Supporting Information

For the

Manuscript

Luminescent Cd^{II} metal-organic frameworks based on isoniazid using mixed ligand approach

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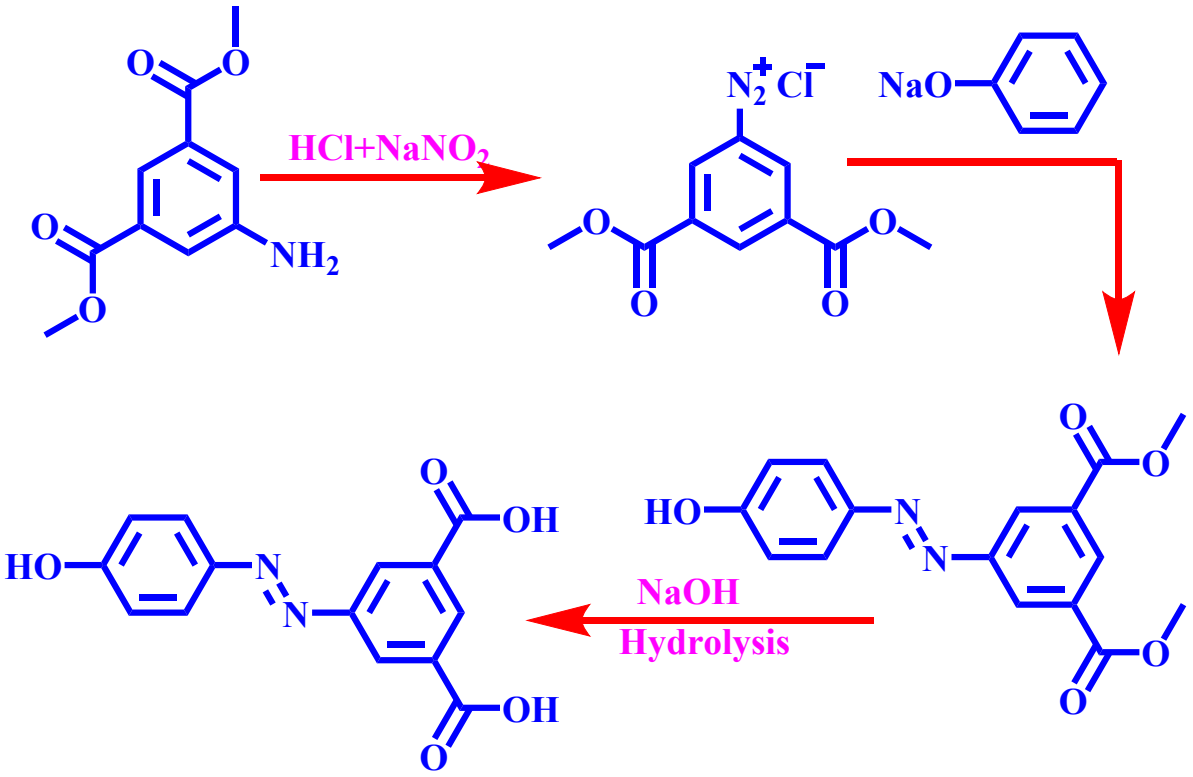
Synthesis of hpdia (5-(4-hydroxyphenylazo)isophthalic acid)

