Electronic Supporting Information (ESI)

Fabrication of Cd(II) metal-organic framework as a dual functional material: Efficient iodine capture and selective adsorption of cationic dye

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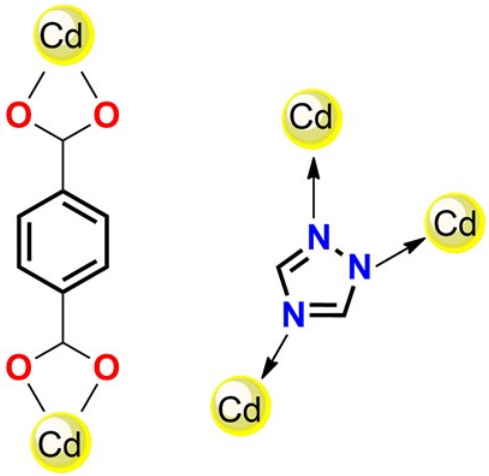

Fig. S1. The different coordination mode of H_2tpa and tz^- ligands are depicted.

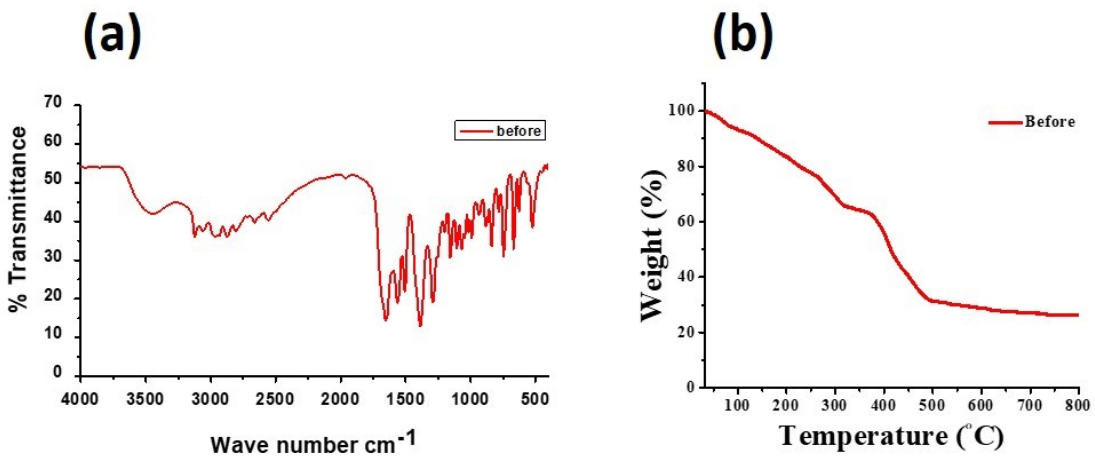

Fig. S2. **(a)** FTIR spectrum and **(b)** TGA before iodine adsorption.

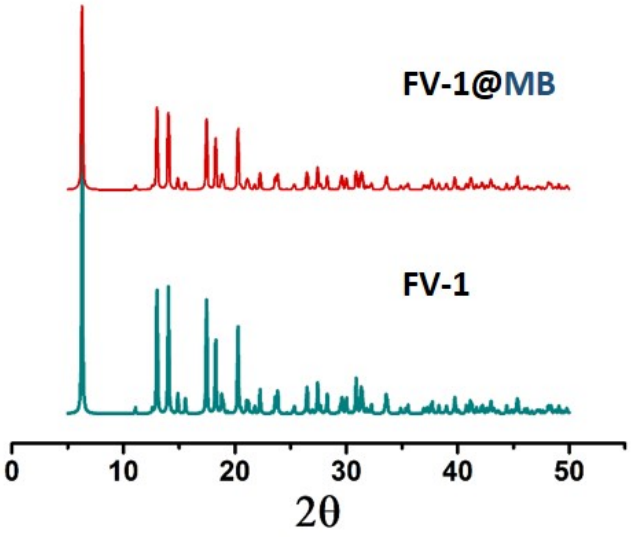

Fig. S3. PXRD pattern of **FV-1** before and after adsorption of MB.

