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Two viologen-based photoluminescence compounds: excitation-wavelength-dependent and photoirradiation-time-dependent photoluminescence switches

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Content

1. Figure

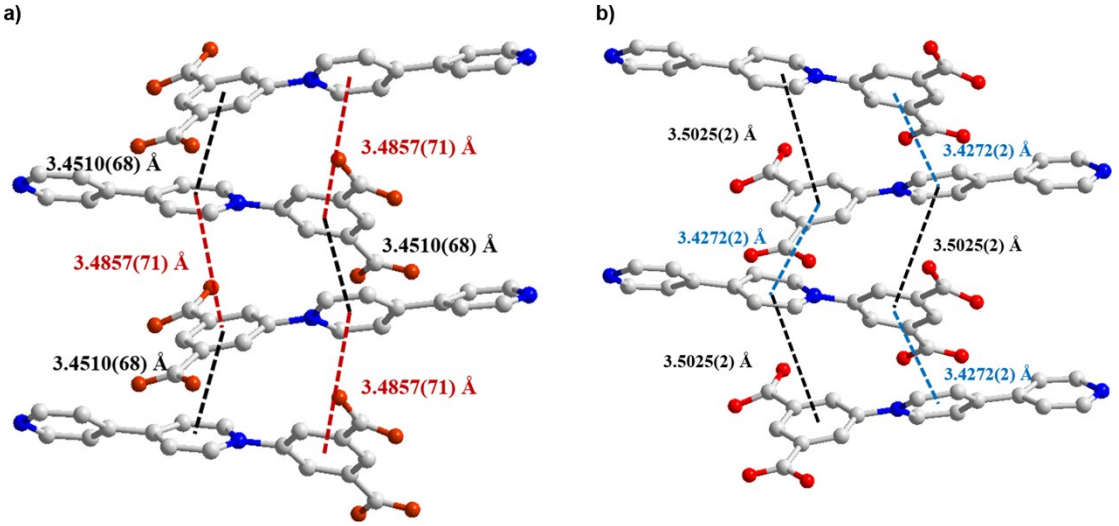

Fig. S1 The π-π interactions of **1** (a) and **2** (b).

