Electronic Supplementary Information (ESI)

[2+2] cycloaddition reaction and luminescent sensors of Fe^{3+} and $Cr_2O_7^{2-}$ ions of a cadmium-based coordination polymer

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Table S1 Crystallographic data and structure refinement summary for compounds **1** and **1a**.

Compound	1	1a
Formula	$C_{46}H_{42}Cd_3N_4O_{16}$	$C_{46}H_{42}Cd_3N_4O_{16}$
Formula weight	1244.03	1244.03
Crystal system	triclinic	triclinic
Space group	P-1	P-1
a (Å)	10.299(5)	10.284(2)
b (Å)	10.721(6)	11.203(2)
c (Å)	11.773(6)	11.577(2)
α (°)	97.149(6)	100.459(3)
β (°)	112.393(6)	114.617(3)
γ (°)	90.846(6)	91.162(3)
V (Å^3)	1189.8(11)	1185.6(4)
Z	1	1
D_{calcd} (g cm^{-3})	1.736	1.742
μ (mm^{-1})	1.403	1.408
F (000)	618.0	618.0
R1 [I > 2σ(I)]	0.0247	0.0469
wR2 [I > 2σ(I)]	0.0521	0.0708
R1 (all data)	0.0355	0.1042
wR2 (all data)	0.0555	0.0843
GOF on F^2	1.000	0.923

Table S2 Selected Bond Distances (Å) and Angles (deg) for Complexes **1** and **1a**.

Complex **1**			
Cd1—O6^{i}	2.273 (2)	O6—Cd1—N1^{i}	90.1 (4)
Cd1—O6	2.273 (2)	O1—Cd1—O1^{i}	180.0
Cd1—O1	2.274 (2)	O1—Cd1—N1	87.9 (5)
Cd1—O1^{i}	2.274 (2)	O1^{i}—Cd1—N1^{i}	87.9 (5)
Cd1—N1	2.327 (7)	O1^{i}—Cd1—N1	92.1 (5)
Cd1—N1^{i}	2.327 (7)	O1—Cd1—N1^{i}	92.1 (5)
Cd2—O6	2.279 (2)	N1—Cd1—N1^{i}	180.0
Cd2—O4^{ii}	2.211 (2)	O6—Cd2—N2^{iii}	96.4 (4)
Cd2—O2^{i}	2.237 (2)	O6—Cd2—O1W	142.58 (7)
Cd2—N2^{iii}	2.333 (9)	O4^{ii}—Cd2—O6	88.74 (9)

Cd2—O1W	2.283 (2)	O4^{ii}—Cd2—O2^{i}	92.09 (10)
O6^{i}—Cd1—O6	180.0	O4^{ii}—Cd2—N2^{iii}	174.6 (5)
O6—Cd1—O1	87.34 (7)	O4^{ii}—Cd2—O1W	87.83 (8)
O6—Cd1—O1^{i}	92.66 (7)	O2^{i}—Cd2—O6	103.41 (8)
O6^{i}—Cd1—O1	92.66 (7)	O2^{i}—Cd2—N2^{iii}	88.5 (4)
O6^{i}—Cd1—O1^{i}	87.34 (7)	O2^{i}—Cd2—O1W	113.94 (8)
O6^{i}—Cd1—N1	90.1 (4)	O1W—Cd2—N2^{iii}	87.0 (5)
O6^{i}—Cd1—N1^{i}	89.9 (4)	Cd1—O6—Cd2	118.68 (9)
O6—Cd1—N1	89.9 (4)		
Complex **1a**			
Cd1—O6	2.247 (4)	O1—Cd1—O1^{i}	180.00 (19)
Cd1—O6^{i}	2.247 (4)	O1^{i}—Cd1—N2^{ii}	86.2 (7)
Cd1—O1^{i}	2.256 (5)	O1^{i}—Cd1—N2^{iii}	93.8 (7)
Cd1—O1	2.256 (5)	O1—Cd1—N2^{ii}	93.8 (7)
Cd1—N2^{ii}	2.401 (18)	O1—Cd1—N2^{iii}	86.2 (7)
Cd1—N2^{iii}	2.401 (18)	N2^{ii}—Cd1—N2^{iii}	180.0 (8)
Cd2—O6	2.281 (4)	O6—Cd2—N1A	94.3 (8)
Cd2—O4^{iv}	2.198 (5)	O4^{iv}—Cd2—O6	91.91 (18)
Cd2—O2^{i}	2.239 (5)	O4^{iv}—Cd2—O2^{i}	96.5 (2)
Cd2—O1W	2.281 (4)	O4^{iv}—Cd2—O1W	87.77 (18)
Cd2—N1A	2.335 (11)	O4^{iv}—Cd2—N1A	172.6 (9)
O6—Cd1—O6^{i}	180.0	O2^{i}—Cd2—O6	97.58 (17)
O6^{i}—Cd1—O1	91.66 (17)	O2^{i}—Cd2—O1W	112.13 (17)
O6^{i}—Cd1—O1^{i}	88.34 (17)	O2^{i}—Cd2—N1A	86.7 (6)
O6—Cd1—O1	88.34 (17)	O1W—Cd2—O6	150.14 (17)
O6—Cd1—O1^{i}	91.66 (17)	O1W—Cd2—N1A	84.8 (9)
O6—Cd1—N2^{ii}	90.5 (9)	Cd1—O6—Cd2	124.4 (2)
O6^{i}—Cd1—N2^{ii}	89.5 (9)		

