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Supporting information for article:

Three novel topologically different metal–organic frameworks built from 3-nitro-4-(pyridin-4-yl)benzoic acid

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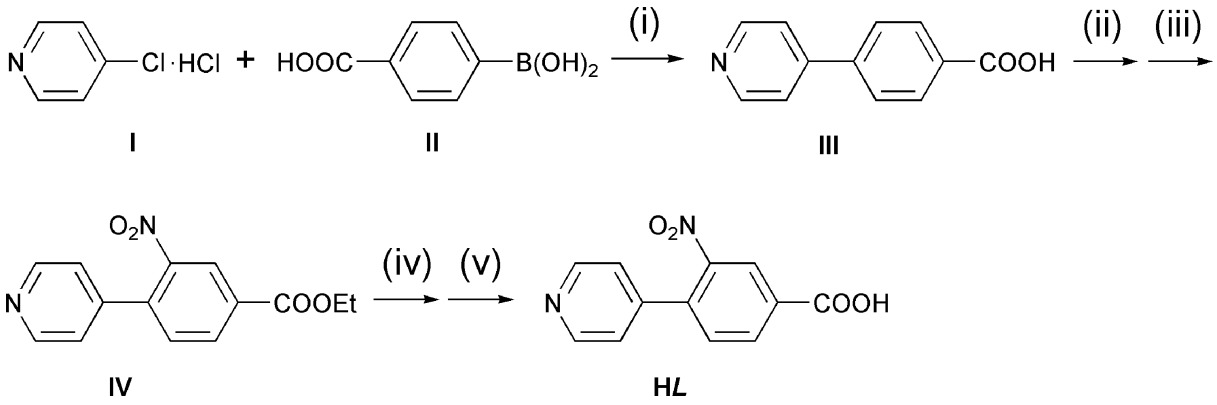
Supporting information



Scheme S1

Synthesis of 3-nitro-4-(4'-pyridyl)benzoic acid (H*L*): (i) $Pd(PPh_3)_4$, K_2CO_3, Ar atmosphere, 100 °C, 24 h, (ii) H_2SO_4, HNO_3, 80 °C, 2 h, (iii) EtOH, H^+, 80 °C, 24 h, (iv) NaOH, EtOH, 60 °C, 4 h, (v) H^+.

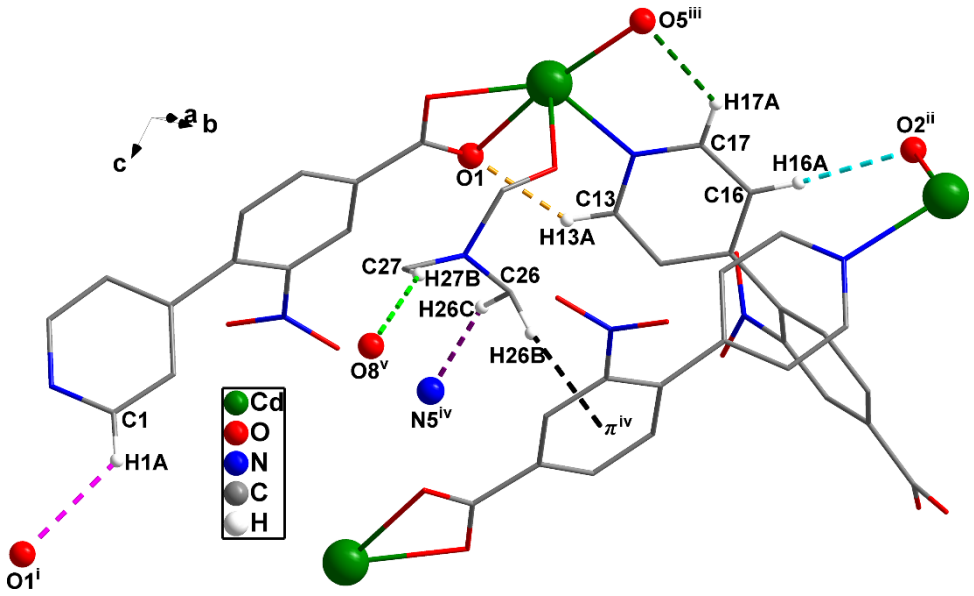


Figure S1 Hydrogen bonds and C-H···π interaction (dotted lines) in MOF (**1**).

