Supplementary Information

Study on synthesis and host-guest luminescence properties of a novel Cd(II)-Picolinate coordination polymer

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Materials and Instrumentation: All solvents and reagents were commercially available A.R. grade and used without further purification unless otherwise noted. Powder X-Ray diffraction (PXRD) patterns were collected with a PAN alytical X'Pert Pro Diffractometer operated at 40kV and 40mA with Cu-Kα radiation. The FT-IR spectra were recorded from KBr pellets in the range from 4000 to 400cm^{-1} on a Bruker VERTEX 70 spectrometer. Thermogravimetric analyses (TGA) were obtained on a NETZSCH STA 449 F3 Jupiter® under an Ar atmosphere. Luminescence spectra were measured using a Hitachi F-7000 luminescence spectrometer. UV-visible spectra were recorded using an Agilent Cary 5000 spectrophotometer. Fluorescent quantum yields were determined by an absolute method using an integrating sphere on FLS920 of Edinburgh Instrument.

X-ray Structural Crystallography: The single-crystal X-ray diffraction data was collected on a Rigaku XtaLAB Synergy DW system HyPix Diffractometer equipped with graphite-monochromatic Mo-Kα source (λ=0.71073Å). The crystal was kept at 150.15K during data collection. Using Olex2[1], the structure was solved with the SHELXT[2] structure solution program using Intrinsic Phasing and refined with the XL[3] refinement package using Least Squares minimisation. All the non-hydrogen atoms were refined anisotropically. The crystal data are listed in Table S1-S4.

Calculations of Luminescent Quantum Yield: Luminescent quantum yield data were measured in the solid state at 298K, and the emission was monitored from 450 to 700nm. The overall luminescent quantum yields of the solid-state samples were determined by an absolute method using an integrating sphere on FLS920 of Edinburgh Instrument (150 mm diameter, $BaSO_4$ coating) and acquired using the following equation:

$$\Phi_{overall} = (A_H) / (R_{ST} - R_H) \quad (1)$$

where A_H is the area under emission spectrum of the sample and R_{ST} and R_H are diffuse reflectance of the reflecting standard and the sample, respectively[4].