To a solution of dimethyl-5-aminoisophthalate (10 mmol, 2.1 g) in 20 mL of H_2O was added 1 mL of conc. HCl, the solution was cooled to 5ºC. A solution of $NaNO_2$ (11 mmol, 0.75 g) in 2 mL of ice cold water, was added drop wise with vigorous stirring to the above solution. In a separate flask, a mixture of phenol (12 mmol, 1.13 g) and NaOAc (110 mmol, 9 g) in 20 mL of ice water was prepared. The diazonium solution was added to the phenolic solution drop wise over 20 min with vigorous stirring. The mixture was allowed to warm up to room temperature naturally, then filtered, and washed with distilled water (3 × 100 mL). The orange-red precipitate was air dried to yield 2.9 g, 92% of dimethyl-5-(4-hydroxyphenylazo)isophthalate. In a typical hydrolysis reaction, dimethyl-5-(4-hydroxyphenylazo)isophthalate was added to a round bottom flask containing methanol (150 mL). An aqueous NaOH solution (6g in 20mL H_2O) was added to this mixture and then refluxed at 50ºC/12h. The solution was acidified to pH=1 using concentrated HCl. The precipitate was separated by filtration, washed with cold H_2O to yield 2.5 g, 88% of 5-(4-hydroxyphenylazo)isophthalic acid. Elemental analysis for $C_{14}H_{10}N_2O_5$ (%), calc: C, 58.74; H, 3.52; N, 9.79; found: C, 58.61; H, 3.58; N, 9.69. FT-IR (KBr, cm^{-1}): 3390(ν_{O-H}), 1704($\nu_{C=O}$), 1600, 1506, 1417, 1319, 1271, 1234, 1149, 1108, 979, 919, 838, 759, 744, 605.



Scheme S1. Synthetic route for ligand **hpdia**.

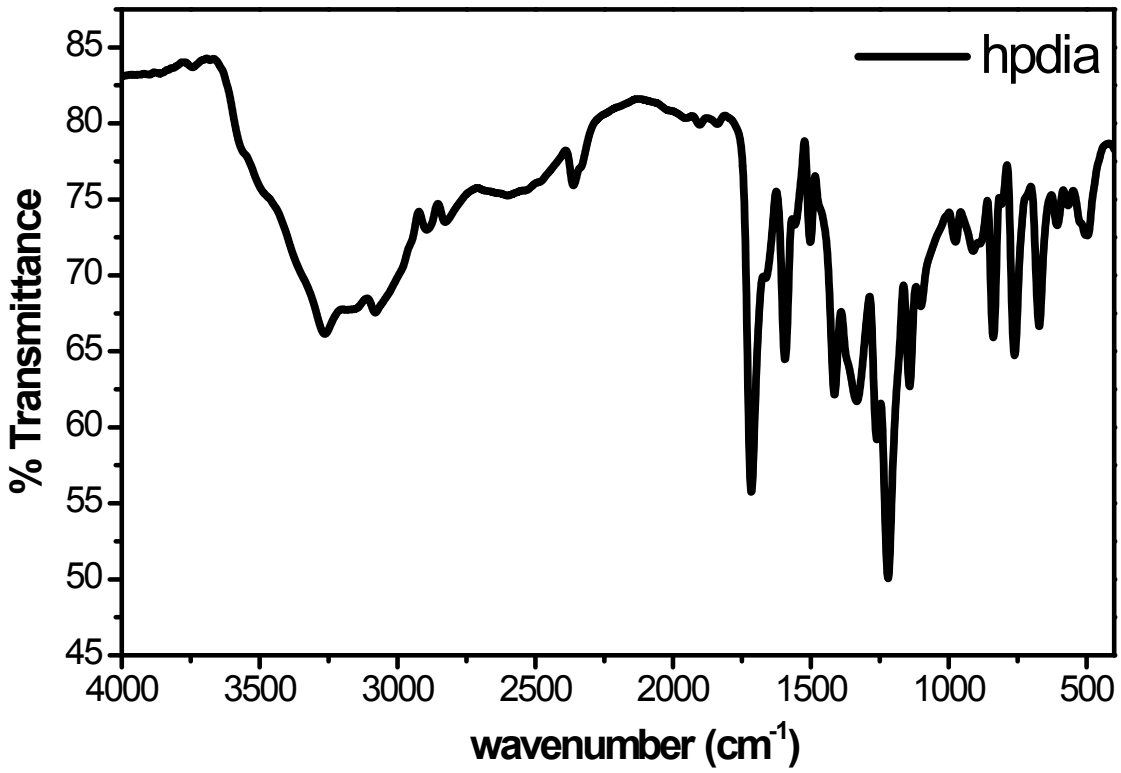


Figure S1. FT-IR spectrum of ligand **hpdia**.