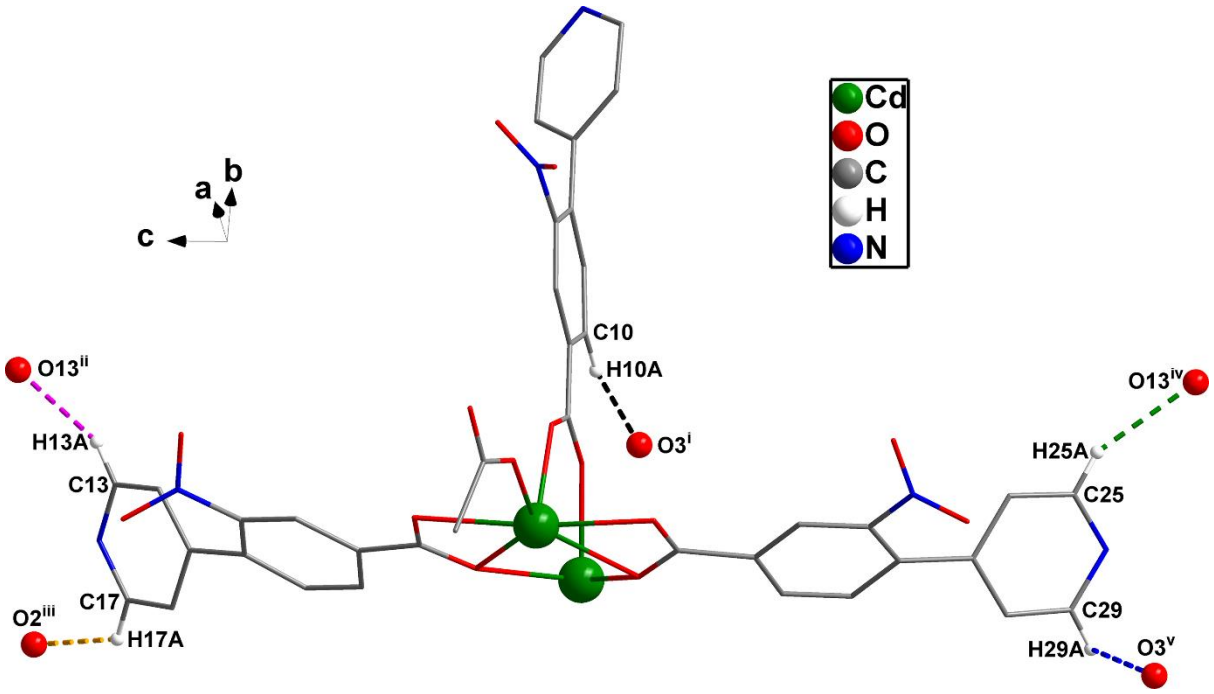


Figure S2 Hydrogen bonds (dotted lines) in MOF (**2**).

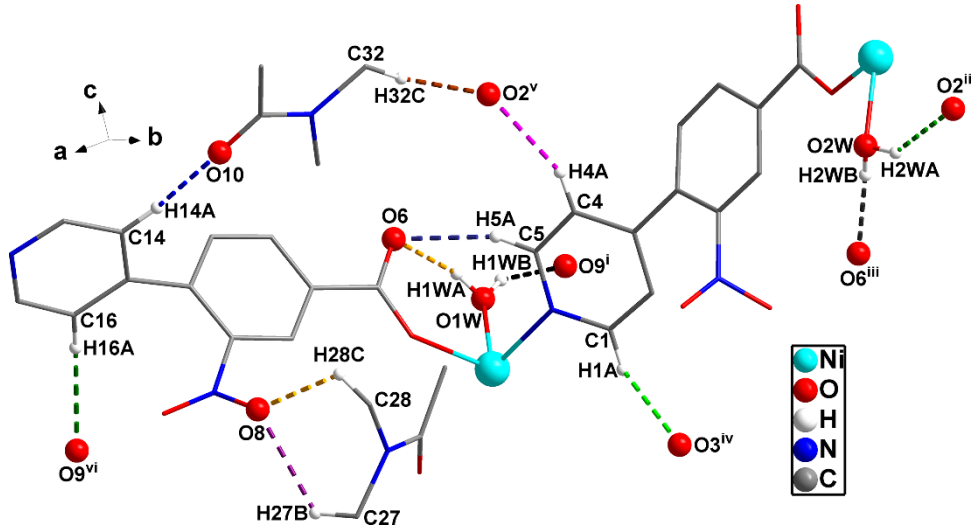


Figure S3 Hydrogen bonds (dotted lines) in MOF (**3**).

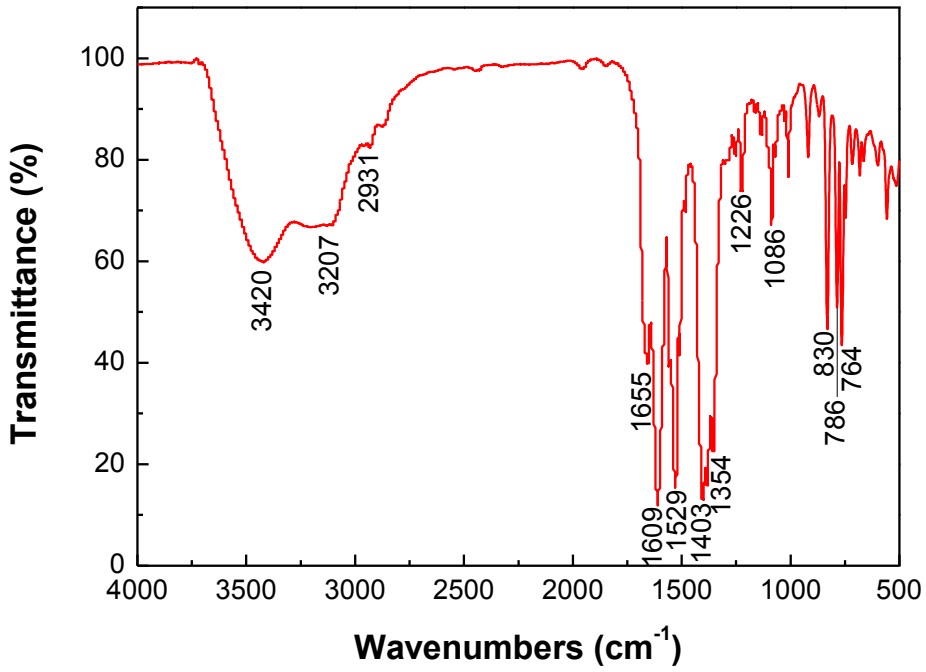


Figure S4 FT-IR spectrum of MOF (**1**).