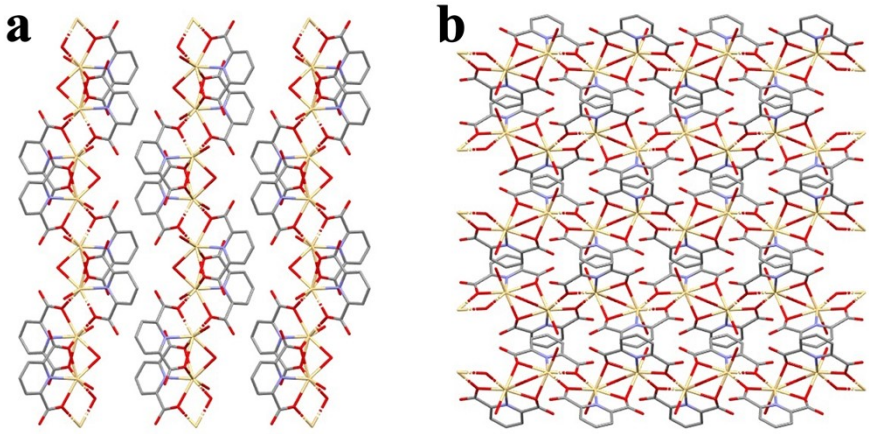

Figure S1. Framework structure of CdL (a) along the a-axis, (b) along the b-axis

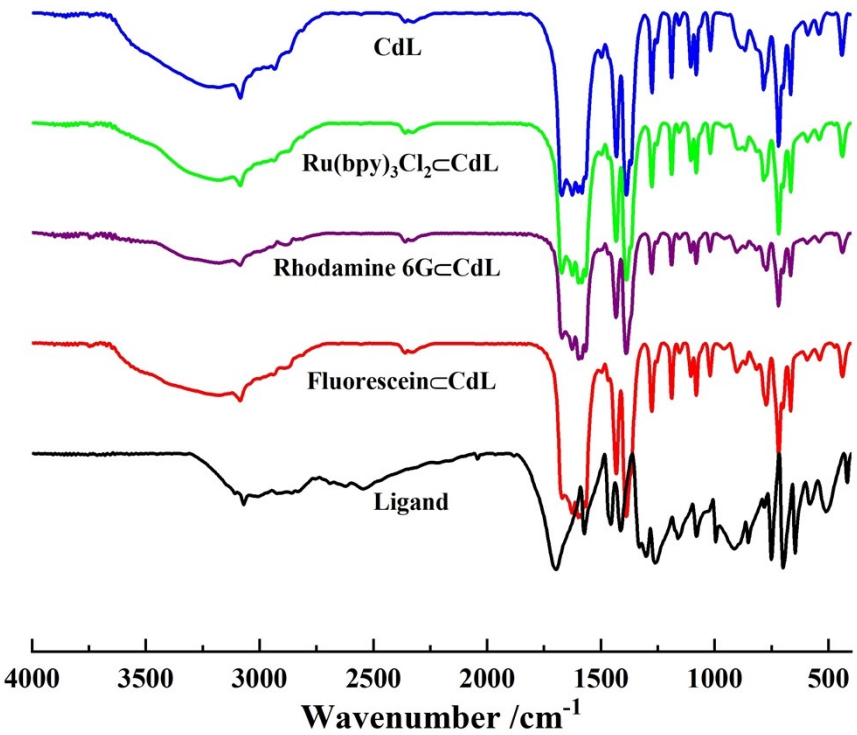

Figure S2. FTIR spectra of L, CdL and dye⊂CdL.

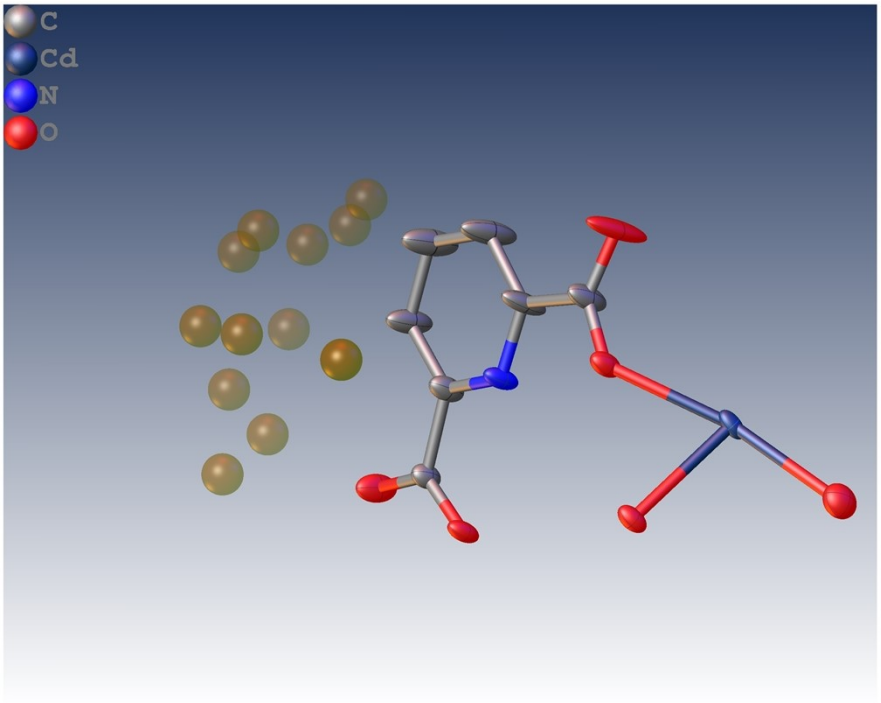

Figure S3. Main frame and residual Q peaks of CdL.

