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Supporting information for article:

**A new three-dimensional twofold interpenetrated cadmium(II)
metal–organic framework: synthesis, structure and
photoluminescence properties**

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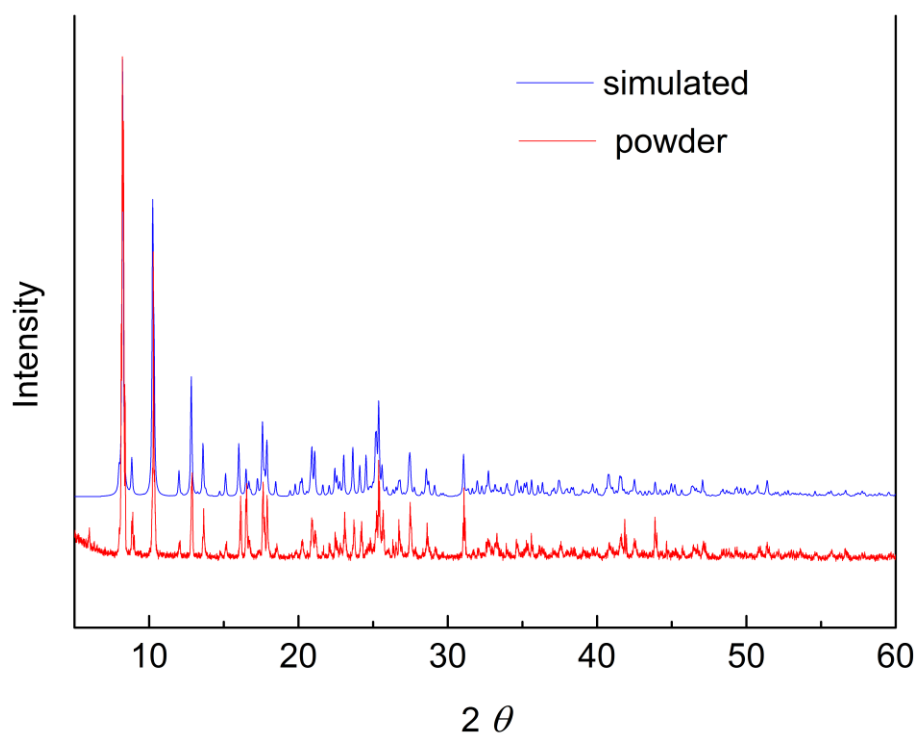
Figure S1 The PXRD patterns of title MOF (I).

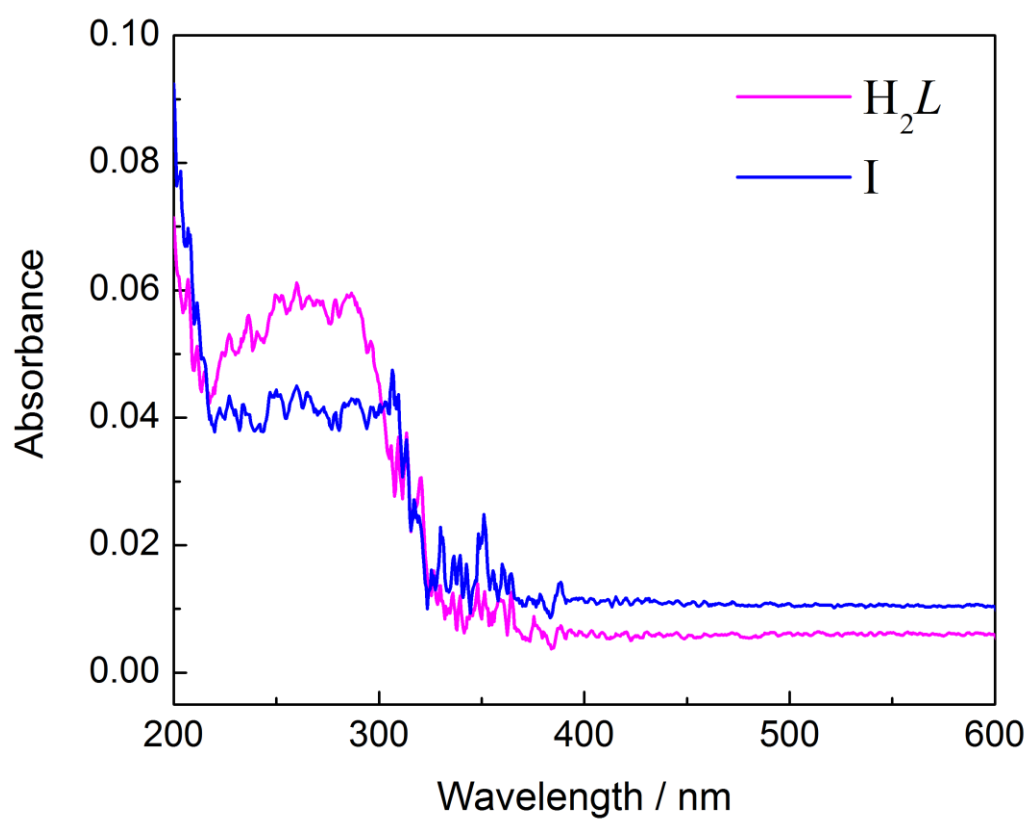
Figure S2 The solid UV–Vis absorption spectra of the free H_2L and MOF (I).