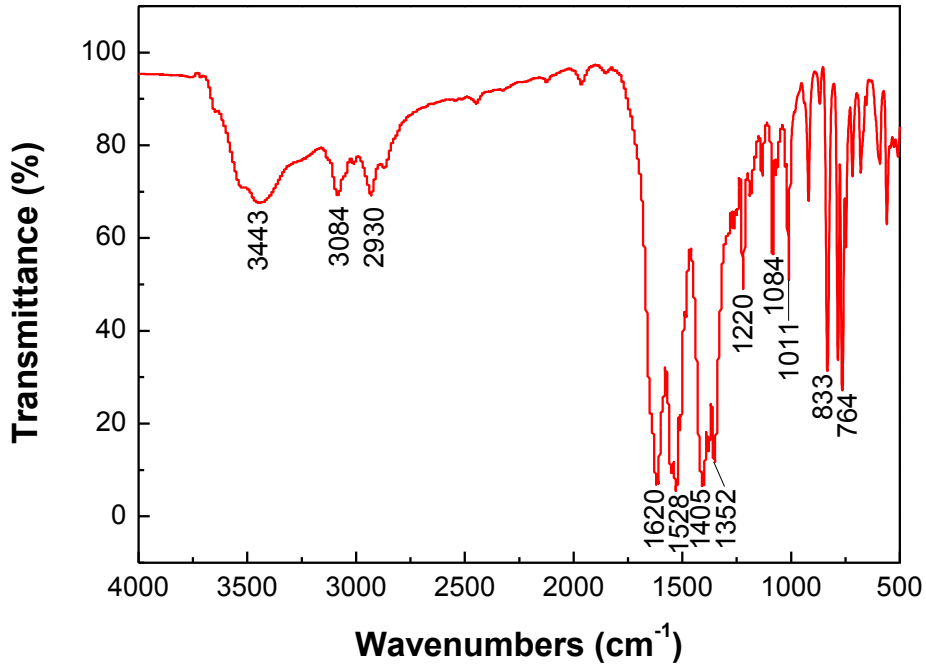


Figure S5 FT-IR spectrum of MOF (**2**).

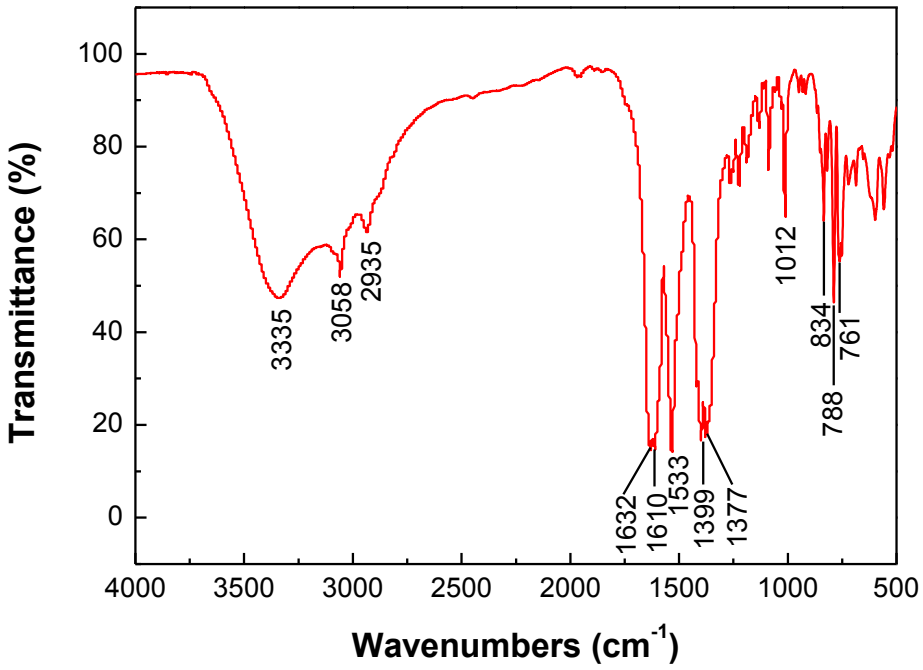


Figure S6 FT-IR spectrum of MOF (**3**).