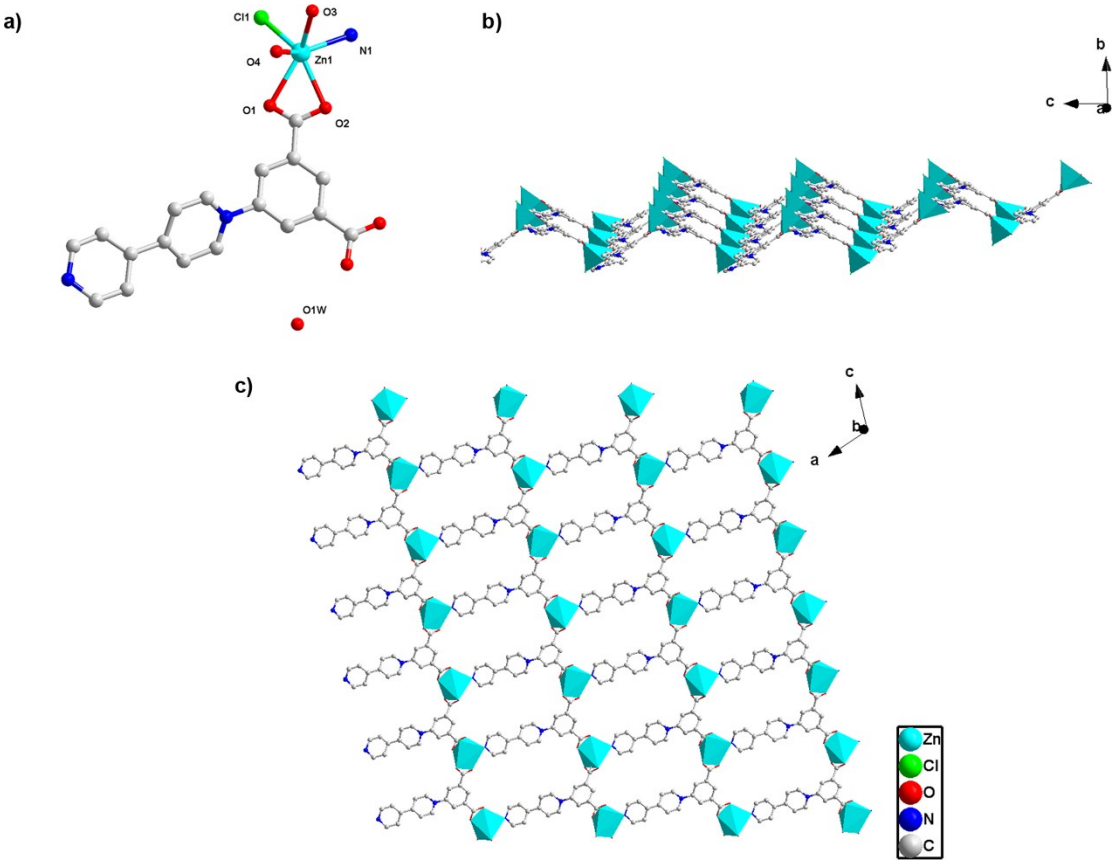

Fig. S2 Crystal structures of **2**. (a) Coordination environments of the Zn^{2+} ion (b) Stack *Z*-shaped non-planar layers in the direction **[**001**]**. (c) A 2D layer with topology.

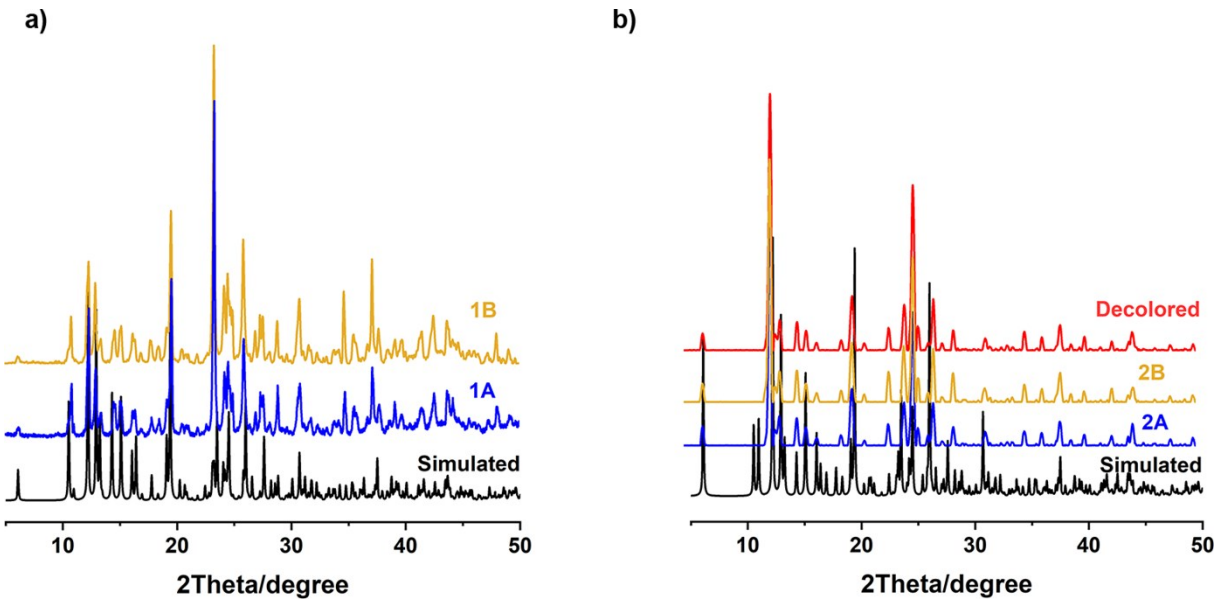

Fig. S3 The PXRD patterns of **1** (a) and **2** (b) simulated (**Simulated**), before irradiation (**1A** and **2A**), after irradiation (**1B** and **2B**) and discoloration in the dark (**Decolored**) at 25℃.