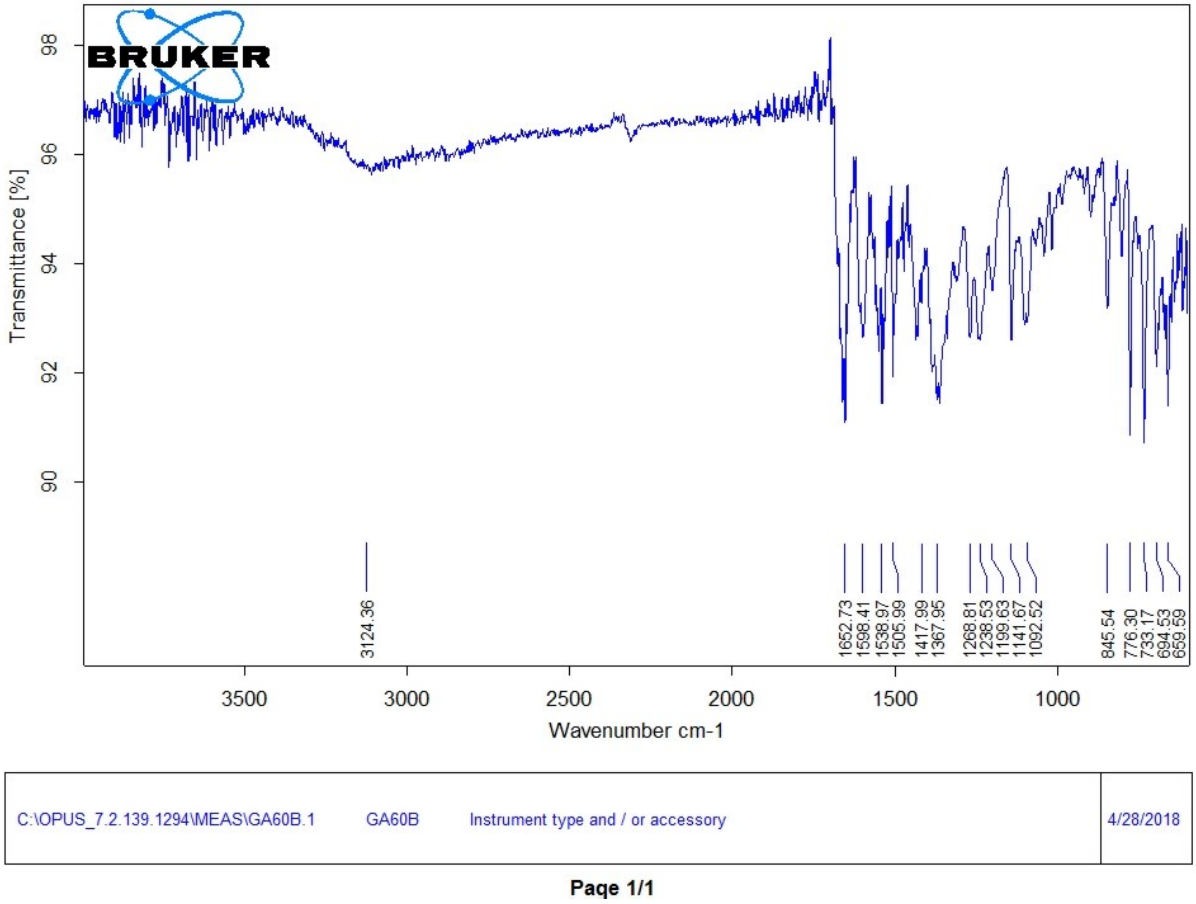


Figure S2. FT-IR spectra of **Cd-MOF-1**.