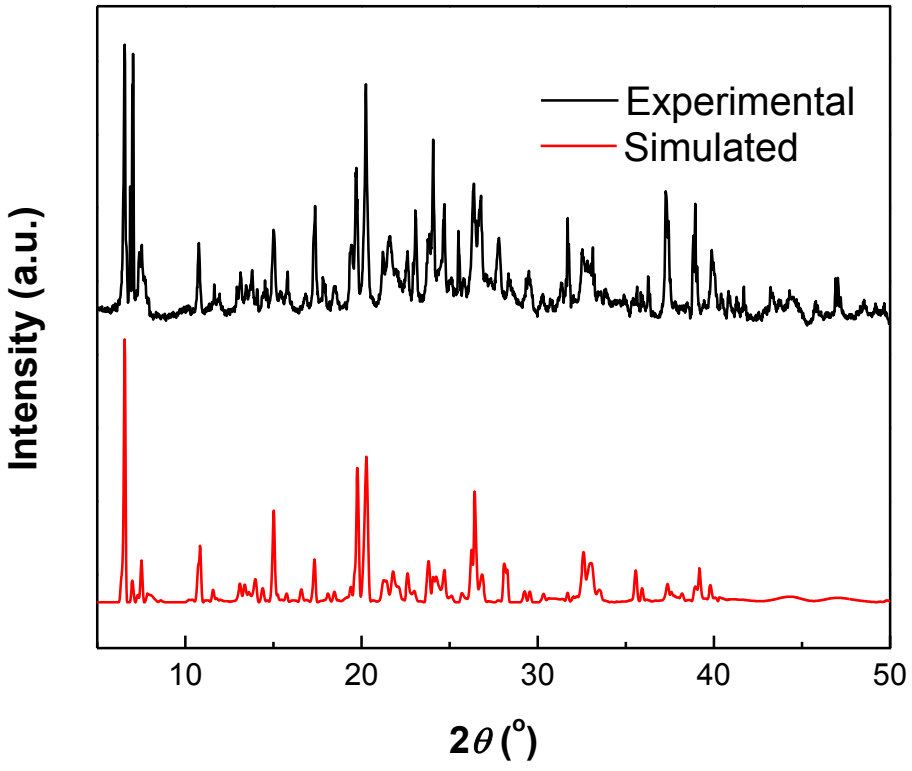


Figure S7 PXRD pattern of MOF (**1**).

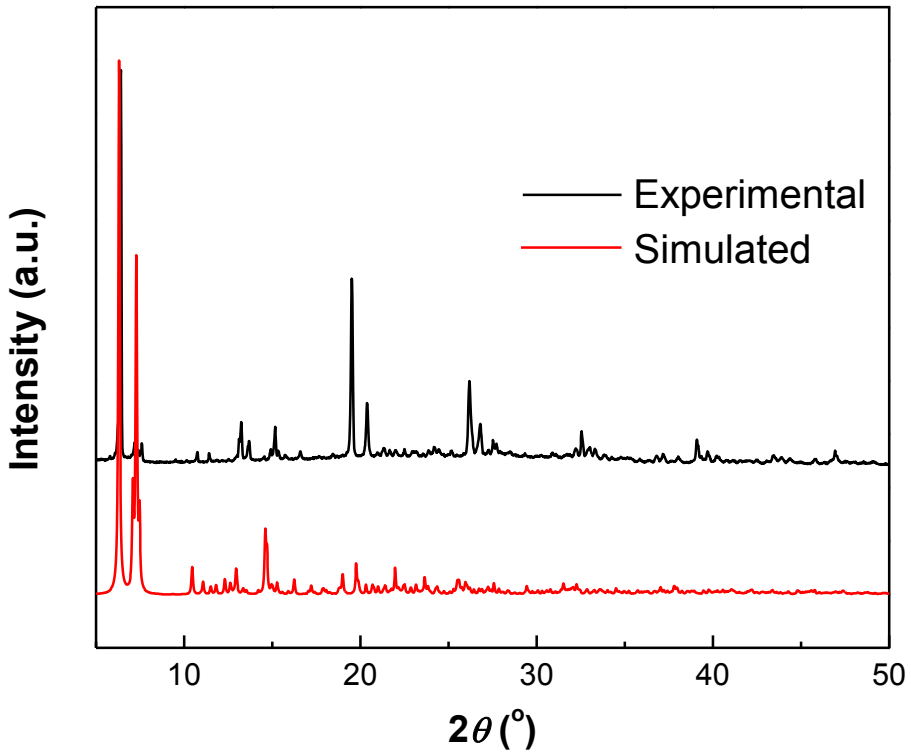


Figure S8 PXRD pattern of MOF (**2**).