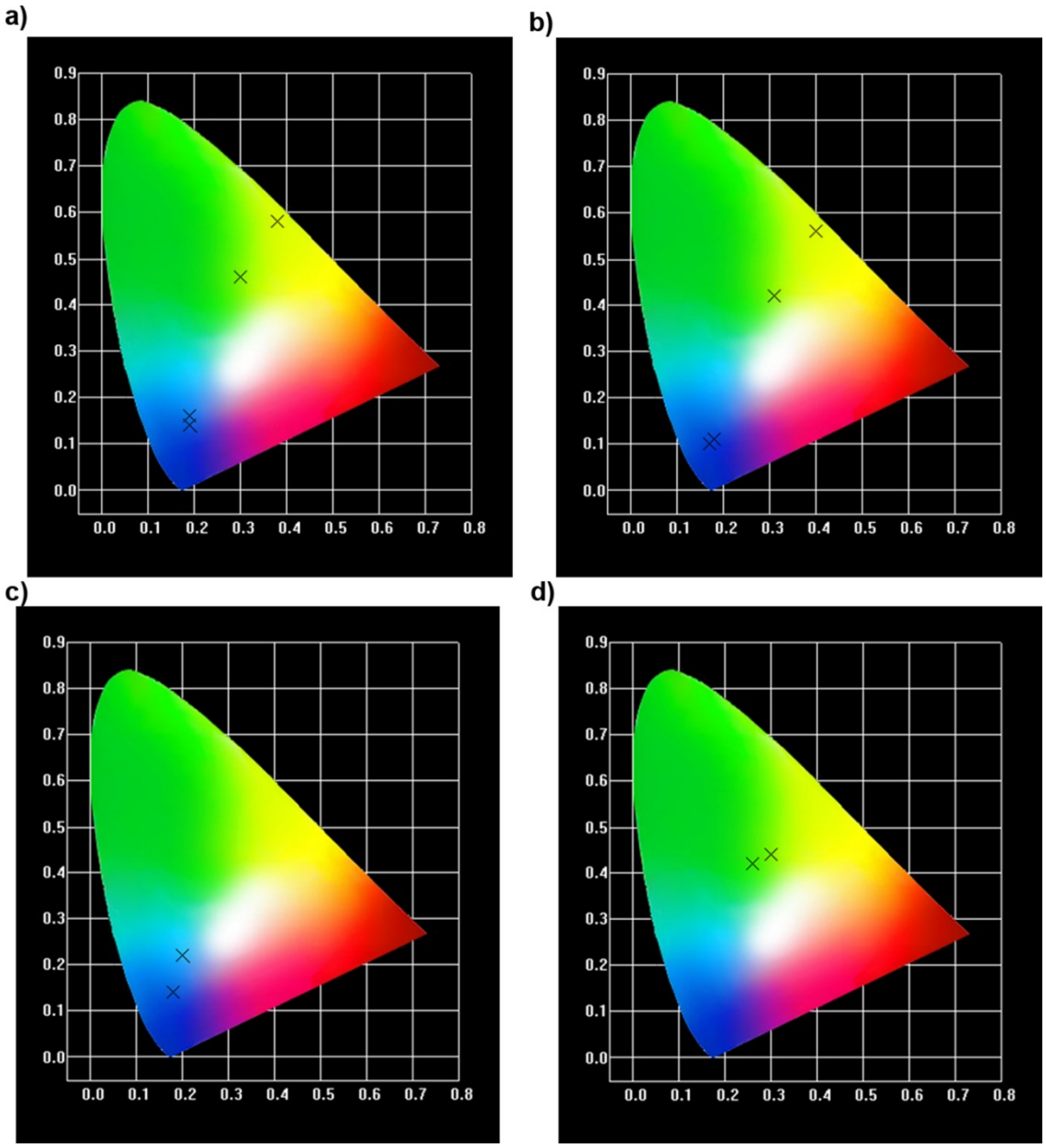

Fig. S4 CIE chromaticity diagram showing the excitation wavelengths dependence (λ_{ex}= 260nm, 330nm, 360nm, 460nm) of the (x, y) color coordinates of **1** (a) and **2** (b); and the CIE chromaticity diagram of **1** before and after photoirradiation when excitation wavelengths are 330 nm (c) and 265 nm (d).