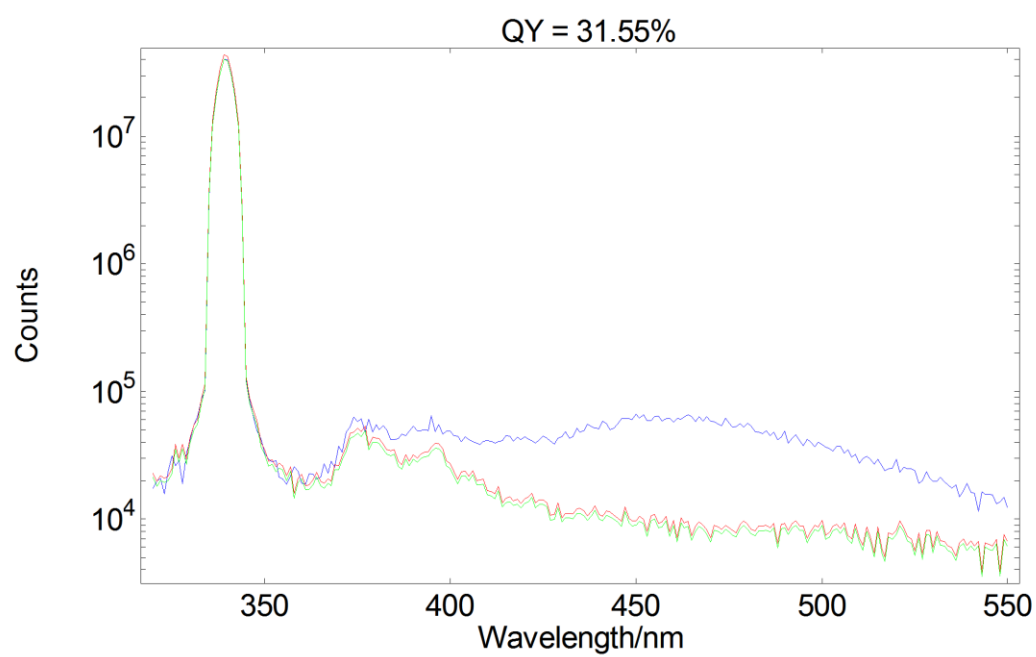
Figure S3 The quantum yield (Φ) of (I) excited at 338 nm.