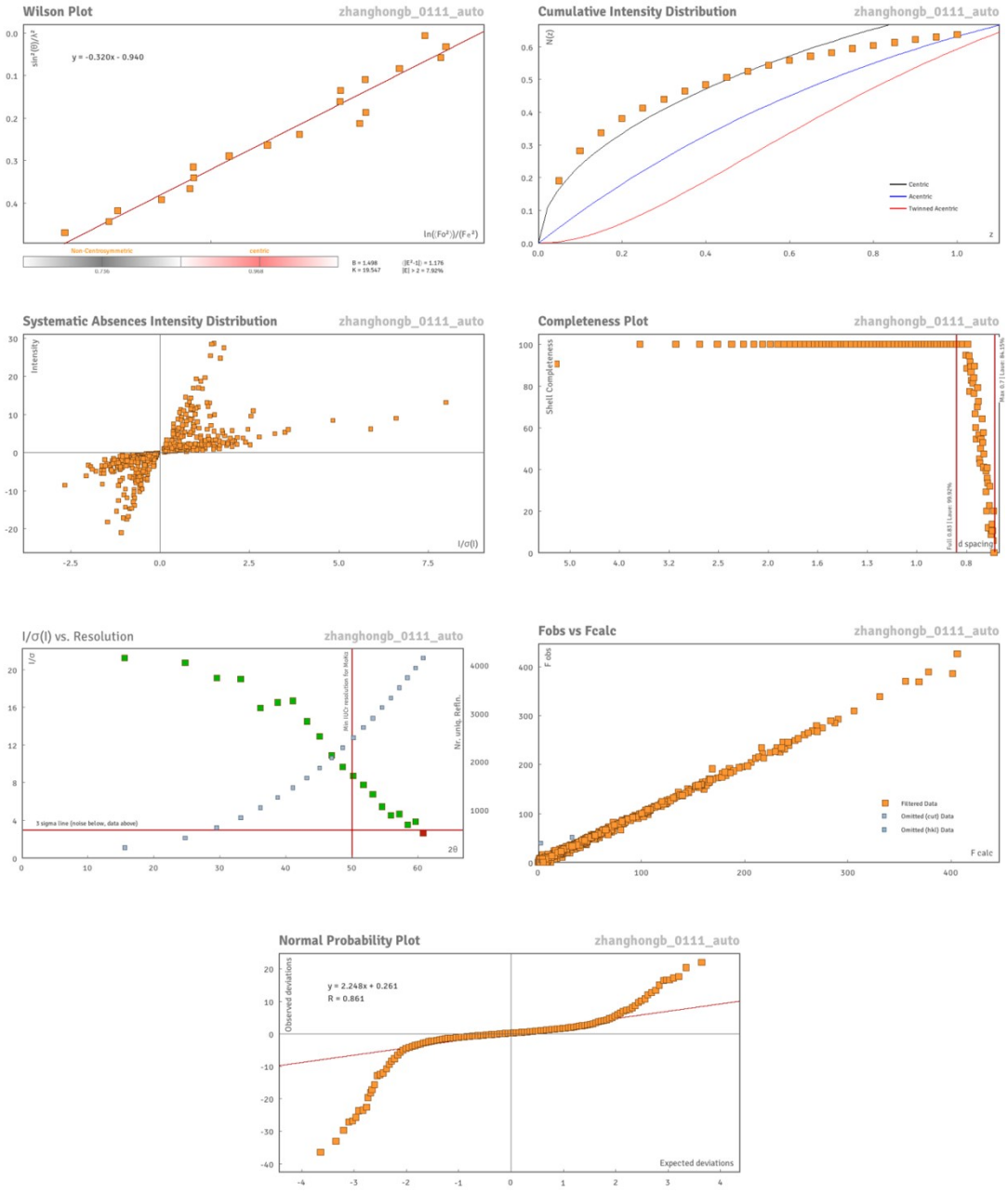

Figure S4. Diffraction Data and Refinement Data.

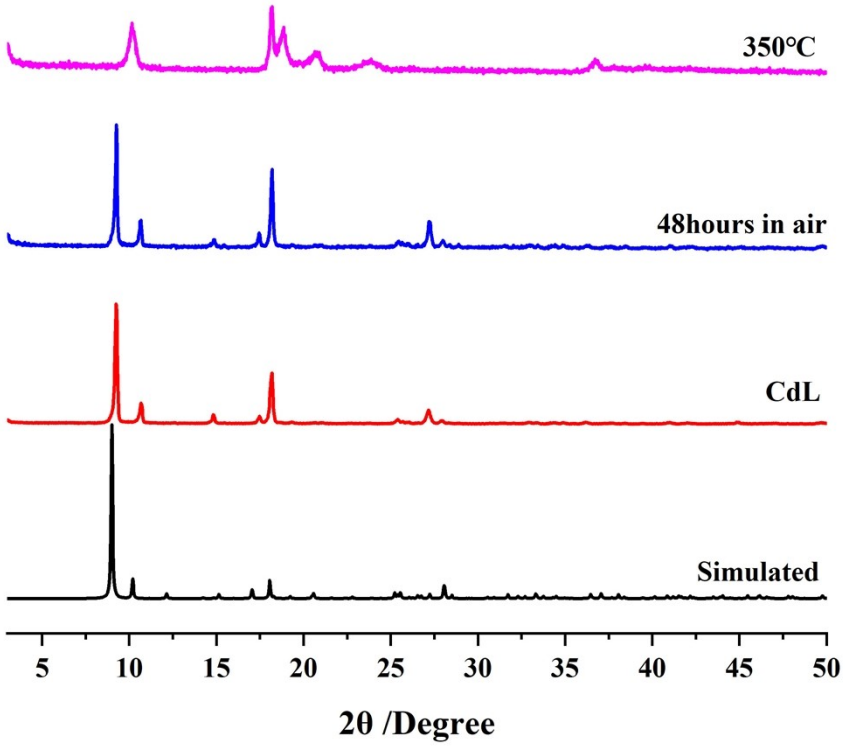

Figure S5. PXRD patterns of CdL.