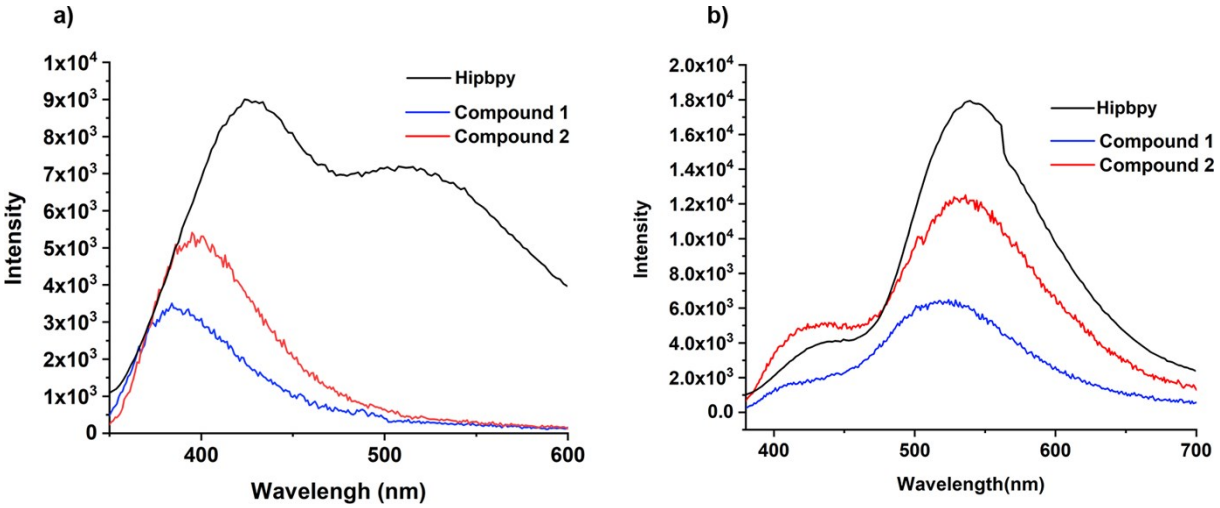

Fig. S5 The fluorescence emission spectrum of **1**, **2** and Hipbpy ligand at λ_{ex}=330nm (a) and λ_{ex}=360nm (b).

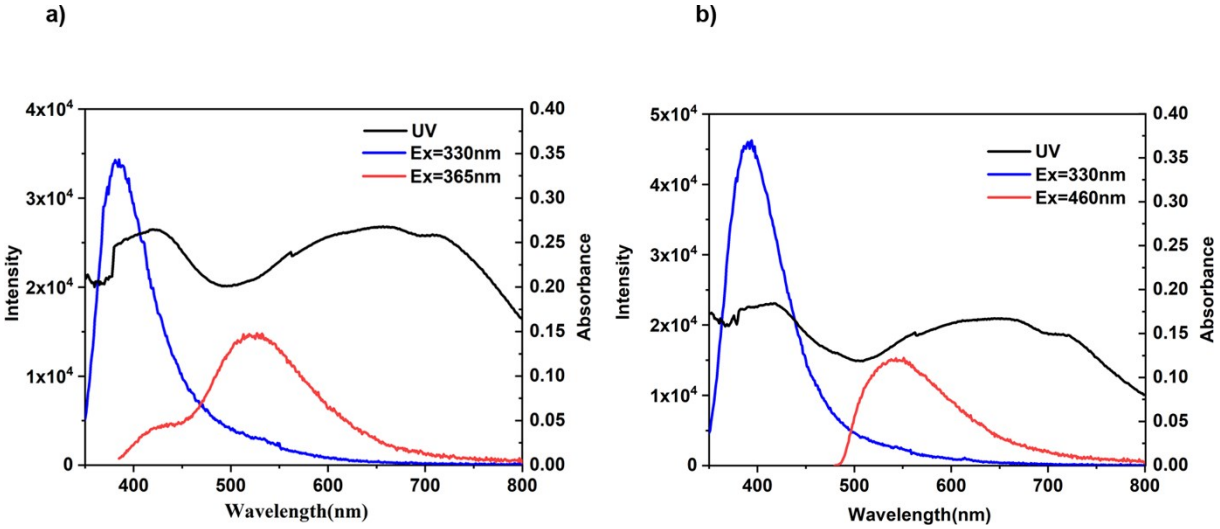

Fig. S6 (a) The fluorescence emission spectrum of **1** at Ex=330nm and Ex=365nm and the UV-vis spectrum after illumination. (b) The fluorescence emission spectrum of **2** at Ex=330nm and Ex=460nm and the UV-vis spectrum after illumination.