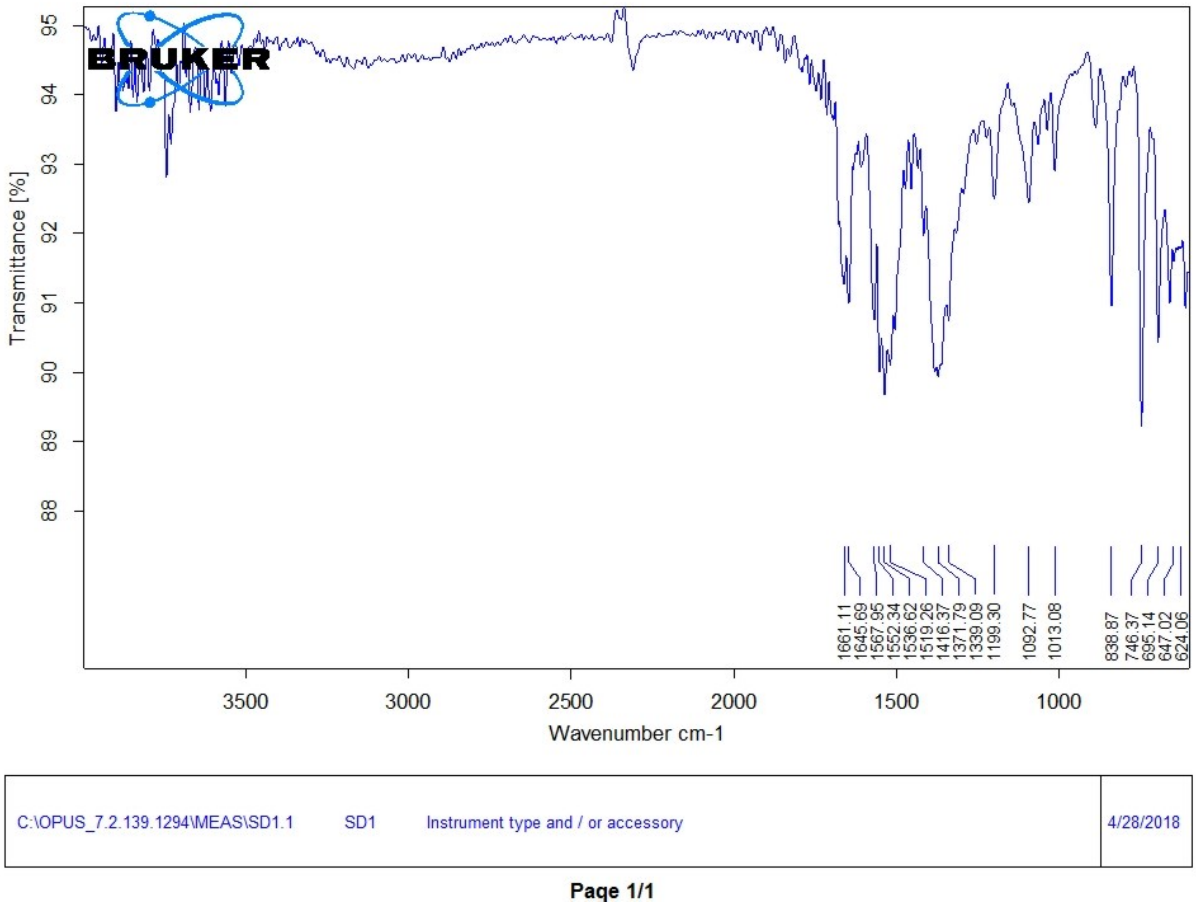


Figure S3. FT-IR spectra of **Cd-MOF-2**.

