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Supporting information for article:

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Topological identification of the first uninodal 8-connected lsz MOF built from 2,2′-difluoro-4,4′-biphenyldicarboxylate pillars and Cd(II)-triazolate layers

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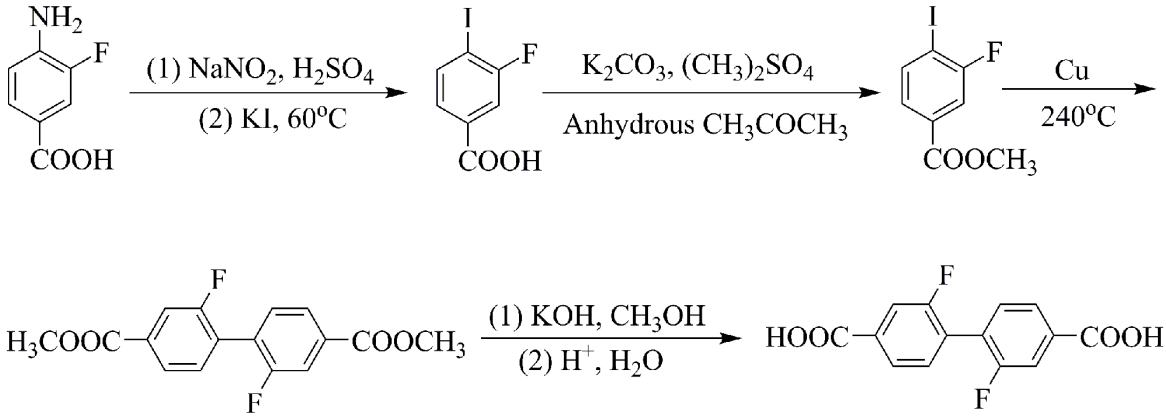

Scheme S1 Synthetic route of 2,2′-difluoro-4,4′-biphenyldicarboxylic acid (H_2L).