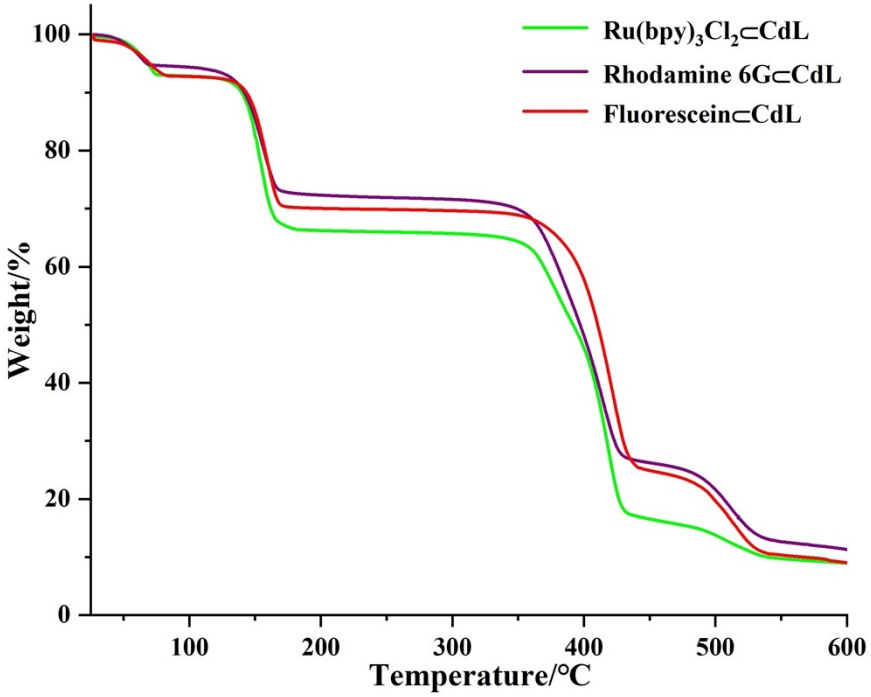

Figure S6. TGA curve of dye⊂CdL.

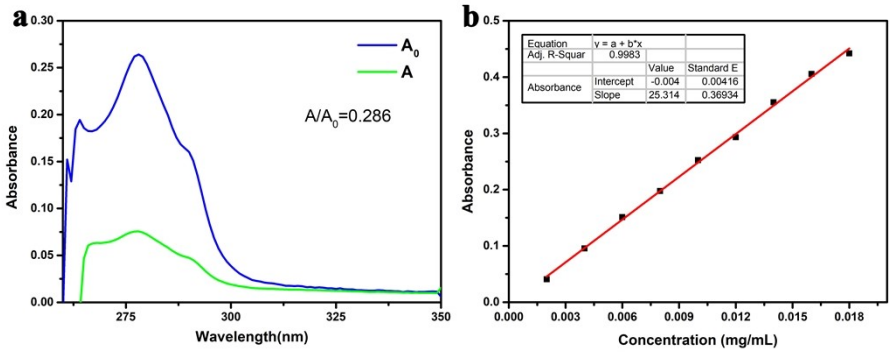

Figure S7. (a)Absorption spectra of Fluorescein solution before and after CdL immersion adsorption. (b) The relationship between the UV-Vis absorbance (monitored the sorption peak at 278nm) and Fluorescein concentration in DMF.

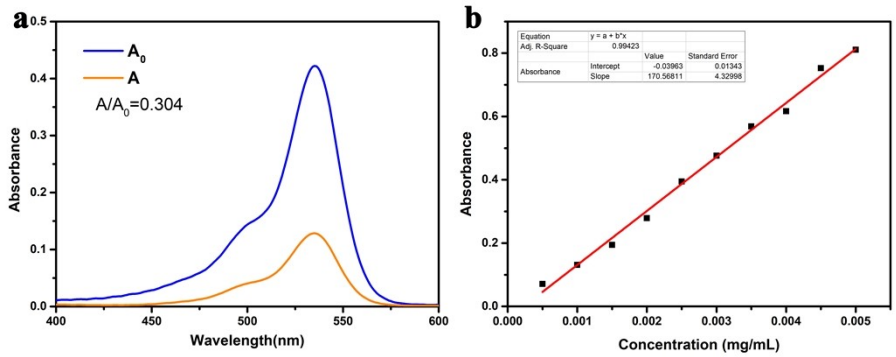

Figure S8. (a)Absorption spectra of Rhodamine 6G solution before and after CdL immersion adsorption. (b) The relationship between the UV-Vis absorbance (monitored the sorption peak at 535nm) and Rhodamine 6G concentration in DMF.

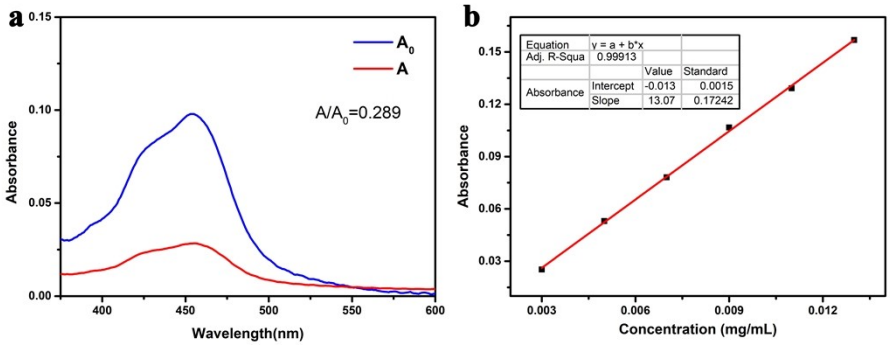

Figure S9. (a)Absorption spectra of $Ru(bpy)_3Cl_2$ solution before and after CdL immersion adsorption. (b) The relationship between the UV-Vis absorbance (monitored the sorption peak at 545nm) and $Ru(bpy)_3Cl_2$ concentration in DMF.

