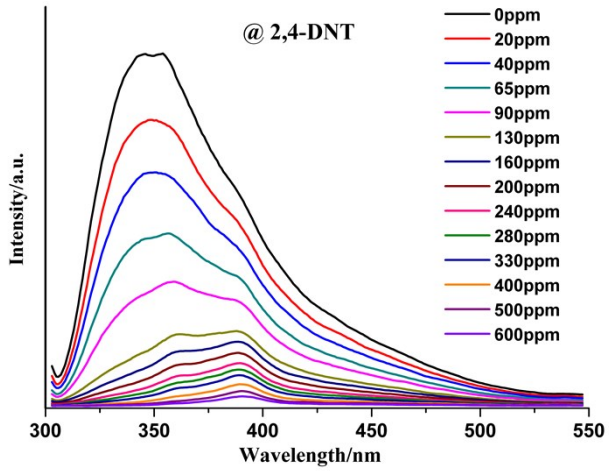
20ppm
40ppm
65ppm
90ppm
130ppm
160ppm
200ppm
240ppm
280ppm
330ppm
400ppm
500ppm
600ppm
Intensity/a.u.
300
350
400
450
500
550
(Wavelength/nm)

（e）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20ppm
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160ppm
200ppm
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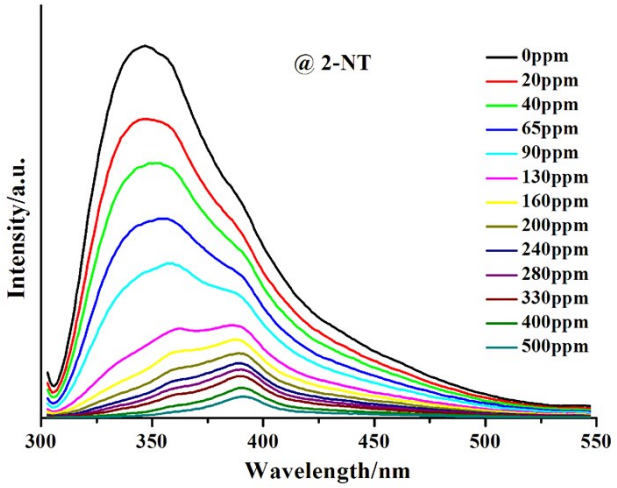
280ppm
330ppm
400ppm
500ppm
600ppm
Intensity/a.u.
300
350
400
450
500
550
Wavelength/nm

（f）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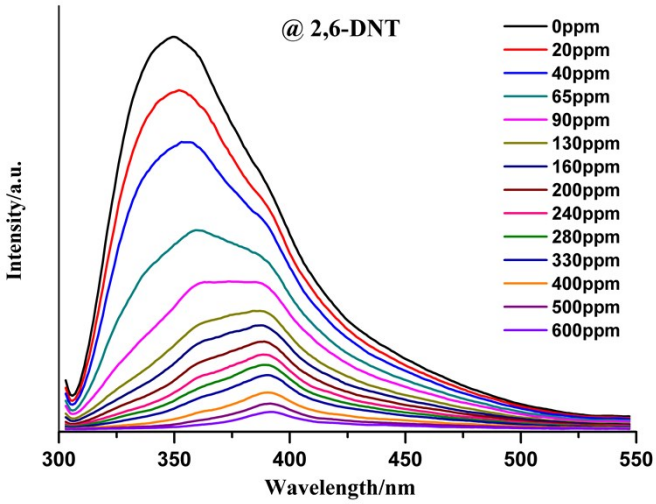
20ppm
40ppm
65ppm
90ppm
130ppm
160ppm
200ppm
240ppm
280ppm
330ppm
400ppm
500ppm
Intensity/a.u.
300
350
400
450
500
550
Wavelength/nm