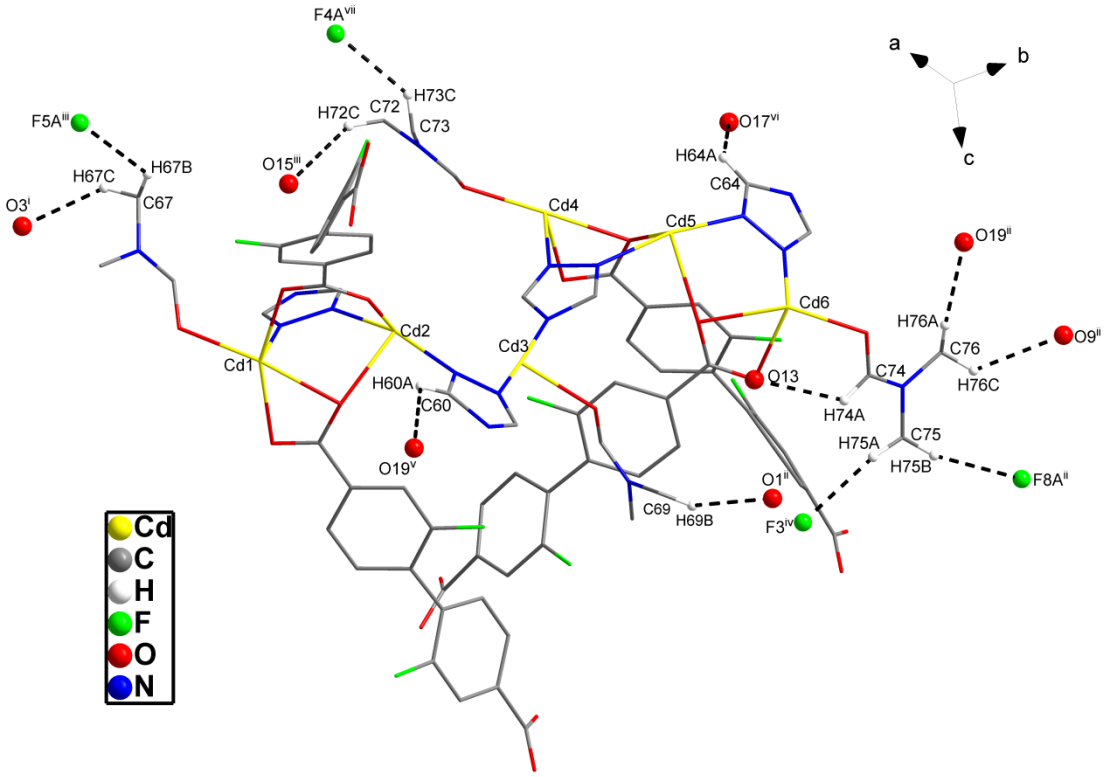

Figure S1 The network of (I) was stabilized by intermolecular C–H···F and C–H···O hydrogen bonds (black dotted lines).

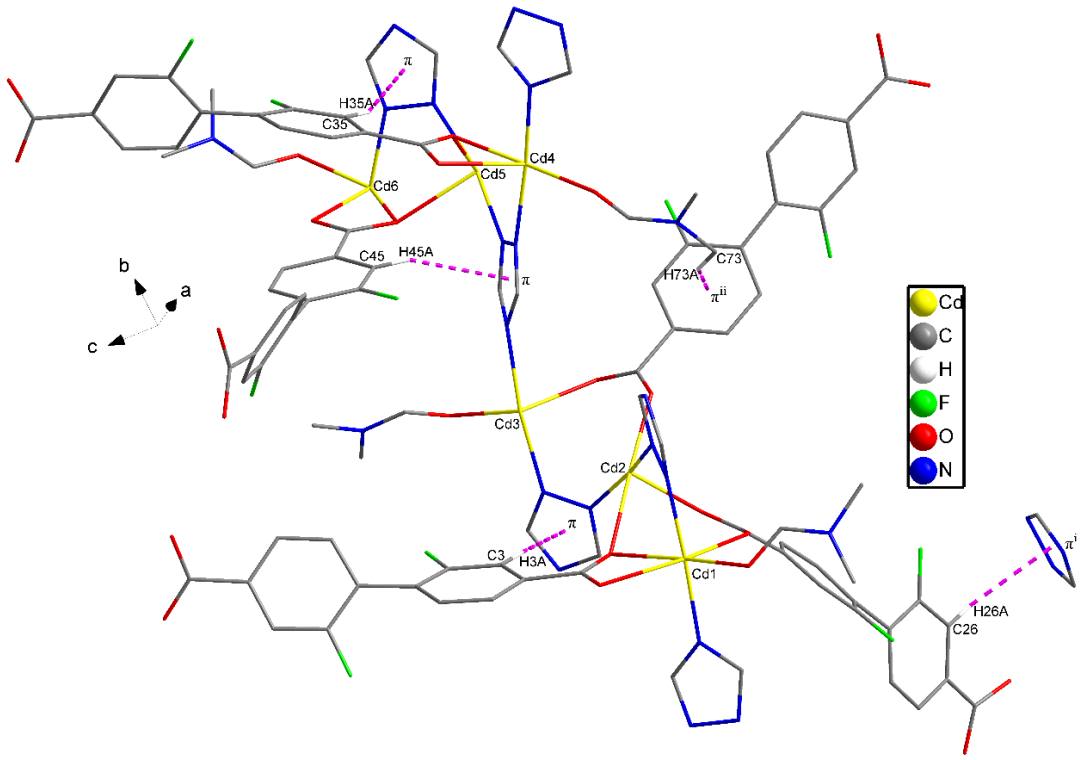

Figure S2 The intermolecular C–H···π interactions in (I) (pink dotted lines).