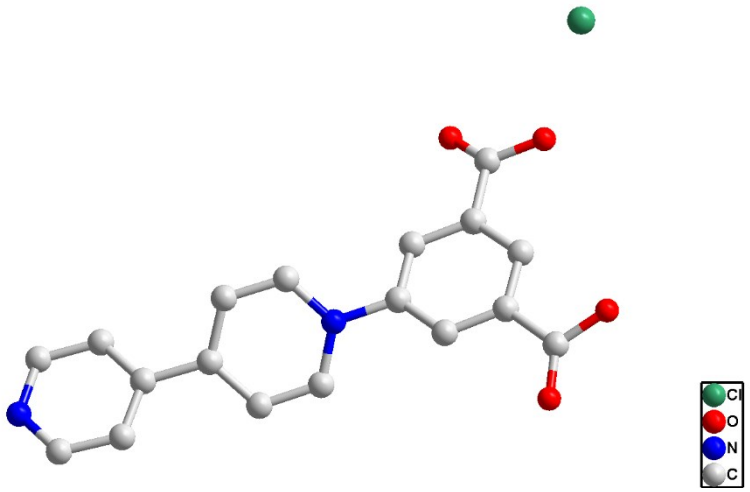

Fig. S7 Crystal structures of H_2ipbpCl.