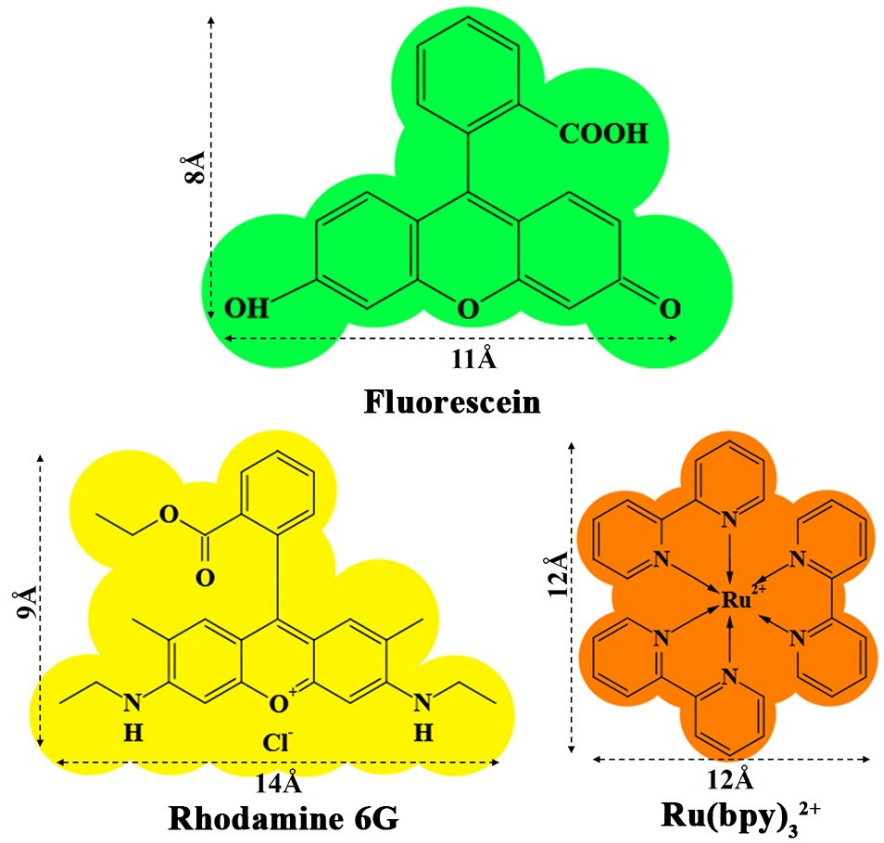

Figure S10. Molecular structure and size of dye.

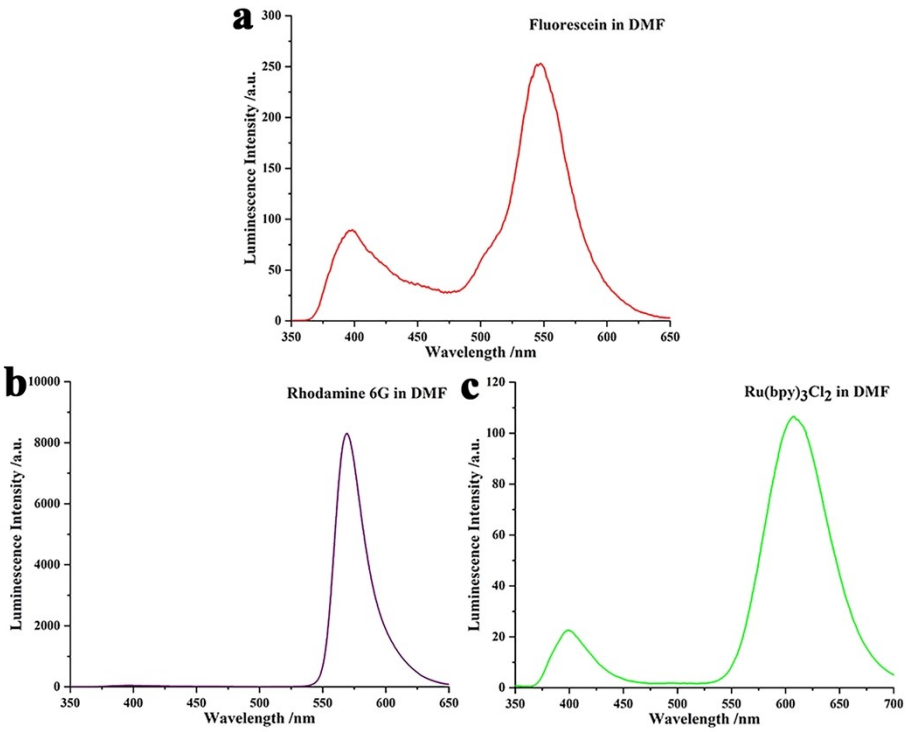

Figure S11. The emission spectrum of dye in DMF. (a) Fluorescein, (b) Rhodamine 6G and (c) $Ru(bpy)_3Cl_2$ (ex=320nm)