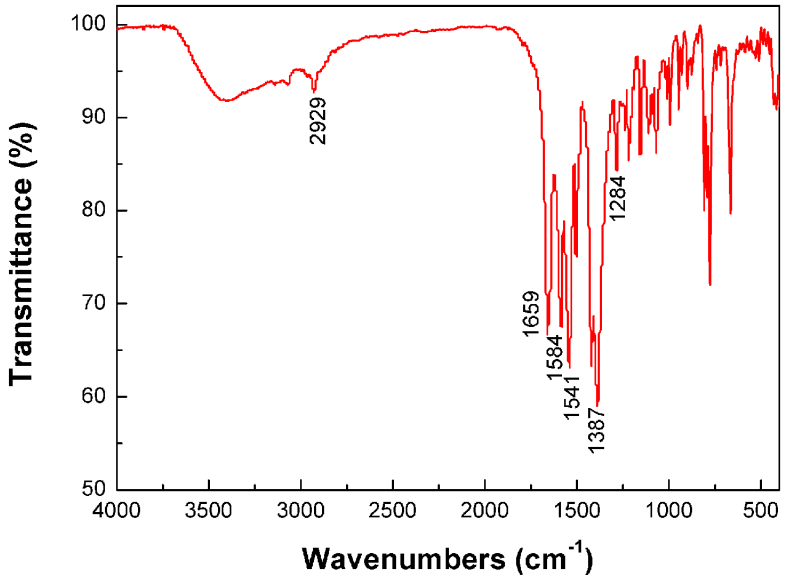

Figure S3 The IR spectrum of (I).

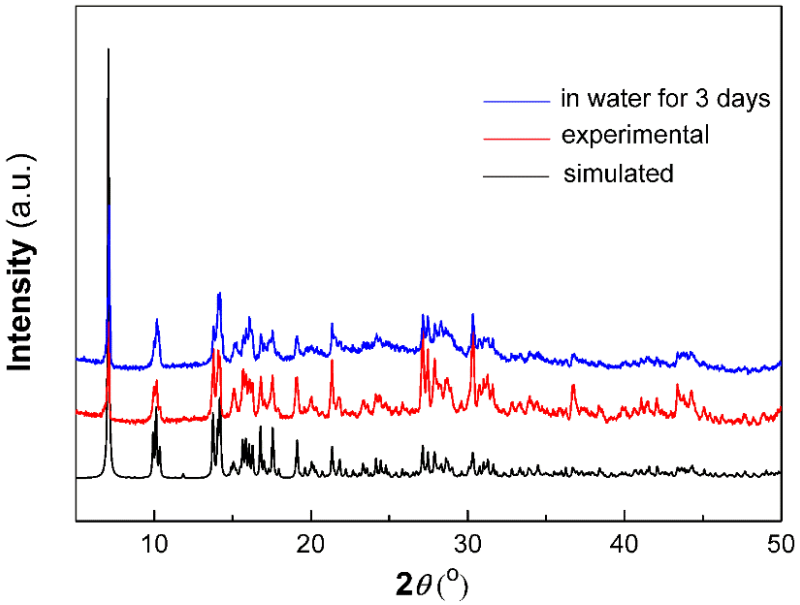

Figure S4 Experimental and simulated powder X-ray diffraction patterns for (I) and the water-treated sample.

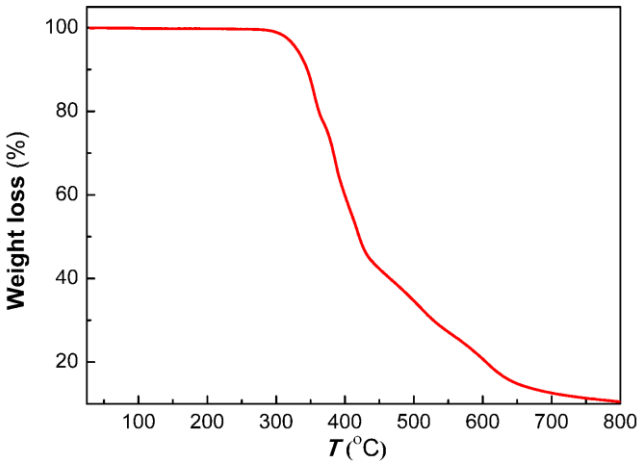

Figure S5 TGA curve for (I).