FLASH EA 1112 SERIES CHN REPORT
THERMO FINNIGAN

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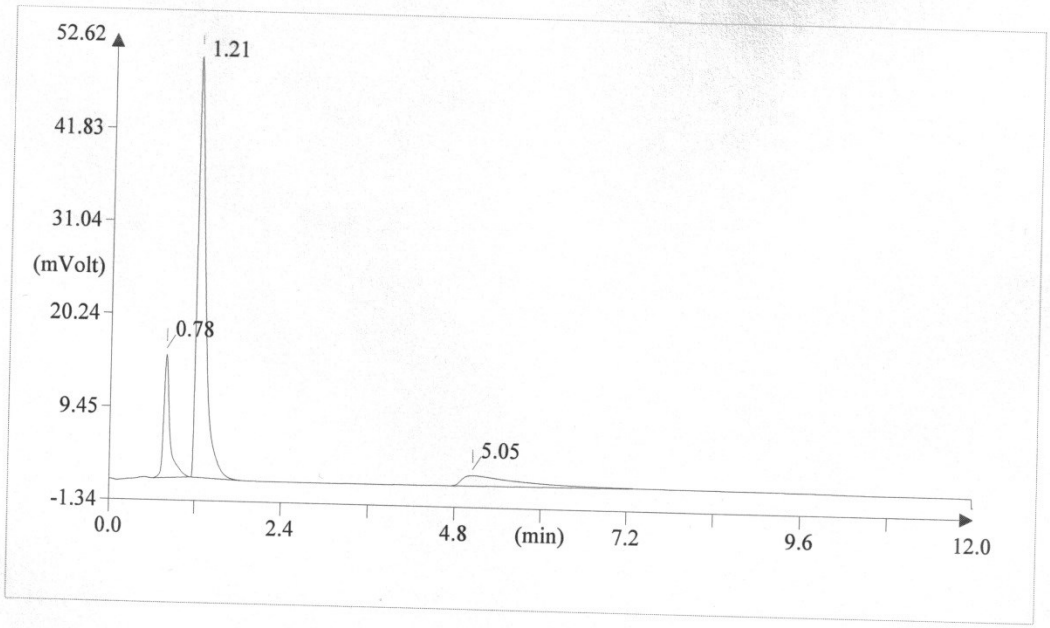

Element Name	Element %	Ret. Time
Nitrogen	11. 49	0. 78
Carbon	39. 65	1. 21
Hydrogen	3. 62	5. 05

Figure S4. Elemental analysis of **Cd-MOF-1**.

FLASH EA 1112 SERIES CHN REPORT
THERMO FINNIGAN

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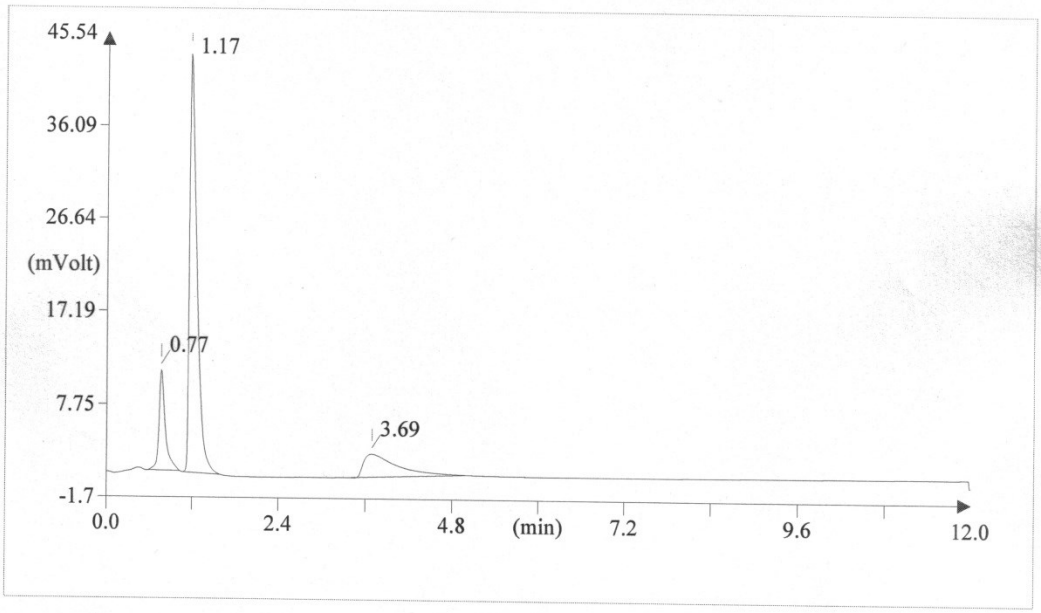

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Nitrogen	12. 45	0. 77
Carbon	42. 85	1. 17
Hydrogen	4. 56	3. 69

Figure S5. Elemental analysis of **Cd-MOF-2**.