（g）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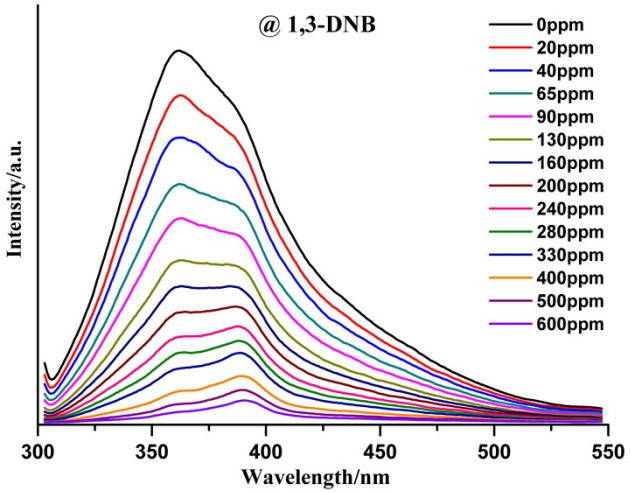
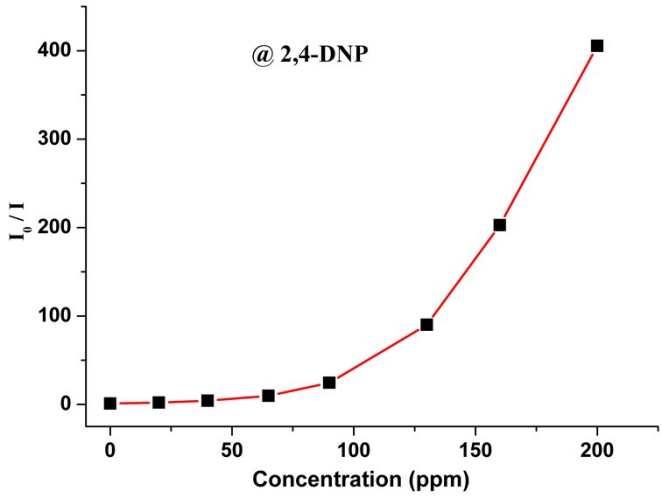
0ppm
20ppm
40ppm
65ppm
90ppm
130ppm
160ppm
200ppm
240ppm
280ppm
330ppm
400ppm
500ppm
600ppm
Intensity/a.u.
300
350
400
450
500
550
Wavelength/nm