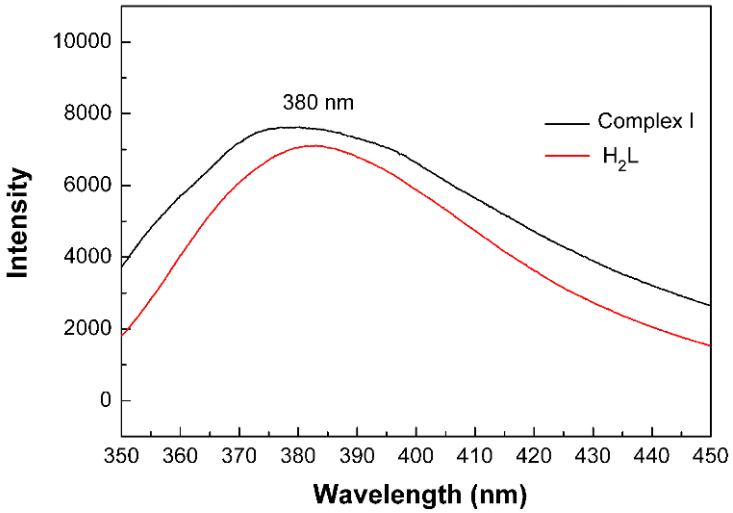

Figure S6 Solid state photoluminescence spectra for (I) and the free H_2L (λ_{ex} = 320 nm).

Table S1 Selected geometric parameters (Å, º) of (I)

Cd1—N1	2.214 (8)	Cd4—N6^{iv}	2.246 (7)
Cd1—N12^{i}	2.242 (7)	Cd4—N7	2.286 (8)
Cd1—O5	2.277 (6)	Cd4—O11^{v}	2.266 (7)
Cd1—O17	2.285 (6)	Cd4—O19	2.288 (7)
Cd1—O1	2.367 (7)	Cd4—O9	2.367 (7)
Cd1—O2	2.391 (7)	Cd4—O10	2.410 (7)
Cd2—N2	2.243 (8)	Cd5—N8	2.248 (7)
Cd2—N4	2.255 (7)	Cd5—N10	2.258 (7)
Cd2—O6	2.233 (7)	Cd5—O12^{v}	2.235 (7)

Cd2—O4^{ii}	2.263 (7)	Cd5—O16^{vi}	2.249 (7)
Cd2—O2	2.436 (7)	Cd5—O10	2.401 (6)
Cd2—O8^{iii}	2.444 (7)	Cd5—O14	2.456 (7)
Cd3—N5	2.239 (8)	Cd6—N11	2.212 (7)
Cd3—N9	2.244 (8)	Cd6—N3^{vii}	2.223 (7)
Cd3—O18	2.294 (8)	Cd6—O15^{vi}	2.293 (7)
Cd3—O3^{ii}	2.300 (7)	Cd6—O20	2.300 (7)
Cd3—O8^{iii}	2.378 (6)	Cd6—O13	2.354 (6)
Cd3—O7^{iii}	2.410 (7)	Cd6—O14	2.410 (6)
Cd1···Cd2	3.670(8)	Cd4···Cd5	3.675(10)
Cd2···Cd3	3.652(9)	Cd5···Cd6	3.666(10)