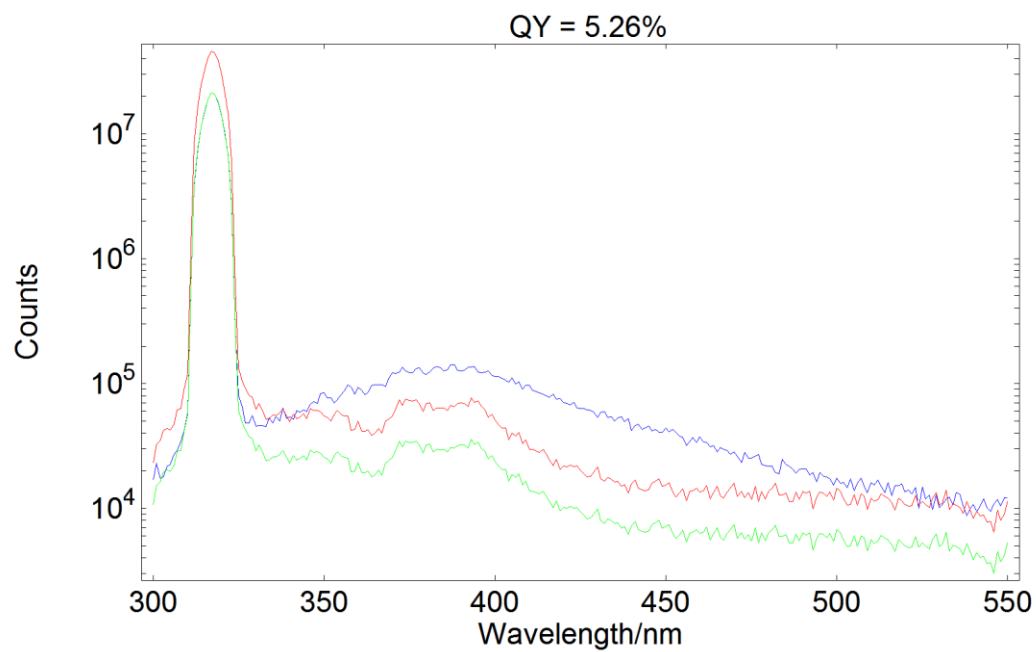
Figure S4 The quantum yield (Φ) of H_2L excited at 318 nm.

Table 1 Experimental details

	I
Crystal data	
Chemical formula	C ₂₈ H ₃₄ Cd ₂ N ₄ O ₁₅ ·2(H ₂ O)
<i>M</i> _r	927.42
Crystal system, space group	Orthorhombic, <i>P</i> 2 ₁ 2 ₁ 2 ₁
Temperature (K)	298
<i>a</i> , <i>b</i> , <i>c</i> (Å)	13.8013 (8), 14.5077 (8), 17.1208 (10)
<i>V</i> (Å ³)	3428.0 (3)
<i>Z</i>	4
Radiation type	Mo <i>K</i> α
μ (mm ⁻¹)	1.32
Crystal size (mm)	0.33 × 0.15 × 0.10
Data collection	
Diffractometer	CCD area detector
Absorption correction	Multi-scan <i>SADABS</i> (Bruker, 2004)
<i>T</i> _{min} , <i>T</i> _{max}	0.673, 0.876
No. of measured, independent and observed [<i>I</i> > 2σ(<i>I</i>)] reflections	29962, 7906, 7587
<i>R</i> _{int}	0.028
(sin θ/λ) _{max} (Å ⁻¹)	0.651
Refinement	
<i>R</i> [<i>F</i> ² > 2σ(<i>F</i> ²)], <i>wR</i> (<i>F</i> ²), <i>S</i>	0.020, 0.048, 1.04
No. of reflections	7906
No. of parameters	465
H-atom treatment	H-atom parameters constrained
Δρ _{max} , Δρ _{min} (e Å ⁻³)	0.34, -0.40
Absolute structure	Flack <i>x</i> determined using 3249 quotients [(<i>I</i> ⁺)-(<i>I</i> ⁻)]/[(<i>I</i> ⁺)+(<i>I</i> ⁻)] (Parsons, Flack and Wagner, Acta Cryst. B69 (2013) 249-259).
Absolute structure parameter	-0.011 (7)

Computer programs: *APEX2* (Bruker, 2004), *SAINT* (Bruker, 2004), *SHELXS97* (Sheldrick, 2008), *SHELXL2014/7* (Sheldrick, 2014), *DIAMOND* (Brandenburg, 2008).