Symmetry codes, **for 1**: (i) -*x*+1, -*y*, -*z*+1; (ii) *x*, *y*+1, *z*; (iii) *x*-1, *y*-1, *z*-1; (iv) *x*, *y*-1, *z*; (v) *x*+1, *y*+1, *z*+1; **for 1a**: (i) -*x*+1, -*y*, -*z*+1; (ii) -*x*+2, -*y*+1, -*z*+2; (iii) *x*-1, *y*-1, *z*-1; (iv) *x*, *y*-1, *z*; (v) *x*, *y*+1, *z*; (vi) *x*+1, *y*+1, *z*+1.

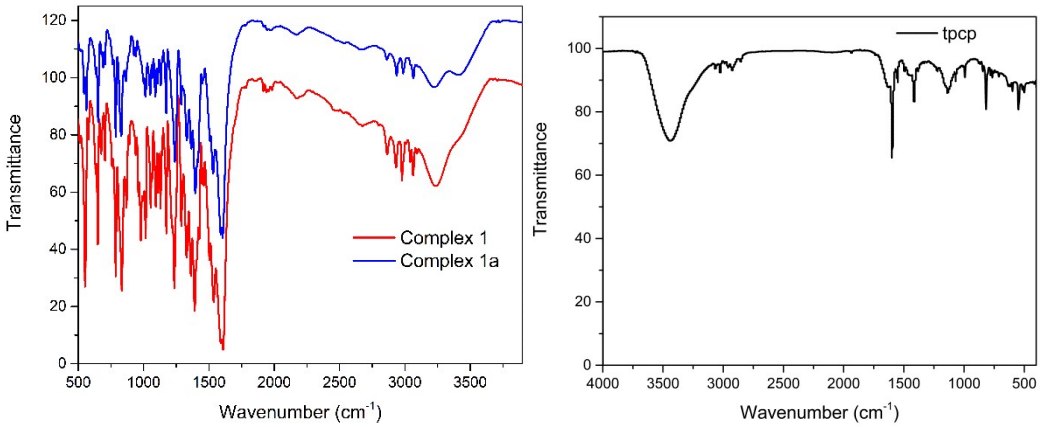

Fig. S1 FT-IR spectrums for **1**, **1a** and *rctt*-tpcb.

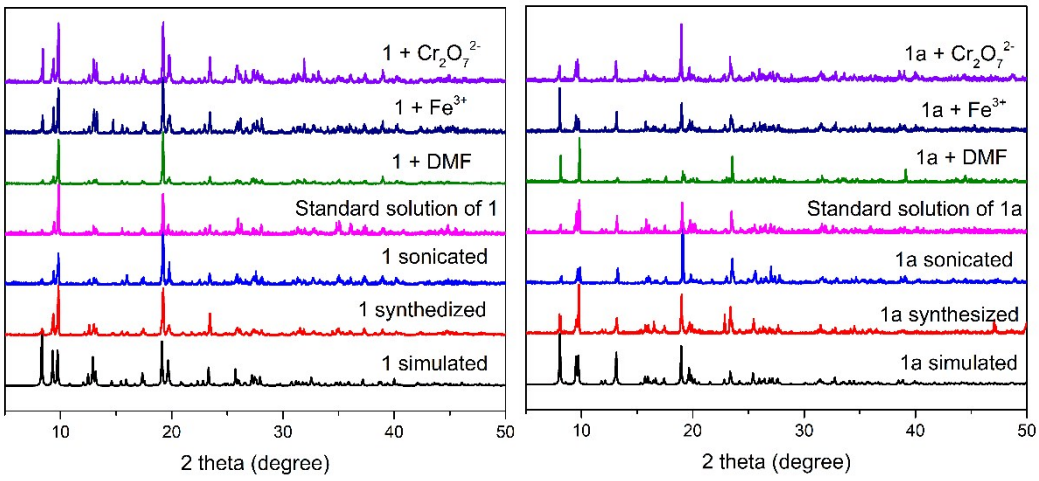

Fig. S2 Powder XRD patterns for **1** and **1a**.