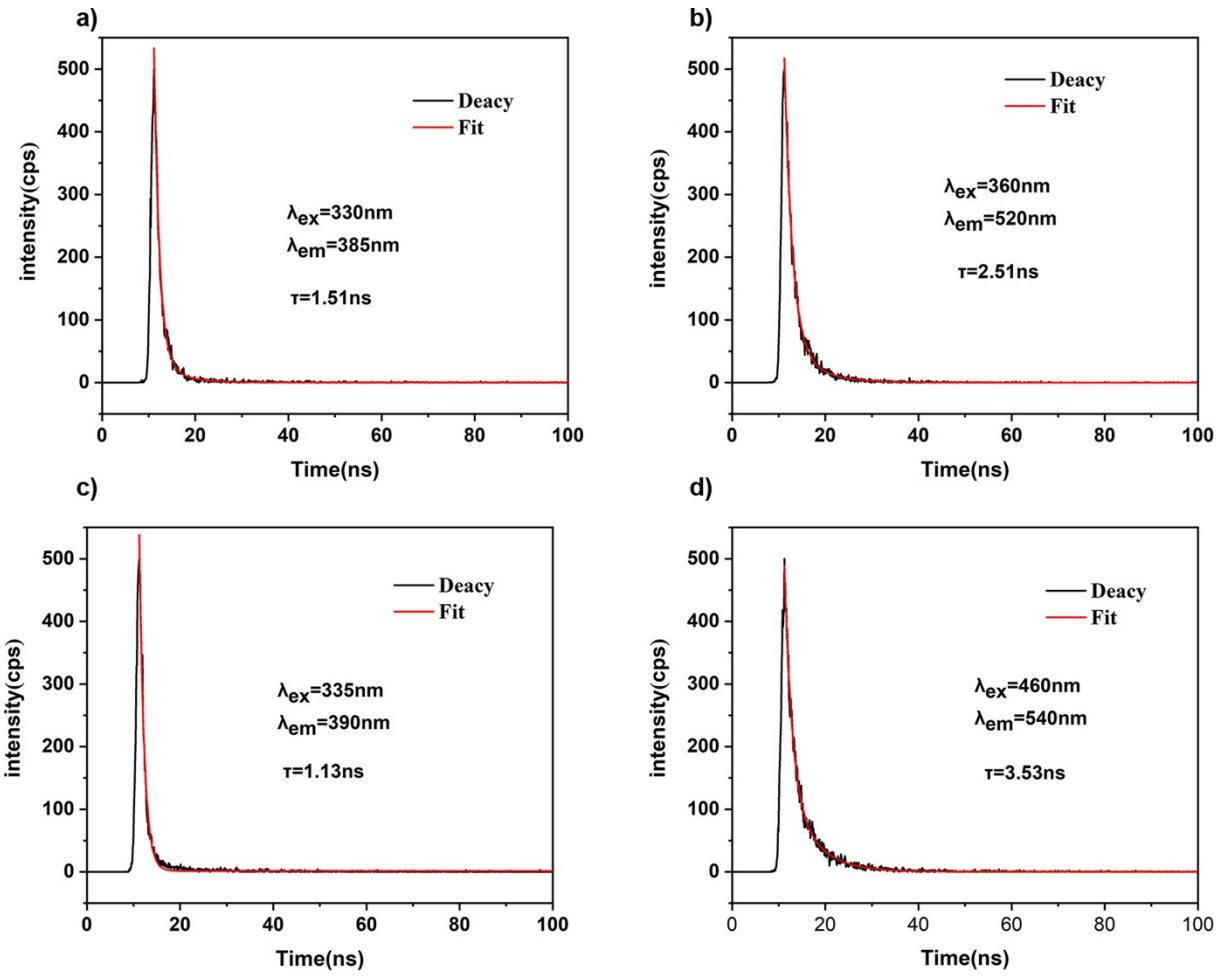

Fig. S8 The lifetime of **1** upon 330 nm(a) and 360nm (b) excitation with their maximum emission; the lifetime of **2** upon 335 nm (c) and 460nm (d) excitation with their maximum.

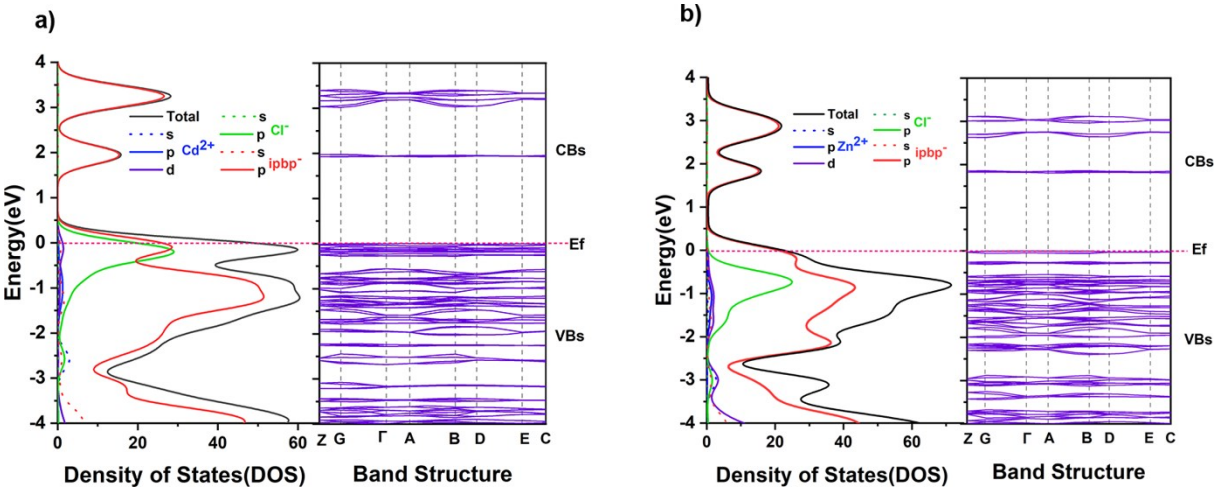

Fig. S9 The Band Structure and the total and partial DOS of **1** (a) and **2** (b). (the position of the Fermi level (Ef) is set at 0 eV).

2. Table

Table S1. Crystal data and structural refinements for **1** and **2**.

Formula	[Cd(ipbp)Cl]·H_2O(**1**)	[Zn(ipbp)Cl]·H_2O(**2**)
Fw	485.15	438.12
Crystal system	monoclinic	monoclinic
Space group	$P2_1/c$	$P2_1/c$
a /Å	15.4911(4)	15.5044(13)
b /Å	7.5672(2)	7.5706(5)
c /Å	17.2289(5)	17.2282(15)
α /°	90	90
β /°	110.483(3)	110.423(2)
γ /°	90	90
V /Å^3	1891.95(10)	1895.1(3)
Z	4	4
D_c /g.cm^{-3}	1.633	1.491
μ /mm^{-1}	1.318	1.466
Goodness-of-fit on F^2	1.436	0.928
R_1, wR_2 [$I > 2\sigma(I)$]	0.0497, 0.1791	0.1015, 0.3359
R_1, wR_2 (all data)	0.0578, 0.1873	0.1133, 0.3645

$R_1 = \sum||F_o|-|F_c||/\sum|F_o|$, $wR_2 = \{\sum w[(F_o)^2-(F_c)^2]^2/\sum w[(\underline{F}_o)^2]^2\}^{1/2}$.