N1—Cd1—N12^{i}	177.1 (3)	N6^{iv}—Cd4—O11^{v}	92.1 (3)
N1—Cd1—O5	92.8 (3)	N6^{iv}—Cd4—N7	174.8 (3)
N12^{i}—Cd1—O5	89.7 (3)	O11^{v}—Cd4—N7	93.2 (3)
N1—Cd1—O17	92.7 (3)	N6^{iv}—Cd4—O19	88.6 (3)
N12^{i}—Cd1—O17	88.9 (3)	O11^{v}—Cd4—O19	83.8 (3)
O5—Cd1—O17	86.9 (3)	N7—Cd4—O19	92.2 (3)
N1—Cd1—O1	90.3 (3)	N6^{iv}—Cd4—O9	83.8 (3)
N12^{i}—Cd1—O1	86.7 (3)	O11^{v}—Cd4—O9	152.0 (2)
O5—Cd1—O1	155.5 (2)	N7—Cd4—O9	91.5 (3)
O17—Cd1—O1	117.3 (3)	O19—Cd4—O9	123.6 (2)
N1—Cd1—O2	86.6 (3)	N6^{iv}—Cd4—O10	91.7 (3)
N12^{i}—Cd1—O2	91.5 (3)	O11^{v}—Cd4—O10	97.3 (2)
O5—Cd1—O2	100.7 (3)	N7—Cd4—O10	87.4 (3)
O17—Cd1—O2	172.4 (3)	O19—Cd4—O9	123.6 (2)
O1—Cd1—O2	55.2 (2)	O9—Cd4—O10	55.3 (2)
O6—Cd2—N2	102.8 (3)	O12^{v}—Cd5—N8	102.9 (3)
O6—Cd2—N4	86.5 (3)	O12^{v}—Cd5—O16^{vi}	94.6 (3)
N2—Cd2—N4	165.6 (3)	N8—Cd5—O16^{vi}	89.2 (3)
O6—Cd2—O4^{ii}	94.8 (3)	O12^{v}—Cd5—N10	87.5 (3)
N2—Cd2—O4^{ii}	90.4 (3)	N8—Cd5—N10	166.7 (3)
N4—Cd2—O4^{ii}	99.8 (3)	O16^{vi}—Cd5—N10	98.3 (3)
O6—Cd2—O2	85.6 (3)	O12^{v}—Cd5—O10	88.0 (3)
N2—Cd2—O2	84.4 (3)	N8—Cd5—O10	85.3 (2)
N4—Cd2—O2	85.4 (3)	O16^{vi}—Cd5—O10	174.3 (2)
O4^{ii}—Cd2—O2	174.7 (3)	N10—Cd5—O10	86.9 (2)
O6—Cd2—O8^{iii}	172.9 (2)	O12^{v}—Cd5—O14	174.0 (2)

N2—Cd2—O8^{iii}	84.3 (2)	N8—Cd5—O14	82.8 (3)
N4—Cd2—O8^{iii}	86.5 (2)	O16^{vi}—Cd5—O14	83.7 (3)
O4^{ii}—Cd2—O8^{iii}	85.5 (3)	N10—Cd5—O14	87.1 (2)
O2—Cd2—O8^{iii}	94.7 (2)	O10—Cd5—O14	94.3 (2)
N5—Cd3—N9	170.3 (3)	N11—Cd6—N3^{vii}	167.1 (3)
N5—Cd3—O18	90.0 (3)	N11—Cd6—O15^{vi}	87.2 (2)
N9—Cd3—O18	91.2 (3)	N3^{vii}—Cd6—O15^{vi}	80.2 (3)
N5—Cd3—O3^{ii}	89.4 (3)	N11—Cd6—O20	89.2 (3)
N9—Cd3—O3^{ii}	81.4 (3)	N3^{vii}—Cd6—O20	93.8 (3)
O18—Cd3—O3^{ii}	117.0 (3)	O15^{vi}—Cd6—O20	115.9 (3)
N5—Cd3—O8^{iii}	87.5 (3)	N11—Cd6—O13	100.8 (3)
N9—Cd3—O8^{iii}	97.4 (3)	N3^{vii}—Cd6—O13	91.9 (3)
O18—Cd3—O8^{iii}	141.4 (3)	O15^{vi}—Cd6—O13	156.5 (2)
O3^{ii}—Cd3—O8^{iii}	101.4 (2)	O20—Cd6—O13	86.5 (3)
N5—Cd3—O7^{iii}	104.0 (3)	N11—Cd6—O14	87.6 (2)
N9—Cd3—O7^{iii}	85.7 (3)	N3^{vii}—Cd6—O14	97.9 (2)
O18—Cd3—O7^{iii}	88.5 (3)	O15^{vi}—Cd6—O14	103.2 (2)
O3^{ii}—Cd3—O7^{iii}	151.4 (3)	O20—Cd6—O14	140.5 (3)
O8^{iii}—Cd3—O7^{iii}	55.1 (2)	O13—Cd6—O14	55.7 (2)

