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Supporting information for article:

A two-dimensional calcium (II) coordination polymer constructed from 2,2′-[terephthaloylbis(azanediyl)]diacetate: synthesis, structure and properties

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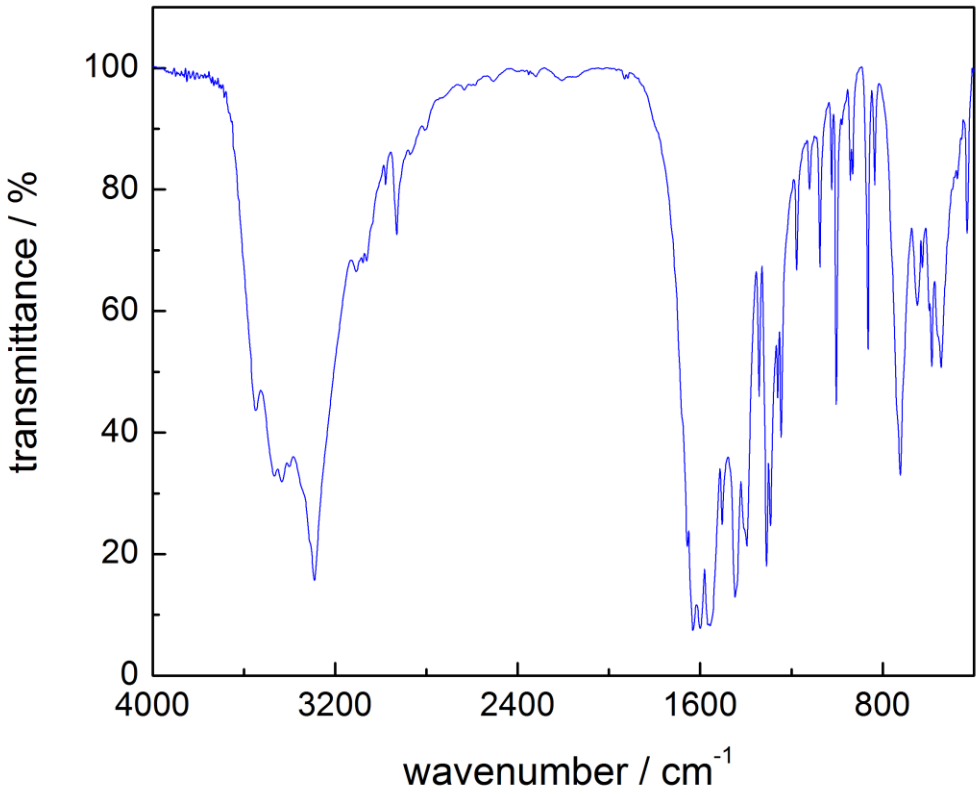

Figure S1 The IR spectrum of the title complex (I).

Figure S2

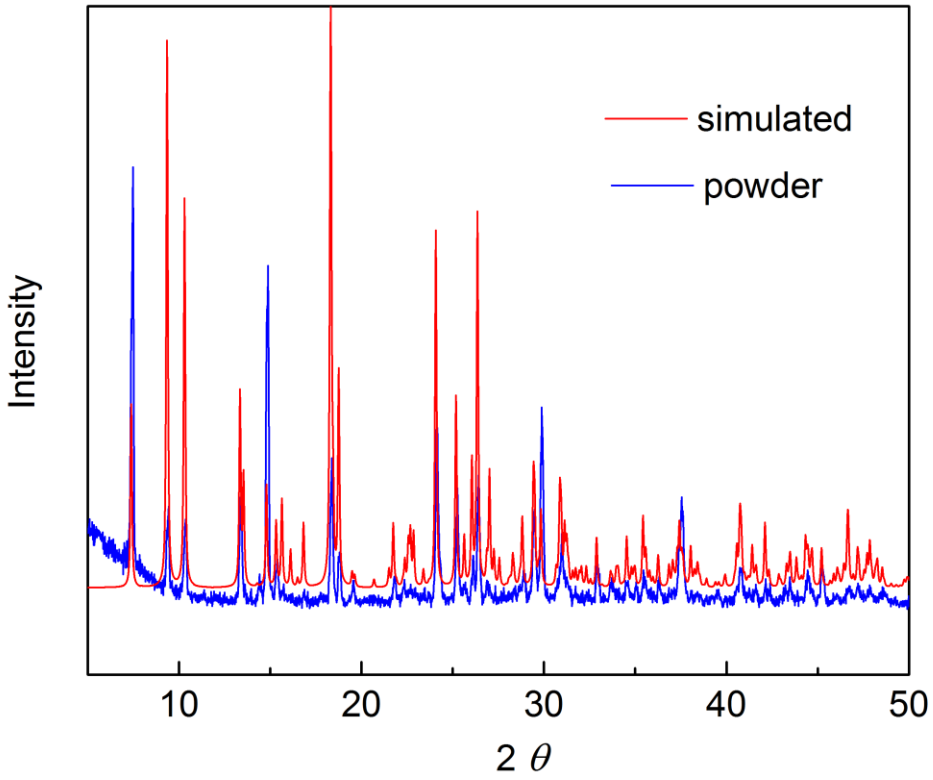

Figure S3

Figure S2 The PXRD patterns of title complex (I).