Table S2. The bond lengths (Å) and bond angles (o) in **1**.

The bond lengths (Å) in **1**			
Cd1–Cl1	2.4533(14)	C2–C1	1.364(8)
Cd1–O1#1	2.404(3)	C12–C11	1.386(7)
Cd1–O2#1	2.334(4)	C12–C13	1.377(7)
Cd1–N1	2.306(4)	C11–C18	1.363(6)
Cd1–O3#2	2.444(4)	C13–C15	1.381(6)
Cd1–O4#2	2.347(4)	C13–C14	1.515(7)
Cd1–C14#1	2.673(5)	C6–C5	1.355(6)
Cd1–C17#2	2.722(5)	C16–C18	1.392(6)
O1–C14	1.246(7)	C16–C15	1.387(6)
O2–C14	1.247(7)	C16–C17	1.500(6)
O3–C17	1.242(6)	C5–C4	1.390(7)

O4–C17	1.237(6)	C4–C8	1.400(7)
N2–C11	1.474(6)	C4–C3	1.476(7)
N2–C6	1.359(6)	C10–C9	1.376(8)
N2–C7	1.341(7)	C9–C3	1.379(8)
N1–C10	1.339(7)	C7–C8	1.361(7)
N1–C1	1.336(7)	C3–C2	1.414(7)
The bond angles (º) in **1**			
C13–C14–Cd1#3	169.9(3)	C1–N1–C10	116.8(5)
O1#1–Cd1–Cl1	98.52(9)	C1–C2–C3	118.7(5)
O1#1–Cd1–O3#2	133.61(13)	C2–C3–C4	119.8(5)
O1–C14–O2	124.0(5)	C5–C4–C8	118.1(5)
O1–C14–C13	118.6(5)	C5–C4–C3	121.1(5)
O2#1–Cd1–Cl1	141.92(11)	C5–C6–N2	120.4(4)
O2#1–Cd1–O1#1	55.37(13)	C6–C5–C4	120.1(4)
O2#1–Cd1–O3#2	120.87(13)	C6–N2–C11	118.7(4)
O2#1–Cd1–O4#2	95.30(15)	C7–N2–C11	120.3(4)
O2–C14–C13	117.4(5)	C7–C8–C4	120.1(5)
O3#2–Cd1–Cl1	97.19(10)	C7–N2–C6	121.0(4)
O3–C17–C16	120.0(5)	C8–C4–C3	120.8(4)
O4#2–Cd1–Cl1	107.53(12)	C9–C3–C4	122.7(5)
O4#2–Cd1–O1#1	79.75(14)	C9–C3–C2	117.5(5)
O4#2–Cd1–O3#2	53.90(13)	C10–C9–C3	119.1(5)
O4–C17–O3	122.4(5)	C11–C18–C16	119.0(4)
O4–C17–C16	117.5(5)	C12–C11–N2	118.9(4)
N1–C1–C2	124.0(5)	C12–C13–C15	119.5(4)
N1–Cd1–Cl1	97.78(11)	C12–C13–C14	118.9(4)
N1–Cd1–O1#1	133.92(14)	C13–C12–C11	119.1(4)
N1–Cd1–O2#1	86.66(15)	C13–C15–C16	121.1(4)
N1–Cd1–O3#2	86.12(14)	C15–C16–C18	119.2(4)
N1–Cd1–O4#2	134.21(15)	C15–C16–C17	120.4(4)
N1–C10–C9	123.7(5)	C15–C13–C14	121.6(4)
N2–C7–C8	120.3(5)	C18–C16–C17	120.1(4)
C18–C11–N2	119.0(4)	C18–C11–C12	122.2(5)

Symmetry transformations used to generate equivalent atoms: #1 -1+X, +Y, +Z; #2-1+X, 1/2-Y, -1/2+Z; #3 1+X, +Y, +Z; #4 1+X, 1/2-Y, 1/2+Z

Table S3. The bond lengths (Å) and bond angles (o) in **2**.