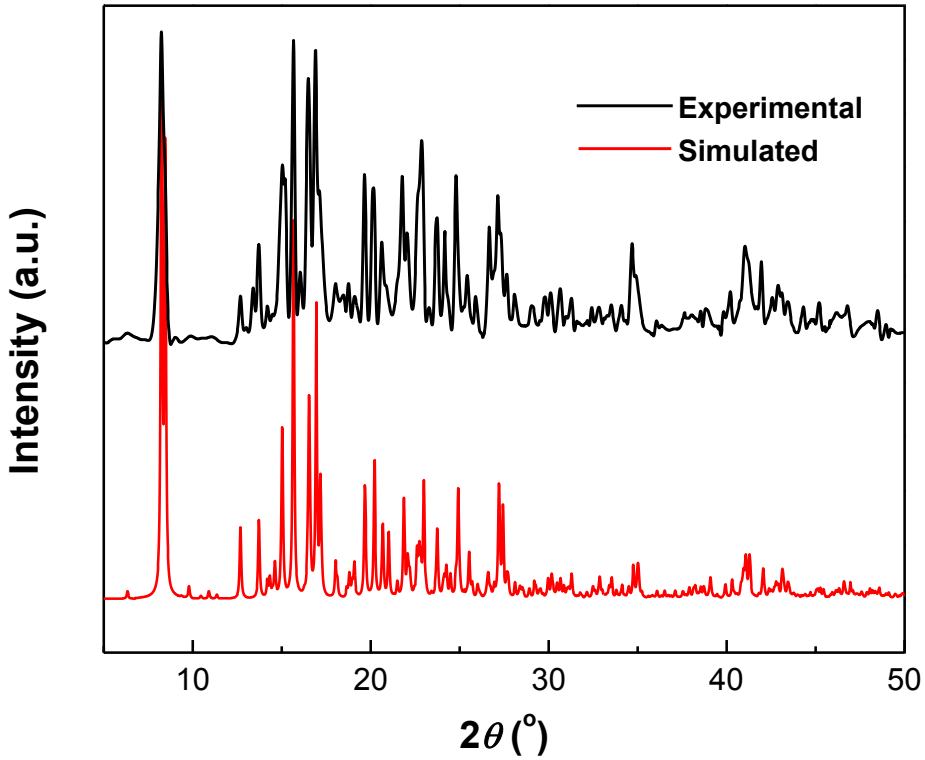


Figure S9 PXRD pattern of MOF (**3**).

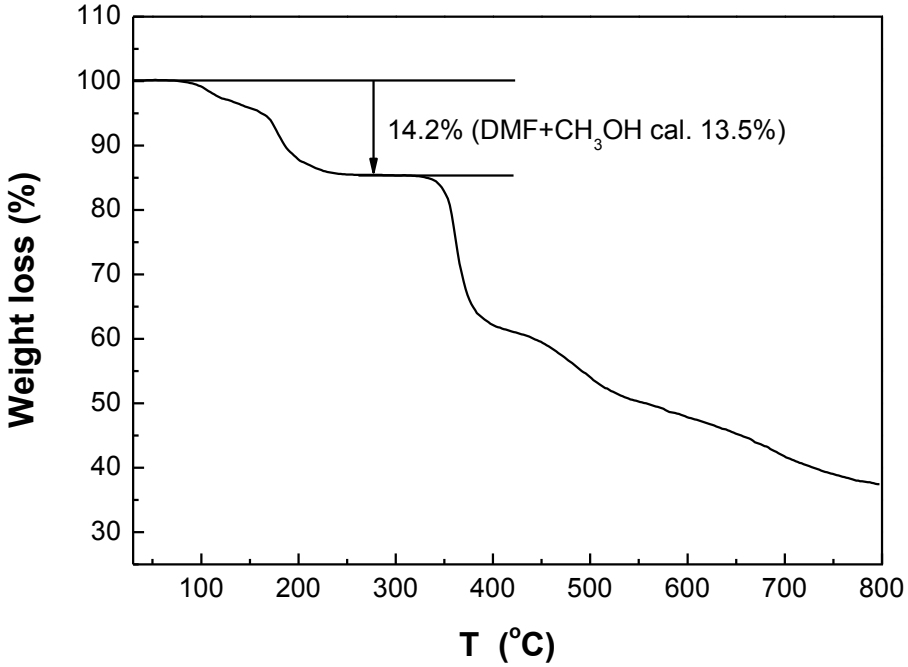


Figure S10 TGA curve of MOF (**1**).

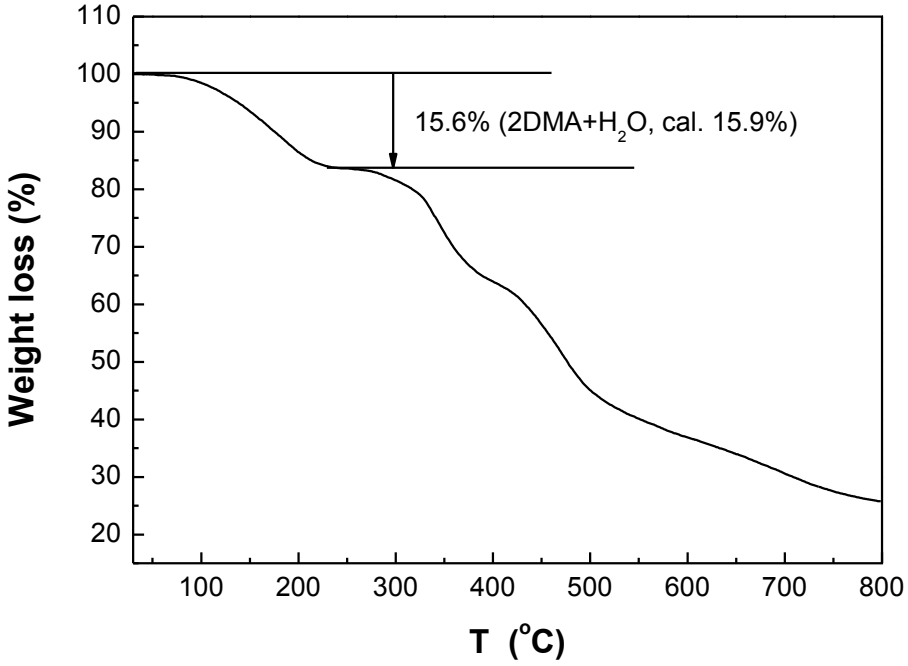


Figure S11 TGA curve of MOF (**2**).