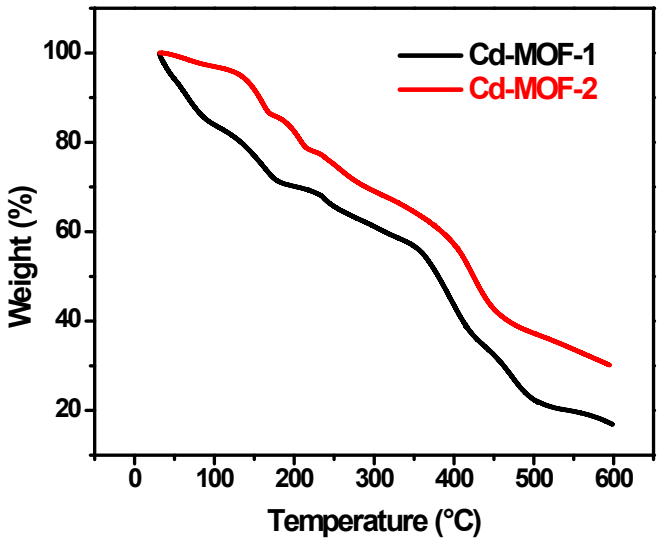

Figure S6. TGA plots for Cd-MOFs **Cd-MOF-1** and **Cd-MOF-2**.

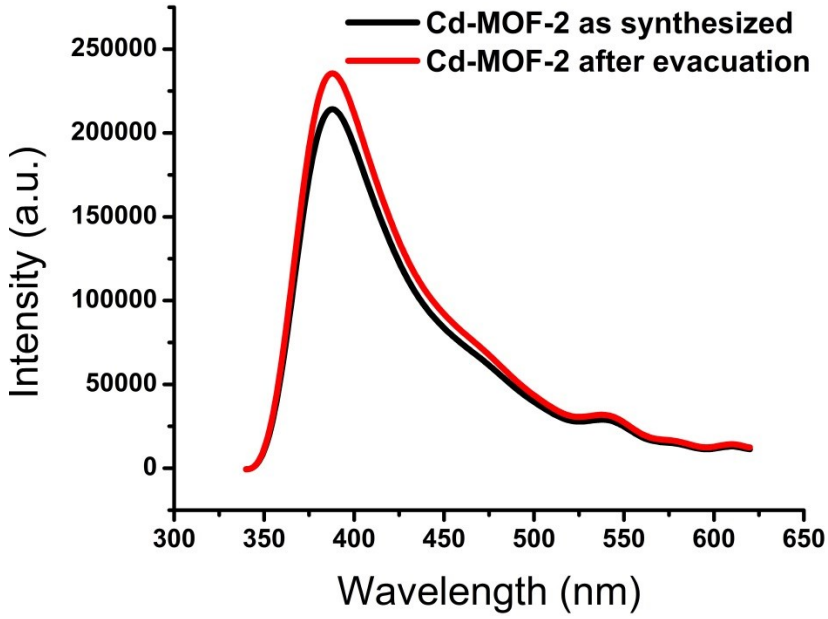

Figure S7. Comparison of photoluminescence intensities of as synthesised Cd-MOF-2 and after heating it at 140°C.

Table S1. Selected bond lengths (Å) and bond angles (°) for **Cd-MOF-1 and Cd-MOF-2.**