Table 2 Selected geometric parameters (Å, °)

Cd1—O14	2.236 (2)	Cd2—O12 ⁱⁱⁱ	2.252 (2)
Cd1—O11 ⁱ	2.253 (2)	Cd2—O15	2.262 (3)
Cd1—O5 ⁱⁱ	2.256 (2)	Cd2—O13	2.323 (3)
Cd1—O1	2.332 (2)	Cd2—O6	2.351 (2)
Cd1—O6	2.360 (2)	Cd2—O4 ⁱⁱ	2.431 (2)
Cd1—O2	2.442 (2)	Cd2—O5 ⁱⁱ	2.442 (3)
		Cd1—O1 ⁱⁱⁱ	2.678(2)
O12—C1—C2—N1	115.8 (3)	O7—C15—C16—C17	−75.0 (4)
O1—C1—C2—N1	−62.3 (4)	N3—C18—C19—C20	12.8 (5)
O12—C1—C2—C3	−6.7 (4)	C23—C22—C25—N4	167.9 (3)
N1—C4—C5—C10	145.2 (3)	N4—C26—C28—O10	18.0 (5)
O2—C4—C5—C6	149.1 (3)	C1—C2—N1—C4	87.1 (3)
C9—C8—C11—O3	17.4 (6)	O3—C11—N2—C12	−5.0 (6)
C9—C8—C11—N2	−160.1 (3)	C14—C12—N2—C11	60.8 (5)
N2—C12—C14—O4	30.0 (5)	O8—C18—N3—C16	2.5 (5)
C13—C12—C14—O5	86.8 (4)	C15—C16—N3—C18	57.9 (4)
O7—C15—C16—N3	45.3 (4)	C27—C26—N4—C25	−168.4 (4)

Symmetry code(s): (i) $-x+1, y-1/2, -z+1/2$; (ii) $x-1, y, z$; (iii) $-x+1, y+1/2, -z+3/2$.

Table 3 Selected hydrogen-bond parameters

$D-H\cdots A$	$D-H$ (Å)	$H\cdots A$ (Å)	$D\cdots A$ (Å)	$D-H\cdots A$ (°)
C21—H21 \cdots O16 ⁱ	0.93	2.45	3.368 (5)	168.9
O17—H17E \cdots O10 ⁱⁱ	0.79	1.94	2.727 (4)	179.2
O17—H17D \cdots O8 ⁱⁱⁱ	0.82	1.86	2.672 (4)	170.4
O16—H16B \cdots O9 ⁱⁱⁱ	0.91	1.81	2.710 (4)	170.7
O16—H16A \cdots O4 ^{iv}	0.81	2.02	2.798 (4)	161.1
O15—H15B \cdots O2	0.85	2.22	2.930 (3)	141.1
O15—H15A \cdots O11 ^v	0.85	2.01	2.621 (3)	127.7
O13—H13E \cdots O3 ^{vi}	0.85	1.99	2.720 (4)	142.8
O13—H13D \cdots O17 ^{vii}	0.85	1.98	2.710 (4)	143.6
O14—H14B \cdots O7	0.85	1.99	2.640 (3)	132.8
O14—H14A \cdots O16	0.85	2.10	2.729 (4)	130.5
N4—H4 \cdots O16 ⁱ	0.86	2.19	3.011 (4)	160.3
N3—H3 \cdots O13 ^{viii}	0.86	2.33	3.117 (4)	153.2
N2—H2A \cdots O17 ^{ix}	0.86	2.26	3.049 (4)	151.8
N1—H1 \cdots O7 ^x	0.86	2.14	2.979 (3)	163.9

Symmetry code(s): (i) $-x+3/2, -y+1, z-1/2$; (ii) $x, y-1, z$; (iii) $-x+1, y-1/2, -z+1/2$; (iv) $-x+2, y-1/2, -z+3/2$; (v) $x, y, z+1$; (vi) $x-1, y, z$; (vii) $-x+1, y+1/2, -z+1/2$; (viii) $x+1/2, -y+3/2, -z+1$; (ix) $x+1/2, -y+1/2, -z+1$; (x) $-x+3/2, -y+1, z+1/2$.