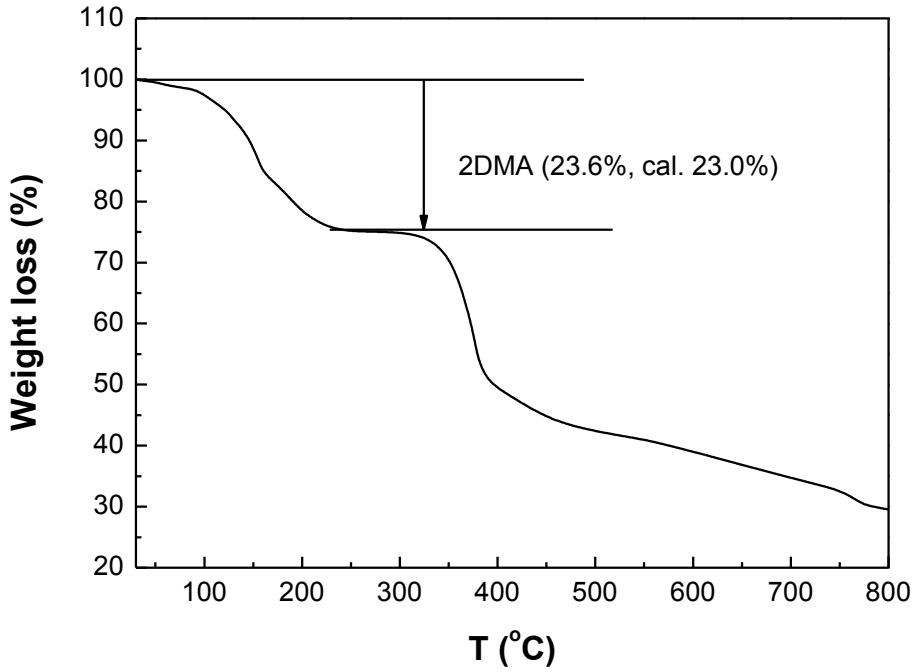


Figure S12 TGA curve of MOF (**3**).

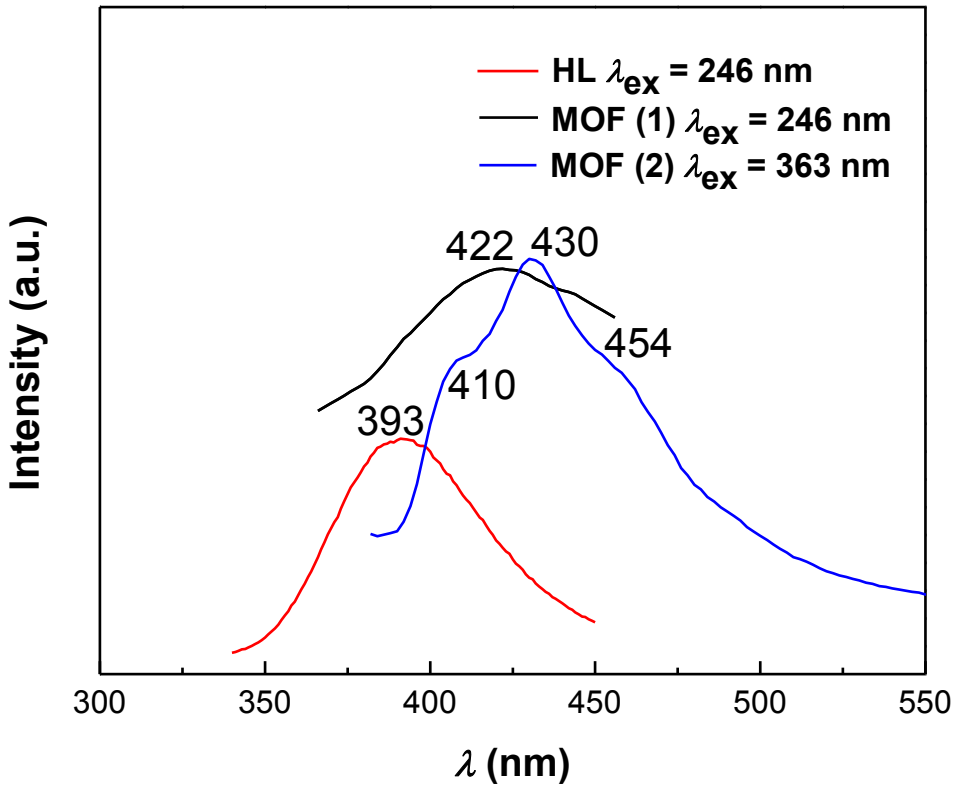


Figure S13 Solid photoluminescent emission spectra of H*L*, MOFs (**1**) and (**2**).

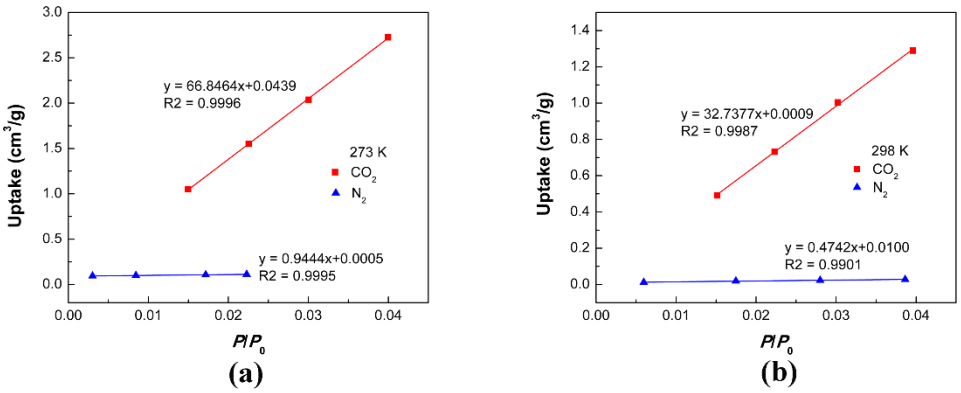


Figure S14 Initial slope calculation for CO_2 and N_2 isotherms of (**2**) collected at 273 K (a) and 298 K (b). (CO_2: red squares; N_2: blue triangles)