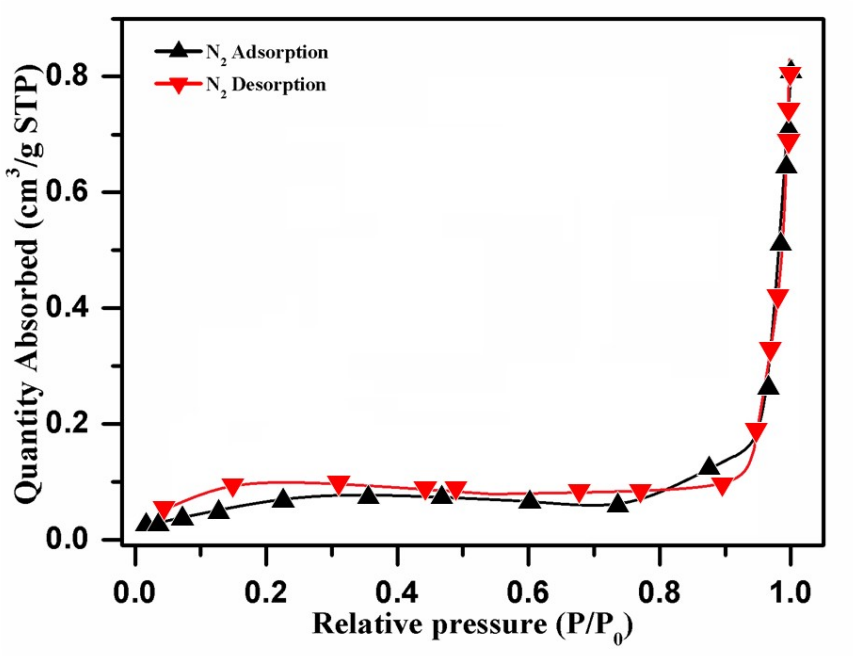

Fig. S4. N_2 adsorption/desorption isotherm for **FV-1** showing no noticeable porosity.

Table S1. Bond Lengths for **FV-1.**

Atom	**Atom**	**Length/Å**
Cd1	O1	2.314(2)
Cd1	O2	2.433(2)
Cd1	O3	2.401(2)
Cd1	N1	2.244(2)
Cd1	N2[1]	2.318(2)
Cd1	N3[2]	2.256(2)
O1	C3	1.249(5)
O2	C3	1.240(4)
O3	C7	1.189(5)
N1	N2	1.365(3)
N1	C1	1.314(3)
N2	C2	1.314(4)
N3	C1	1.326(3)
N3	C2	1.334(4)
N4	C7	1.288(6)
N4	C8	1.400(8)
N4	C9	1.434(10)
C3	C4	1.517(4)
C4	C5	1.359(6)
C4	C6	1.363(5)
C5	C6[3]	1.392(5)

Table S2. Bond Angles for **FV-1.**

Atom	**Atom**	**Atom**	**Angle/°**
O2	Cd1	O1	54.91(9)
O3	Cd1	O1	86.59(10)
O3	Cd1	O2	88.94(9)
N1	Cd1	O1	108.16(10)
N1	Cd1	O2	162.05(9)
N1	Cd1	O3	83.67(9)
$N2^{1}$	Cd1	O1	95.34(9)
$N2^{1}$	Cd1	O2	89.14(8)
$N2^{1}$	Cd1	O3	175.82(10)
$N2^{1}$	Cd1	N1	99.22(8)
$N3^{2}$	Cd1	O1	146.17(9)
$N3^{2}$	Cd1	O2	92.14(9)
$N3^{2}$	Cd1	O3	85.19(10)
$N3^{2}$	Cd1	N1	103.46(9)
$N3^{2}$	Cd1	$N2^{1}$	91.17(9)
C3	Cd1	O1	27.55(11)
C1	N1	Cd1	127.41(18)
C1	N1	N2	105.7(2)
N1	N2	$Cd1^{1}$	133.62(17)
C2	N2	$Cd1^{1}$	120.90(18)
C2	N2	N1	105.3(2)
C1	N3	$Cd1^{3}$	128.79(19)
C2	N3	$Cd1^{3}$	129.24(19)
C2	N3	C1	101.9(2)
C8	N4	C7	121.9(6)
C9	N4	C8	117.3(7)
N3	C1	N1	113.6(2)
N3	C2	N2	113.5(2)
O1	C3	Cd1	58.98(16)
O2	C3	Cd1	64.46(16)
O2	C3	O1	123.4(3)
C3	Cd1	O2	27.37(10)
C3	Cd1	O3	87.31(10)
C3	O1	Cd1	93.5(2)
C3	O2	Cd1	88.2(2)
C7	O3	Cd1	126.5(3)
N2	N1	Cd1	126.74(17)
C4	C3	Cd1	177.0(3)
C4	C3	O1	118.1(3)
C4	C3	O2	118.5(3)
C5	C4	C3	120.8(3)
C6	C4	C3	120.4(3)
C6	C4	C5	118.8(3)
$C6^{4}$	C5	C4	120.5(4)
$C5^{4}$	C6	C4	120.7(4)

Explanation of Alert B in the Checkcif:

start Validation Reply Form
_vrf_PLAT230_ALERT_2_B
;
PROBLEM:Hirshfeld Test Diff for O3 --C7 8.5 s.u.
RESPONSE:Due to unresolved disorders, some atoms were still not ideally shaped, however, this does not indicate an incorrect atom-type assignment.
;
_vrf_PLAT232_ALERT_2_B
;
PROBLEM:Hirshfeld Test Diff (M-X) Cd1 --O2 13.9 s.u.
RESPONSE:Due to unresolved disorders, some atoms were still not ideally shaped, however, this does not indicate an incorrect atom-type assignment.
;
_vrf_PLAT242_ALERT_2_B
;
PROBLEM:Low 'MainMol' Ueq as Compared to Neighbors of N4 Check
RESPONSE:This may be also due to disorders in the atoms, but the atom-type assignment is correct.
end Validation Reply Form

Table S3. Determination of zeta potential at varying pH for **FV-1**.

pH	Zeta Potential (mV)
2	-4.06
3	-4.10
4	-4.11
5	-4.19
6	-4.21
7	-5.61
8	0.00
9	+0.56
10	+0.55
11	+0.54
12	+0.60