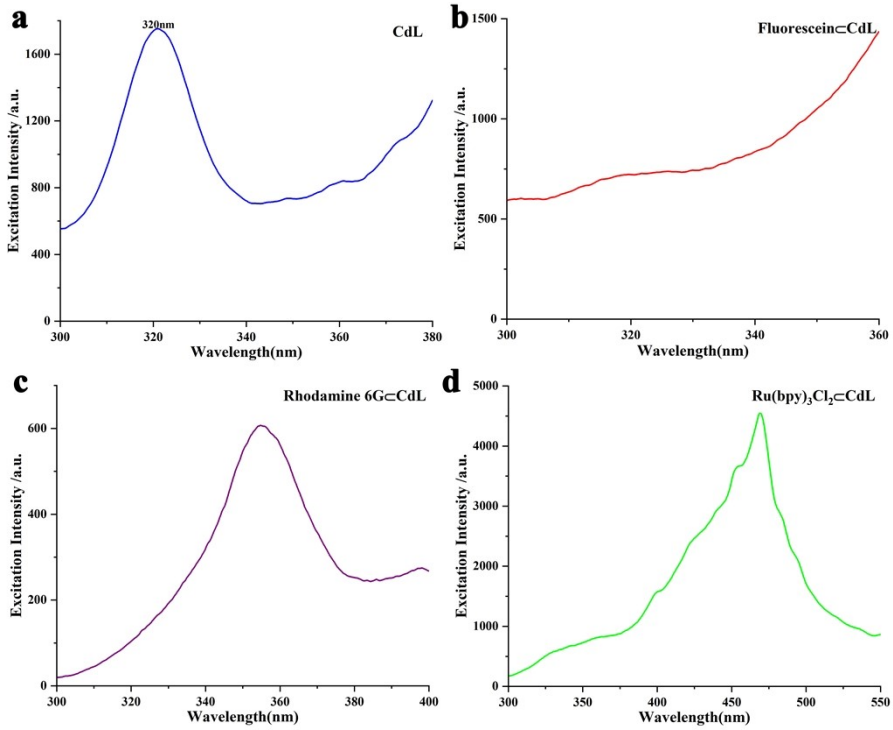

Figure S12. Excitation spectrum of (a)CdL (em=420nm), (b) Fluorescein⊂CdL (em=468nm), (c) Rhodamine 6G⊂CdL (em=562nm) and (d) $Ru(bpy)_3Cl_2$⊂CdL (em=586nm).

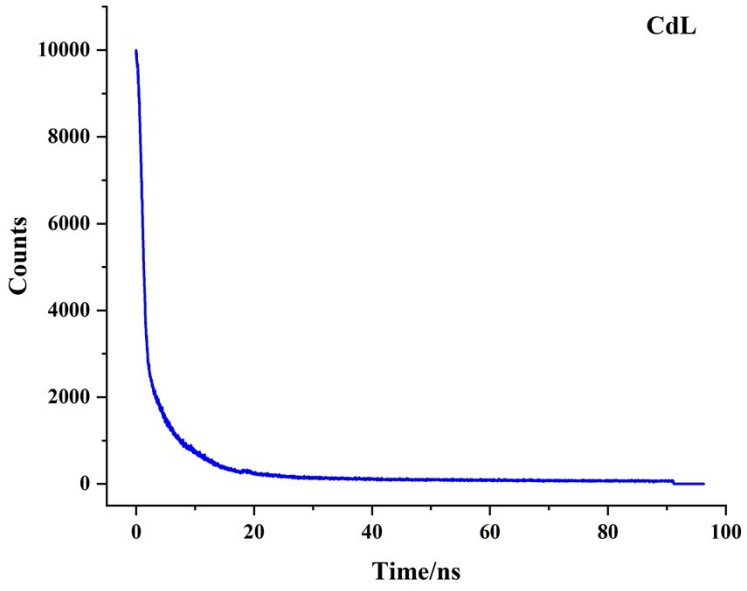

Figure S13. Photoluminescence decay curve of CdL.