Table S1 Selected geometric parameters of MOF (**1**) (Å, °)

Cd1—N3	2.318 (4)	Cd1—O9	2.386 (5)
Cd1—O6^{i}	2.339 (4)	Cd1—O5^{i}	2.438 (3)
Cd1—N1^{ii}	2.344 (4)	Cd1—O1	2.484 (3)
Cd1—O2	2.372 (3)	Cd1···Cd1^{iii}	8.246 (2)
Cd1···Cd1^{iv}	13.478 (2)	Cd1···Cd1^{v}	13.542 (2)
N3—Cd1—O6^{i}	141.28 (13)	O6^{i}—Cd1—O5^{i}	54.27 (13)
N3—Cd1—N1^{ii}	99.57 (14)	N1^{ii}—Cd1—O5^{i}	90.53 (14)
O6^{i}—Cd1—N1^{ii}	88.85 (16)	O2—Cd1—O5^{i}	136.94 (13)
N3—Cd1—O2	132.17 (13)	O9—Cd1—O5^{i}	88.0 (2)
O6^{i}—Cd1—O2	83.37 (14)	N3—Cd1—O1	82.73 (13)
N1^{ii}—Cd1—O2	96.54 (14)	O6^{i}—Cd1—O1	135.55 (13)
N3—Cd1—O9	81.6 (2)	N1^{ii}—Cd1—O1	88.53 (14)
O6^{i}—Cd1—O9	89.2 (2)	O2—Cd1—O1	52.94 (14)
N1^{ii}—Cd1—O9	178.0 (2)	O9—Cd1—O1	93.2 (2)
O2—Cd1—O9	83.69 (19)	O5^{i}—Cd1—O1	170.09 (12)
N3—Cd1—O5^{i}	87.70 (12)		

Symmetry codes: (i) *x*-1, -*y*+3/2, *z*-1/2; (ii) *x*, -*y*+1/2, *z*-1/2; (iii) -*x*+1, *y*+1/2, -*z*+1/2; (iv) *x*+1, -*y*+3/2, *z*+1/2; (v) *x*, -*y*+1/2, *z*+1/2.

Table S2 Selected geometric parameters of MOF (**2**) (Å, °)

Cd1—O14^{i}	2.221 (8)	Cd2—O1	2.284 (5)
Cd1—O2	2.253 (5)	Cd2—N1^{iv}	2.323 (6)
Cd1—N3^{ii}	2.337 (6)	Cd2—O10	2.365 (6)
Cd1—N5^{iii}	2.337 (6)	Cd2—O5	2.412 (6)

Cd1—O9	2.397 (6)	Cd2—O6	2.452 (5)
Cd1—O6	2.460 (5)	Cd2—O9	2.542 (5)
Cd2—O13	2.262 (7)	Cd1···Cd2^{i}	5.218 (1)
Cd1···Cd2	3.620 (8)		
O14^{i}—Cd1—O2	155.0 (3)	O13—Cd2—O1	87.2 (2)
O14^{i}—Cd1—N5^{iii}	114.0 (3)	O13—Cd2—N1^{iv}	100.5 (2)
O2—Cd1—N5^{iii}	87.56 (19)	O1—Cd2—N1^{iv}	172.0 (2)
O14^{i}—Cd1—N3^{ii}	102.2 (3)	O13—Cd2—O10	87.3 (2)
O2—Cd1—N3^{ii}	88.1 (2)	O1—Cd2—O10	88.41 (18)
N5^{iii}—Cd1—N3^{ii}	93.8 (2)	N1^{iv}—Cd2—O10	89.8 (2)
O14^{i}—Cd1—O9	82.8 (3)	O13—Cd2—O5	85.8 (2)
O2—Cd1—O9	84.7 (2)	O1—Cd2—O5	88.75 (18)
N5^{iii}—Cd1—O9	90.26 (19)	N1^{iv}—Cd2—O5	93.9 (2)
N3^{ii}—Cd1—O9	171.6 (2)	O10—Cd2—O5	172.65 (18)
O14^{i}—Cd1—O6	74.5 (3)	O13—Cd2—O6	138.6 (2)
O2—Cd1—O6	82.78 (18)	O1—Cd2—O6	86.88 (18)
N5^{iii}—Cd1—O6	169.2 (2)	N1^{iv}—Cd2—O6	88.7 (2)
N3^{ii}—Cd1—O6	90.80 (18)	O10—Cd2—O6	133.40 (18)
O9—Cd1—O6	83.96 (17)	O5—Cd2—O6	53.14 (18)
O10—Cd2—O9	52.45 (18)	O13—Cd2—O9	139.7 (2)
O5—Cd2—O9	134.28 (19)	O1—Cd2—O9	89.32 (18)

Symmetry codes: (i) *x*−1, *y*, *z*; (ii) −*x*, −*y*+1, −*z*+1; (iii) −*x*, −*y*+1, −*z*; (iv) *x*, *y*−1, *z*.