（h）

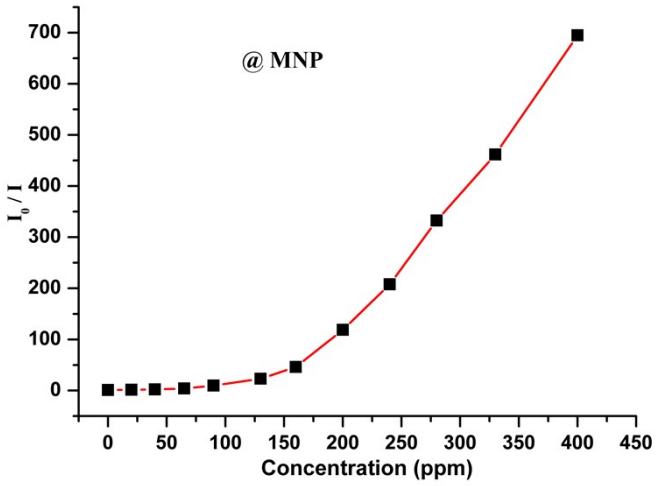


（i）

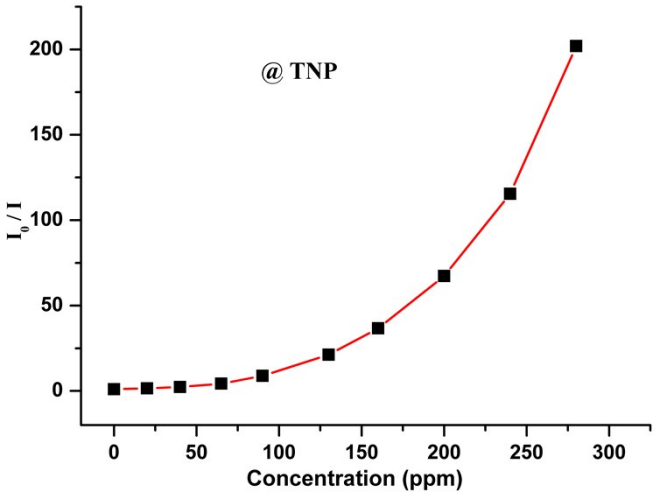
Fig. S3 Luminescence spectra of MOF-**1** upon the incremental addition of nitroaromatic explosives: (a) 2,4-DNP, (b) MNP, (c) TNP, (d) PNP, (e) 4-NT, (f) 2,4-DNT, (g) 2-NT, (h) 2,6-DNT, (i) 1,3-DNB.



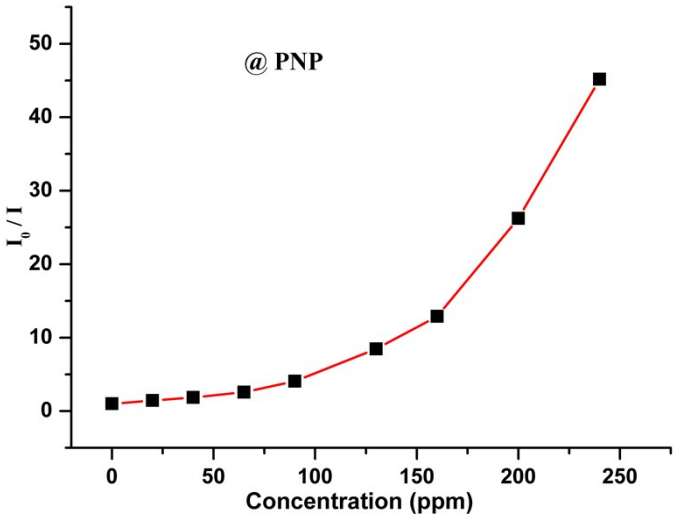
(a)


@ MNP
I_0 / I
Concentration (ppm)

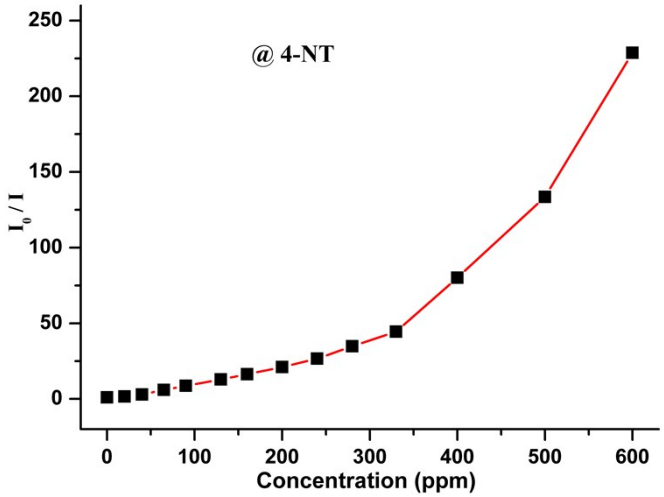
(b)


@ TNP
I_0 / I
Concentration (ppm)

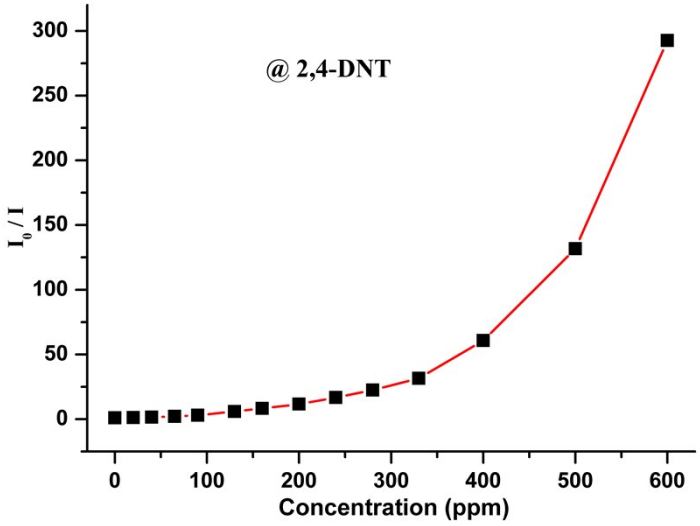
(c)