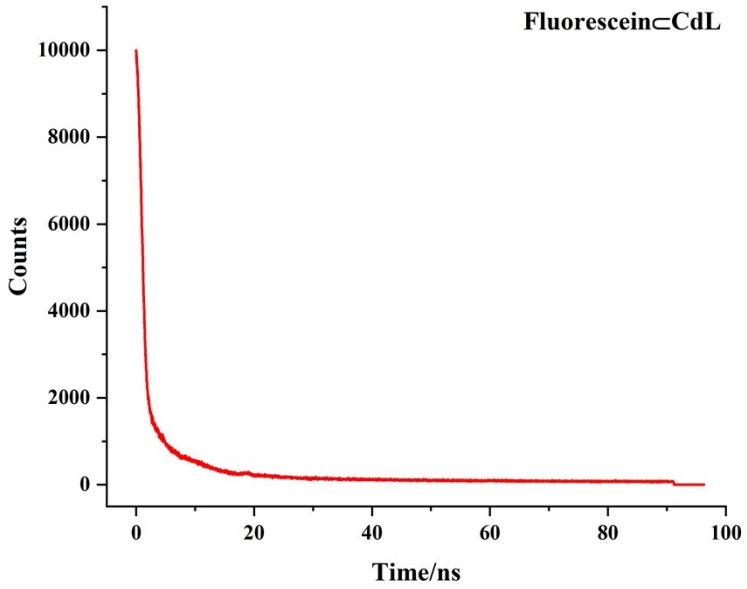

Figure S14. Photoluminescence decay curve of Fluorescein⊂CdL.

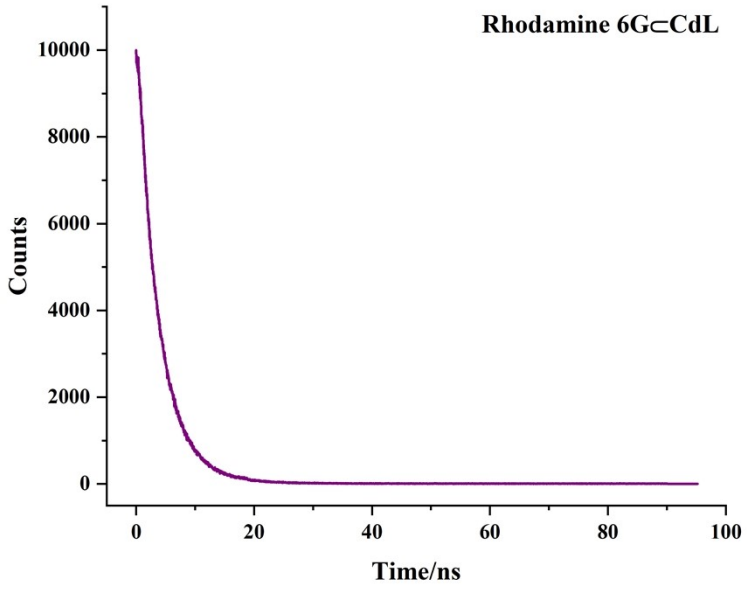

Figure S15. Photoluminescence decay curve of Rhodamine 6G ⊂CdL.

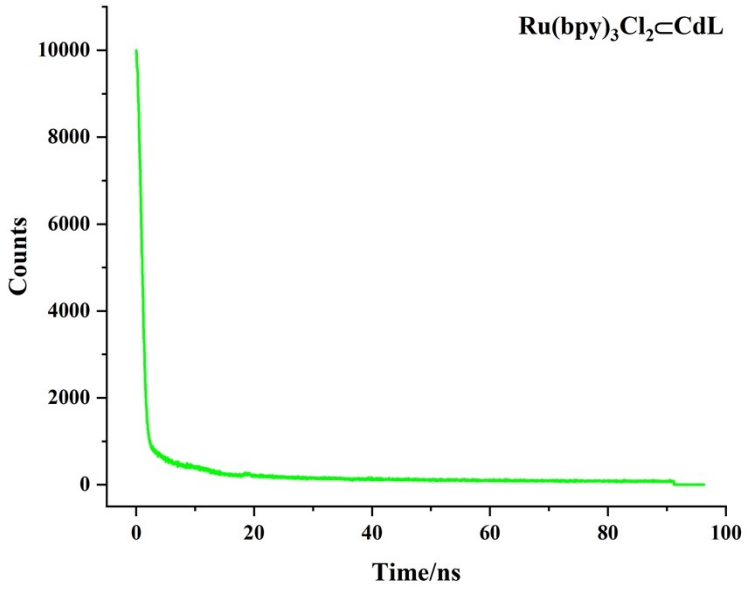

Figure S16. Photoluminescence decay curve of $Ru(bpy)_3Cl_2 \subset CdL$.

Table S1. Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for CdL. U_{eq} is defined as 1/3 of the trace of the orthogonalized U_{IJ} tensor.

Atom	x	y	z	U(eq)
Cd1	4460.3(2)	5066.9(2)	1321.7(2)	18.86(8)
O5	5000	4096.3(12)	2500	20.3(4)
O4	5458.5(13)	5722.9(9)	5239.8(10)	23.2(3)
O1	6124.5(14)	5424.5(9)	1983.9(10)	25.0(4)
O6	2990.8(15)	4383.3(10)	777.2(12)	33.4(4)
O3	6179.2(18)	6666.8(11)	6175.7(11)	37.4(5)
N1	6461.2(18)	6249.5(11)	3620.2(12)	27.4(5)
O2	6972(2)	6304.7(12)	1034.8(13)	64.2(8)
C7	6048.9(19)	6318.9(13)	5376.2(15)	22.9(5)
C6	6641(2)	6632.3(13)	4467.3(15)	28.5(5)
C1	6659(2)	6045.7(15)	1847.3(16)	35.1(6)
C2	6929(3)	6501.7(14)	2775.0(16)	37.2(7)
C3	7610(3)	7149.5(17)	2760.8(19)	57.5(10)
C5	7314(3)	7283.3(15)	4511.9(18)	41.3(7)
C4	7813(4)	7535.9(19)	3644.8(19)	59.4(11)