Symmetry codes: (i) *x*, *y*−1, *z*; (ii) *x*, 2−*y*, *z*−1/2; (iii) *x*+1/2, 3/2−*y*, *z*+1/2; (iv) *x*+1/2, *y*+1/2, *z*; (v) *x*, 3−*y*, *z*−1/2; (vi) *x*−1/2, 5/2−*y*, *z*−1/2; (vii) *x*−1/2, *y*+1/2, *z*.

Table S2 Hydrogen-bond geometry (Å, °) for (I)

D–H···A	d(D–H)	d(H···A)	d(D···A)	∠D–H···A
C60–H60A···O19^{v}	0.95	2.67	3.185(4)	115
C64–H64A···O17^{vi}	0.95	2.65	3.174(4)	115
C67–H67B···F5A^{iii}	0.98	2.63	3.265(4)	123
C67–H67C···O3^{i}	0.98	2.57	3.402(2)	143
C69–H69B···O1^{ii}	0.98	2.62	3.255(9)	122
C72–H72C···O15^{iii}	0.98	2.54	3.389(3)	145
C73–H73C···F4A^{vii}	0.98	2.50	3.300(2)	138
C74–H74A···O13	0.95	2.41	3.015(5)	121
C75–H75A···F3^{iv}	0.98	2.51	3.431(7)	157
C75–H75B···F8A^{ii}	0.98	2.65	3.428(6)	137
C76–H76A···O19^{ii}	0.98	2.54	3.495(4)	165
C76–H76C···O9^{ii}	0.98	2.53	3.232(3)	129

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

Table S3 C–H···π interactions (Å, °) for (I)

D–H···A	d(D–H)	d(H···A)	d(D···A)	∠D–H···A
C3–H3A···π (trz)	0.95	2.70	3.625(11)	165
C26–H26A···π (trz)^{i}	0.78	2.57	3.349(11)	140
C35–H35A···π (trz)	0.95	2.54	3.438(11)	157
C45–H45A···π (trz)	0.95	2.62	3.508(11)	157
C73–H73A···π (Ph)^{ii}	0.98	2.70	3.607(16)	155

Symmetry codes: (i) *x*–1/2, 3/2–*y*, *z*–1/2; (ii) *x*, 2–*y*, *z*–1/2.

Table S4 The dihedral angles for L^{2-} ligand in (I)

L^{2-}	Dihedral angles (°)	
	F-Ph/F-Ph ring	F-Ph ring/CO_2^{2-}
L (F_1/F_2)	54.5(3)	(F1) 3.4(3); (F2) 35.5(3)
L (F_3/F_4)	57.5(3)	(F3) 16.9(2); (F4) 15.0(3)
L (F_5/F_6)	63.3(3)	(F5) 7.2(3); (F6) 16.4(3)
L (F_7/F_8)	55.2(3)	(F7) 2.7(3); (F8) 36.1(3)