@ PNP
I_0 / I
Concentration (ppm)

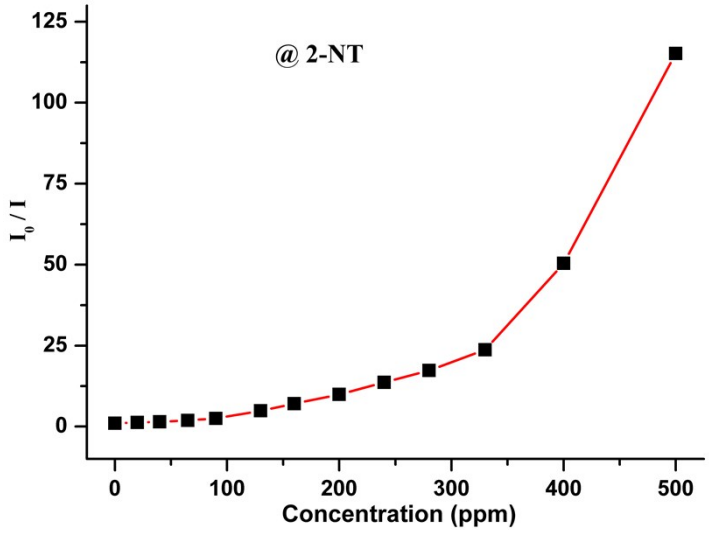
(d)


@ 4-NT
I_0 / I
Concentration (ppm)

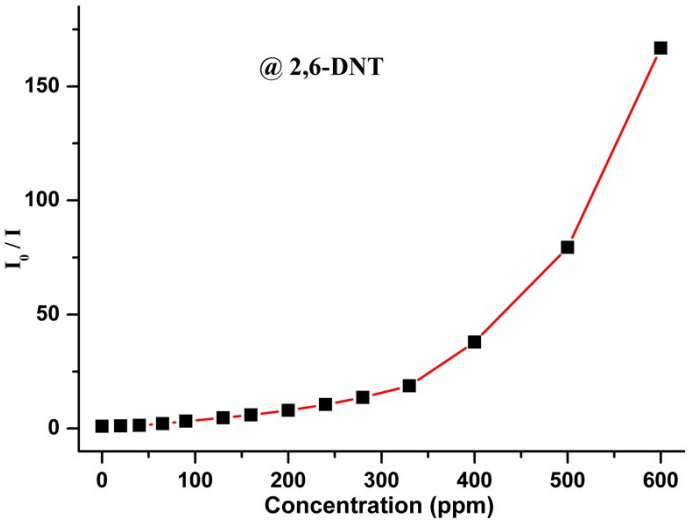
(e)


@ 2,4-DNT
I_0 / I
Concentration (ppm)

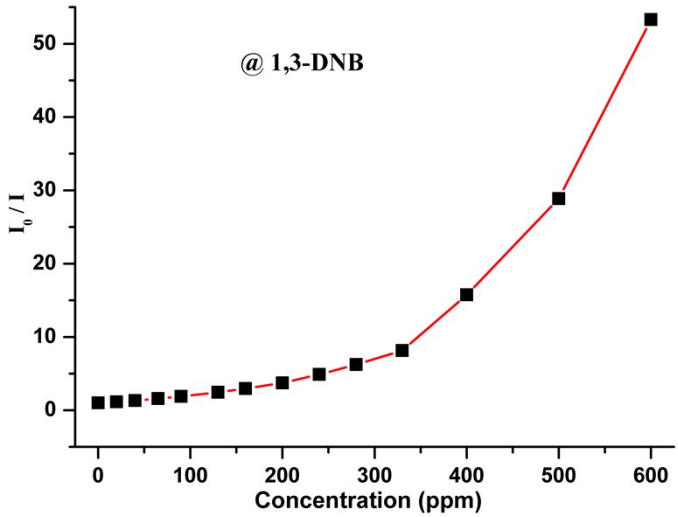
(f)