Table S2. Anisotropic Displacement Parameters ($Å^2 \times 10^3$) for CdL. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\cdots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Cd1	32.78(12)	14.75(12)	9.04(11)	-0.62(5)	-2.70(5)	5.57(6)
O5	33.2(13)	16.0(12)	11.9(10)	0	2.3(9)	0
O4	40.1(9)	18.7(8)	10.9(6)	-0.3(6)	-0.5(6)	-11.0(6)
O1	42.0(10)	19.7(9)	13.3(7)	0.4(6)	-2.7(6)	-8.6(7)
O6	42.1(10)	36.3(10)	21.8(9)	-3.8(7)	-2.4(7)	-0.5(8)
O3	61.1(13)	33.5(12)	17.5(8)	-11.1(7)	6.9(7)	-25.0(9)
N1	47.9(13)	21.5(11)	12.8(9)	-0.4(7)	0.0(8)	-14.8(9)
O2	129(2)	49.8(14)	13.6(8)	-0.9(8)	8.2(11)	-55.0(14)
C7	35.1(13)	19.7(12)	13.9(10)	-0.1(8)	-2.3(8)	-7.4(9)
C6	47.3(15)	22.9(13)	15.4(10)	-1.0(8)	0.2(9)	-13.6(10)
C1	62.5(18)	29.1(14)	13.7(11)	0.0(9)	-1.2(11)	-18.9(12)
C2	73(2)	25.2(13)	13.3(11)	0.4(9)	3.2(11)	-23.7(12)
C3	108(3)	40.9(18)	23.0(14)	-6.0(12)	15.4(15)	-49.9(18)
C5	71(2)	33.1(15)	20.2(12)	-7.3(10)	8.1(11)	-29.2(14)
C4	105(3)	49(2)	24.3(15)	-10.7(11)	13.7(14)	-53(2)

Table S3. Bond Lengths for CdL.

Atom	Atom	Length/Å
Cd1	O5	2.3991(15)
Cd1	O4[1]	2.3883(14)
Cd1	O4[2]	2.3312(14)
Cd1	O1	2.2819(16)
Cd1	O6	2.2536(17)
Cd1	N1[1]	2.3307(19)

[1]1-X, +Y,1/2-Z; [2]+X,1-Y, -1/2+Z

Table S4. Bond Angles for CdL.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
O4[1]	Cd1	O5	154.42(4)	N1[1]	Cd1	O5	136.26(5)
O4[2]	Cd1	O5	82.00(4)	N1[1]	Cd1	O4[1]	68.37(5)
O4[2]	Cd1	O41	73.11(6)	N1[1]	Cd1	O4[2]	141.48(6)
O1	Cd1	O5	72.16(5)	Cd1[1]	O5	Cd1	91.08(7)
O1	Cd1	O4[2]	87.01(5)	Cd1[3]	O4	Cd1[1]	106.89(6)
O1	Cd1	O4[1]	100.24(5)	C7	O4	Cd1[3]	132.67(13)
O1	Cd1	N1[1]	99.70(7)	C7	O4	Cd1[1]	119.41(13)
O6	Cd1	O5	93.45(5)	Cd1	O1	Cd1[1]	92.32(6)
O6	Cd1	O4[1]	89.80(6)	C1	O1	Cd1[1]	119.53(13)
O6	Cd1	O4[2]	84.03(6)	C1	O1	Cd1	128.42(16)
O6	Cd1	O1	164.01(6)	C6	N1	Cd1[1]	118.99(14)
O6	Cd1	N1[1]	95.56(7)	C2	N1	Cd1[1]	120.98(14)

[1]1-X, +Y,1/2-Z; [2]+X,1-Y, -1/2+Z; [3]+X,1-Y,1/2+Z

References

[1] Dolomanov, O.V., Bourhis, L.J., Gildea, R.J, Howard, J.A.K. & Puschmann, H., *J. Appl. Cryst.*, 2009, **42**, 339-341.

[2] Sheldrick, G.M., *Acta Cryst.*, 2015, **A71**, 3-8.

[3] Sheldrick, G.M., *Acta Cryst.*, 2008, **A64**, 112-122.

[4] a) J. C. Mello, H. F. Wittmann and R. H. Friend, *Adv. Mater.*, 1997, **9**, 230–232; b) Q. Zhu, C. Shen, C. Tan, T. Sheng, S. Hu and X. Wu, *Chem. Commun.*, 2012, **48**, 531–533;