Cd-MOF-1		**Cd-MOF-2**	
Cd1–O6$^{\#1}$	2.357(4)	Cd1–O3	2.327(2)
Cd1–O3$^{\#2}$	2.478(4)	Cd1–O2$^{\#1}$	2.2921(18)
Cd1–O5	2.259(4)	Cd1–O2	2.2921(19)
Cd1–O2$^{\#2}$	2.320(4)	Cd1–N1	2.328(3)
Cd1–O4	2.619(5)	Cd1–O1$^{\#1}$	2.556(2)
Cd1–N3	2.305(4)	Cd1–O1	2.556(2)
Cd1–N5$^{\#1}$	2.324(5)	Cd1–N3$^{\#2}$	2.382(2)
O6$^{\#1}$–Cd1–O3$^{\#2}$	80.30(15)	O3–Cd1–N1	71.14(8)
O6$^{\#1}$–Cd1–O4	91.55(15)	O3–Cd1–O1$^{\#1}$	87.21(5)
O3$^{\#2}$–Cd1–O4	171.67(14)	O3–Cd1–O1	87.21(5)
O5–Cd1–O6$^{\#1}$	143.48(15)	O3–Cd1–N3$^{\#2}$	167.90(9)
O5–Cd1–O3$^{\#2}$	136.04(14)	O2–Cd1–O3	94.39(7)
O5–Cd1–O2$^{\#2}$	82.69(14)	O2$^{\#1}$–Cd1–O3	94.39(7)
O5–Cd1–O4	52.01(14)	O2–Cd1–O2$^{\#1}$	76.70(9)
O5–Cd1–N3	93.96(16)	O2–Cd1–N1	139.76(5)
O5–Cd1–N5$^{\#1}$	99.71(16)	O2$^{\#1}$–Cd1–N1	139.76(5)
O2$^{\#2}$–Cd1–O6$^{\#1}$	133.70(14)	O2$^{\#1}$–Cd1–O1$^{\#1}$	52.88(6)
O2$^{\#2}$–Cd1–O3$^{\#2}$	53.41(14)	O2–Cd1–O1	52.88(6)
O2$^{\#2}$–Cd1–O4	134.70(14)	O2$^{\#1}$–Cd1–O1	129.47(6)
O2$^{\#2}$–Cd1–N5$^{\#1}$	106.81(17)	O2–Cd1–O1$^{\#1}$	129.48(6)
N3–Cd1–O6$^{\#1}$	82.94(15)	O2$^{\#1}$–Cd1–N3$^{\#2}$	95.09(8)
N3–Cd1–O3$^{\#2}$	96.53(16)	O2–Cd1–N3$^{\#2}$	95.09(8)
N3–Cd1–O2$^{\#2}$	101.17(17)	N1–Cd1–O1$^{\#1}$	88.24(4)
N3–Cd1–O4	84.02(17)	N1–Cd1–O1	88.24(4)
N3–Cd1–N5$^{\#1}$	150.12(16)	N1–Cd1–N3$^{\#2}$	96.76(9)
N5$^{\#1}$–Cd1–O6$^{\#1}$	70.27(14)	O1–Cd1–O1$^{\#1}$	174.13(11)
N5$^{\#1}$–Cd1–O3$^{\#2}$	91.87(16)	N3$^{\#2}$–Cd1–O1$^{\#1}$	92.54(5)
N5$^{\#1}$–Cd1–O4	83.73(17)	N3$^{\#2}$–Cd1–O1	92.54(5)
Symmetry transformations used to generate equivalent atoms: #1: +X, 0.5-Y, +Z; #2: 1+X, +Y, 1+Z; #3: 2-X, 1-Y, 1-Z; #4: -1+X, +Y, -1+Z;		Symmetry transformations used to generate equivalent atoms: #1: +X, 0.5-Y, 0.5+Z; #2: -1+X, +Y, +Z; #3: +X, 0.5-Y, -0.5+Z; #4: 1+X, +Y, +Z;	

Table S2. Hydrogen bonds for **Cd-MOF-1** and **Cd-MOF-2**.

D–H···A [Å]	d(D–H) [Å]	d(H···A) [Å]	d(D···A) [Å]	<(DHA) [°]
Cd-MOF-1				
N4–H4···O8A$^{\#1}$	0.86	1.95	2.748(11)	154.4
N5–H5A···O5$^{\#1}$	0.86	1.93	2.792(6)	161.7
Cd-MOF-2				
N2–H2···O2$^{\#1}$	0.86	2.22	2.875(3)	133.0
N2–H2···O2$^{\#2}$	0.86	2.22	2.875(3)	133.0

Symmetry transformations used to generate equivalent atoms for **Cd-MOF-1**: #1: -X, -0.5+Y, 1.5-Z; and for **Cd-MOF-2**: #1: -1+X, +Y, +Z; #2: -1+X, 0.5-Y, +Z;