@ 2-NT
I_0 / I
Concentration (ppm)

(g)



(h)



(i)

Fig. 4 The correlation between I_0/I *vs* [C] concentration of different nitroaromatic explosives: (a) 2,4-DNP, (b) MNP, (c) TNP, (d) PNP, (e) 4-NT, (f) 2,4-DNT, (g) 2-NT, (h) 2,6-DNT, (i) 1,3-DNB.

Table S1. Selected bond lengths (Å) and angles (°) of MOF-**1** [a].

Cd1-O1	2.353(3)	Cd1-O5#2	2.316(3)
Cd1-O2	2.382(2)	Cd1-O7#1	2.258(2)
Cd1-O3#3	2.314(3)	Cd2-N1	2.232(4)
Cd2-O3	2.274(3)	Cd2-O6#4	2.346(3)
Cd2-O9	2.264(3)	Cd2-O10	2.331(3)
Cd2-O11	2.272(3)		
O1-Cd1-O2	55.27(9)	O3#3-Cd1-O1	141.83(9)
O3#3-Cd1-O2	90.08(9)	O3#3-Cd1-O5#2	91.87(10)
O5#2-Cd1-O2	126.71(9)	O5#2-Cd1-O1	96.90(10)
O7#1-Cd1-O1	97.32(10)	O7#1-Cd1-O2	133.21(10)
O7#1-Cd1-O3#3	119.83(9)	O7#1-Cd1-O5#2	89.99(9)
O3-Cd2-O6#4	78.32(9)	O3-Cd2-O10	169.91(12)
O9-Cd2-O3	89.79(10)	O9-Cd2-O6#4	77.67(10)
O9-Cd2-O10	84.99(13)	O9-Cd2-O11	159.95(12)
O10-Cd2-O6#4	92.12(13)	O11-Cd2-O6#4	86.83(13)
O11-Cd2-O3	99.54(11)	O11-Cd2-O10	82.94(13)
N1-Cd2-O3	103.40(11)	N1-Cd2-O6#4	178.20(11)
N1-Cd2-O9	101.71(13)	N1-Cd2-O10	86.14(15)
N1-Cd2-O11	93.40(15)		

[a] Symmetry codes: #1 x, y, z+1; #2 x-1, y, z+1; #3 –x+1, -y+1, -z+1; #4 -x+2, -y+1, -z.

Table S2. Standard deviation (δ) calculation for MOF-**1** in different solvent systems.

	Luminescence intensity test of MOF-**1**					Average value	Standard deviation
	1	2	3	4	5		
Water	784.63	785.10	784.26	783.97	784.88	784.57	0.46
DMF	791.28	790.08	790.56	791.44	790.92	790.86	0.55

Table S3. The luminous intensities and quenching effects of MOF-**1** at 200 ppm concentration of different nitroaromatic explosives.

	Luminous intensity before quenching / a.u.	Luminous intensity after quenching / a.u.	Quenching efficiency / %
2,4-DNP	811.36	1.80	99.78
MNP	830.67	7.34	99.12
TNP	807.68	11.96	98.52
PNP	812.72	31.32	96.15
4-NT	800.56	37.96	95.26
2,4-DNT	789.80	68.12	91.38
NB	791.28	76.35	90.35
2-NT	806.46	80.80	89.97
2,6-DNT	834.35	104.57	87.47
1,3-DNB	693.24	185.46	73.25