Table S3 Selected geometric parameters of MOF (**3**) (Å, °)

Ni1—O1W	2.059 (2)	Ni2—O1	2.016 (2)
Ni1—O5	2.068 (2)	Ni2—O2W	2.071 (2)
Ni1—N1	2.116 (2)	Ni2—N3^{iii}	2.126 (3)
Ni1···Ni2	13.255 (2)	Ni1···Ni2^{v}	13.451 (3)
Ni1···Ni2^{vi}	7.124 (2)		
O1W—Ni1—O1W^{i}	180.0	O1—Ni2—O1^{ii}	180.0
O1W—Ni1—O5	89.87 (9)	O1—Ni2—O2W	88.36 (9)
O1W^{i}—Ni1—O5	90.13 (9)	O1^{ii}—Ni2—O2W	91.64 (9)
O1W—Ni1—O5^{i}	90.13 (9)	O1—Ni2—O2W^{ii}	91.64 (9)
O1W^{i}—Ni1—O5^{i}	89.87 (9)	O1^{ii}—Ni2—O2W^{ii}	88.36 (9)
O5—Ni1—O5^{i}	180.0	O2W—Ni2—O2W^{ii}	180.00 (12)
O1W—Ni1—N1^{i}	89.38 (11)	O1—Ni2—N3^{iii}	91.20 (9)
O1W^{i}—Ni1—N1^{i}	90.62 (11)	O1^{ii}—Ni2—N3^{iii}	88.80 (9)
O5—Ni1—N1^{i}	87.91 (9)	O2W—Ni2—N3^{iii}	88.42 (11)
O5^{i}—Ni1—N1^{i}	92.09 (9)	O2W^{ii}—Ni2—N3^{iii}	91.58 (10)
O1W—Ni1—N1	90.62 (10)	O1—Ni2—N3^{iv}	88.80 (9)
O1W^{i}—Ni1—N1	89.38 (10)	O1^{ii}—Ni2—N3^{iv}	91.20 (9)
O5—Ni1—N1	92.09 (9)	O2W—Ni2—N3^{iv}	91.58 (10)
O5^{i}—Ni1—N1	87.91 (9)	O2W^{ii}—Ni2—N3^{iv}	88.42 (11)
N1^{i}—Ni1—N1	180.0	N3^{iii}—Ni2—N3^{iv}	180.0

Symmetry codes: (i) −*x*, −*y*, −*z*; (ii) −*x*, −*y*+2, −*z*+1; (iii) −*x*+1, −*y*+1, −*z*+1; (iv) *x*−1, *y*+1, *z*; (v) *x*+1, *y*−1, *z*; (vi) *x*, *y*−1, *z*.

Table S4 Hydrogen-bonding geometry and C-H···π interaction (Å, °) for MOF (**1**).

D-H···*A*	*D*-H	H···*A*	*D*···*A*	*D*-H···*A*
C1-H1*A*···O1^{i}	0.95	2.58(2)	3.281(7)	131(2)
C13-H13*A*···O1	0.95	2.25(2)	2.994(8)	134(2)
C16-H16*A*···O2^{ii}	0.95	2.57(2)	3.480(6)	161(2)
C17-H17*A*···O5^{iii}	0.95	2.57(2)	3.238(7)	127(2)
C26-H26*C*···N5^{iv}	0.98	1.95(2)	2.73(3)	135(2)
C27-H27*B*···O8^{v}	0.98	2.52(3)	3.26(4)	132(3)
C26-H26*B*···π(Ph)^{iv}	0.98	2.53(3)	3.50(2)	171(3)

Symmetry codes: (i) *x*, -*y*+1/2, *z*+1/2; (ii) –*x*+1, *y*+1/2, -*z*+1/2; (iii) *x*-1, -*y*+3/2, *z*-1/2; (iv) -*x*+1, -*y*+1, -*z*+1; (v) *x*-1, *y*, *z*.

Table S5 Hydrogen-bonding geometry (Å, °) for MOF (**2**).

D-H···*A*	*D*-H	H···*A*	*D*···*A*	*D*-H···*A*
C10-H10*A*···O3^{i}	0.93	2.59(2)	3.491(11)	163(2)
C13-H13*A*···O13^{ii}	0.93	2.56(2)	3.389(11)	149(2)
C17-H17*A*···O2^{iii}	0.93	2.55(3)	3.192(9)	126(3)
C25-H25*A*···O13^{iv}	0.93	2.42(2)	3.264(10)	151(2)
C29-H29*A*···O2^{v}	0.93	2.51(2)	3.152(9)	126(2)

Symmetry codes: (i) *x*-1, *y*, *z*; (ii) 1-*x*, 1-*y*, 1-*z*; (iii) -*x*, 1-*y*, 1-*z*; (iv) 1-*x*, 1-*y*, -*z*; (v) -*x*, 1-*y*, -*z*.

Table S6 Dihedral angles (°) for MOFs (**1**)-(**3**).

MOFs	Py/Ph	-NO_2/Ph	CO_2^-/Ph
(**1**)	69.2(1), 54.3(3)	36.6(3), 35.3(2)	4.6(3), 7.9(5)
(**2**)	56.5(2), 46.5(2), 45.8(3)	41.2(4), 39.8(2), 37.0(3)	2.6(3), 7.3(3), 5.0(2)
(**3**)	37.4(3), 66.4(2)	63.2(2), 45.5(3)	5.5(3), 1.2(1)