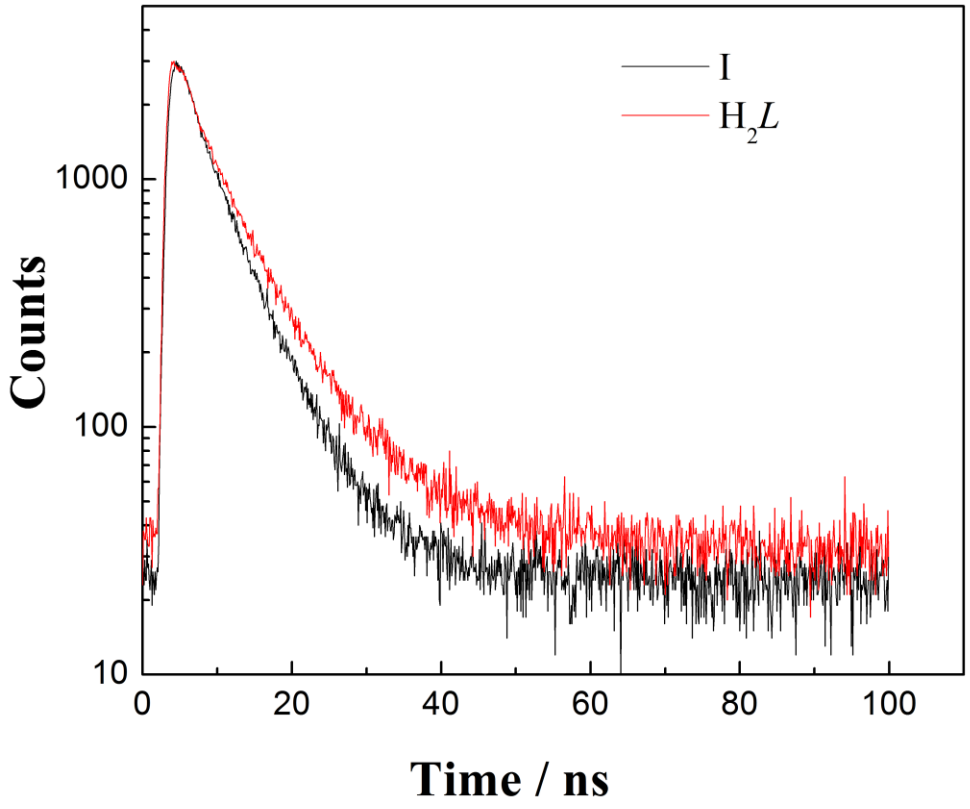

Figure S4

Figure S3 The emission decay behaviours of (I) and free H_2L in solid state.

Table 1 Experimental details

	I
Crystal data	
Chemical formula	$C_{12}H_{14}CaN_2O_8\cdot H_2O$
M_r	372.35
Crystal system, space group	Triclinic, $P\bar{1}$
Temperature (K)	298
a, *b*, *c* (Å)	6.661 (3), 9.833 (5), 12.612 (6)
α, β, γ (°)	74.277 (6), 79.224 (6), 84.609 (7)
V (Å^3)	780.3 (7)
Z	2
Radiation type	Mo *K*α
μ (mm^{-1})	0.45
Crystal size (mm)	0.10 × 0.05 × 0.05
Data collection	

Diffractometer	CCD area detector
Absorption correction	Multi-scan *SADABS* (Bruker, 2004)
T_{min}, T_{max}	0.956, 0.978
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	6752, 3500, 2466
R_{int}	0.030
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.650
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.042, 0.096, 1.00
No. of reflections	3500
No. of parameters	221
No. of restraints	6
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.26, −0.38

Computer programs: *APEX2* (Bruker, 2004), *SAINT* (Bruker, 2004), *SHELXS97* (Sheldrick, 2008), *SHELXL2014*/7 (Sheldrick, 2015), *DIAMOND* (Brandenburg, 2008).

Table 2 Selected geometric parameters (Å, º)

Ca1—O2^{i}	2.3284 (19)	Ca1—O5^{iii}	2.5297 (19)
Ca1—O1^{ii}	2.3778 (19)	Ca1—O2	2.837 (2)
Ca1—O8	2.385 (2)	O5—Ca1^{iii}	2.5297 (19)
Ca1—O7	2.403 (2)	O1—Ca1^{ii}	2.3778 (19)
Ca1—O1	2.4606 (18)	O2—Ca1^{i}	2.3285 (19)
Ca1—O6^{iii}	2.508 (2)	O6—Ca1^{iii}	2.508 (2)
O2—C1—C2—N1	−21.9 (3)	N2—C10—C7—C8	−24.4 (3)
C1—C2—N1—C3	−65.6 (3)	N1—C3—C4—C9	−139.7 (2)
N2—C10—C7—C6	156.9 (2)	N1—C3—C4—C5	41.9 (3)

Symmetry code(s): (i) −*x*+2, −*y*+2, −*z*+1; (ii) −*x*+3, −*y*+2, −*z*+1; (iii) −*x*+1, −*y*+2, −*z*+2.

Table 3 Selected hydrogen-bond parameters

D—H···*A*	*D*—H (Å)	H···*A* (Å)	*D*···*A* (Å)	*D*—H···*A* (°)
N1—H1···O4^{i}	0.86	2.00	2.810 (3)	157.6
N2—H2···O3^{ii}	0.86	2.06	2.828 (3)	148.4
O7—H7A···O6^{iii}	0.90	1.95	2.837 (3)	169.9
O7—H7B···O5^{iv}	0.90	1.89	2.766 (2)	166.2
O8—H8B···O4^{v}	0.90	2.05	2.814 (3)	142.7

C11—H11A···O4	0.97	2.38	2.769 (3)	103.7
O8—H8A···O9^{vi}	0.90	1.97	2.843(8)	164
O8—H8A···O9A^{vi}	0.90	1.90	2.66(3)	140
O9—H9A···O5^{iii}	0.85	2.27	2.986(6)	142
O9—H9B···O6^{vii}	0.85	2.24	3.080(6)	169

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