The bond lengths (Å) in **2**			
Zn1–Cl1	2.439(3)	O4–C17	1.250(13)
Zn1–O1#1	2.399(7)	C12–C11	1.411(15)
Zn1–N1	2.281(10)	C12–C13	1.367(16)
Zn1–O2#1	2.373(11)	C18–C11	1.392(14)
Zn1–O3#2	2.412(8)	C18–C16	1.387(13)
Zn1–O4#2	2.405(9)	C10–C9	1.388(15)

O1–Zn1#3	2.399(7)	C13–C14	1.534(15)
O1–C14	1.200(13)	C13–C15	1.394(14)
N1–C10	1.375(15)	C9–C3	1.426(15)
N1–C1	1.376(15)	C7–C8	1.415(16)
N2–C11	1.423(13)	C6–C5	1.402(16)
N2–C7	1.319(14)	C3–C2	1.365(16)
N2–C6	1.347(14)	C3–C4	1.475(15)
O2–Zn1#3	2.373(11)	C16–C15	1.436(13)
O2–C14	1.262(13)	C16–C17	1.491(13)
O3–Zn1#4	2.412(8)	C1–C2	1.300(18)
O3–C17	1.226(13)	C5–C4	1.387(15)
O4–Zn1#4	2.405(9)	C8–C4	1.379(16)

The bond angles (º) in **2**

O1#1–Zn1–Cl1	99.06(19)	C18–C11–N2	120.4(9)
O1#1–Zn1–O3#2	132.9(3)	C18–C11–C12	120.7(10)
O1#1–Zn1–O4#2	79.8(3)	C12–C13–C14	117.3(10)
N1–Zn1–Cl1	98.9(3)	C12–C13–C15	121.9(10)
N1–Zn1–O1#1	133.3(3)	C15–C13–C14	120.7(10)
N1–Zn1–O2#1	87.5(3)	C10–C9–C3	118.6(10)
N1–Zn1–O3#2	86.4(3)	N2–C7–C8–	121.4(11)
N1–Zn1–O4#2	135.8(4)	N2–C6–C5	122.8(10)
O2#1–Zn1–Cl1	143.7(2)	C9–C3–C4	118.9(10)
O2#1–Zn1–O11	54.4(3)	C2–C3–C9	115.4(10)
O2#1–Zn1–O3#2	118.6(3)	C2–C3–C4	125.7(10)
O2#1–Zn1–O4#2	95.9(3)	C18–C16–C15	118.9(9)
O3#2–Zn1–Cl1	97.5(3)	C18–C16–C17	121.9(9)
O4#2–Zn1–Cl1	103.6(3)	C15–C16–C17	119.2(9)
O4#2–Zn1–O3#2	53.5(3)	C2–C1–N1	124.9(11)
C14–O1–Zn1#3	90.3(6)	C4–C5–C6	116.7(11)
C10–N1–Zn1	124.0(8)	C1–C2–C3	123.4(11)
C10–N1–C1	113.6(10)	O1–C14–O2	124.7(11)
C1–N1–Zn1	122.4(8)	O1–C14–C13	118.8(9)
C7–N2–C11	119.8(10)	O2–C14–C13	116.2(11)
C7–N2–C6	119.7(9)	C4–C8–C7	118.1(10)
C6–N2–C11	120.2(9)	C13–C15–C16	119.1(9)
C14–O2–Zn1#3	90.0(8)	O3–C17–O4	122.2(10)
C17–O3–Zn1#4	91.9(7)	O3–C17–C16	121.3(10)
C17–O4–Zn1#4	91.5(7)	O4–C17–C16	116.2(10)
C13–C12–C11	118.9(11)	C5–C4–C3	118.0(10)
C16–C18–C11	120.4(9)	C8–C4–C3	121.1(10)
N1–C10–C9	123.8(11)	C8–C4–C5	120.9(10)
C12–C11–N2	118.9(10)		

Symmetry transformations used to generate equivalent atoms: #1 1+X, +Y, +Z; #2 1+X, 3/2-Y, 1/2+Z; #3 -

1+X, +Y, +Z; #4 -1+X, 3/2-Y, -1/2+Z