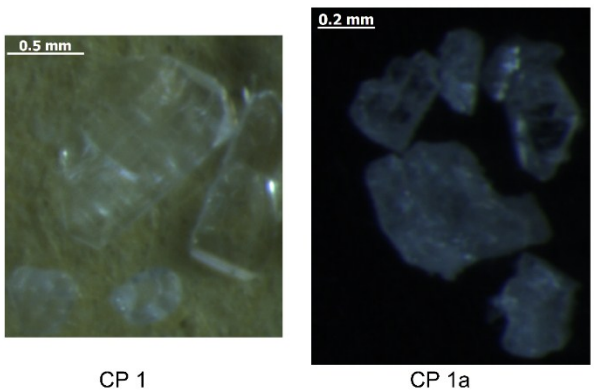

Fig. S3 Photos of the crystal of **1** and **1a**.

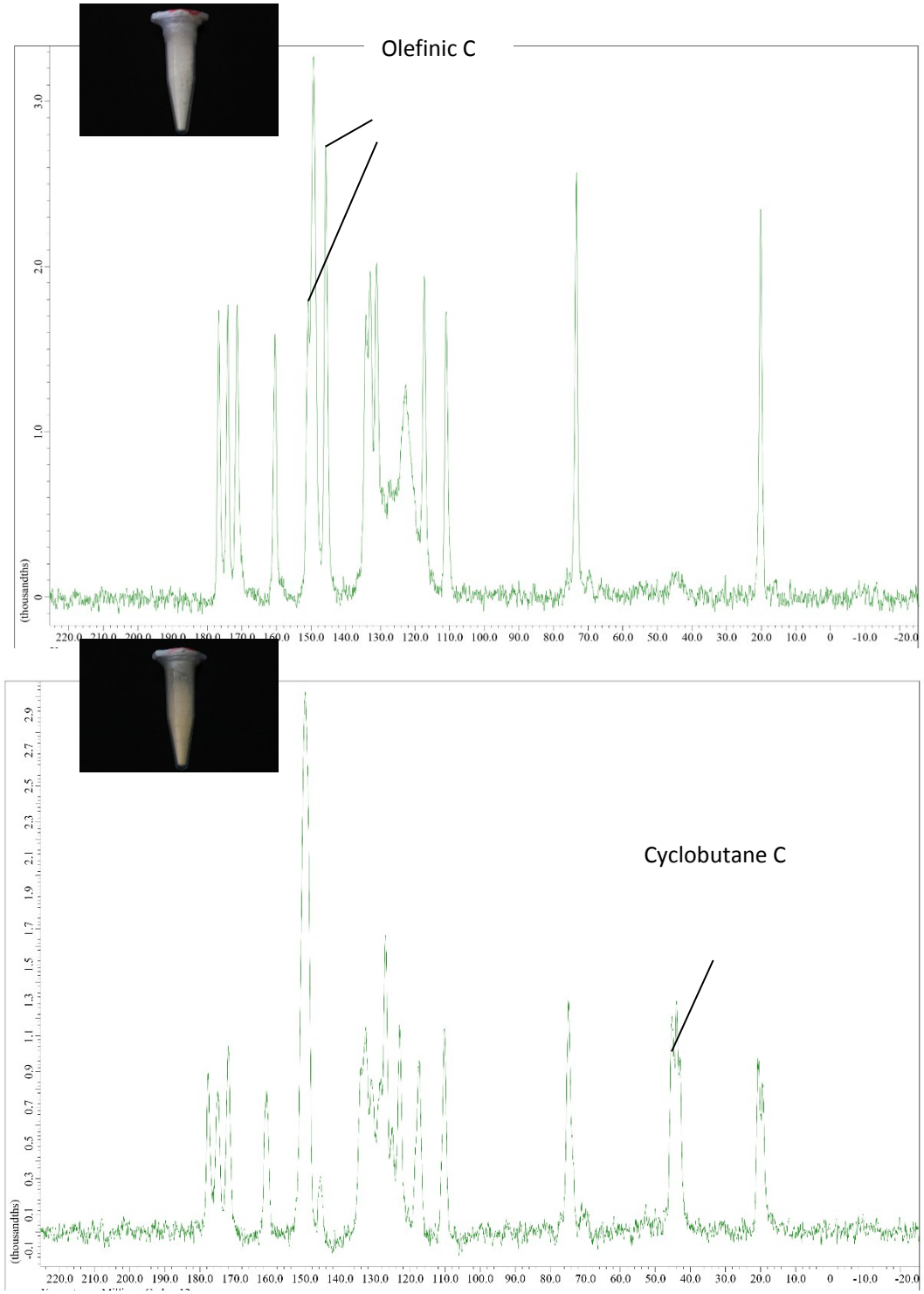

Fig. S4 ^{13}C CPMAS NMR spectra of **1** (top) and **1a** (bottom)

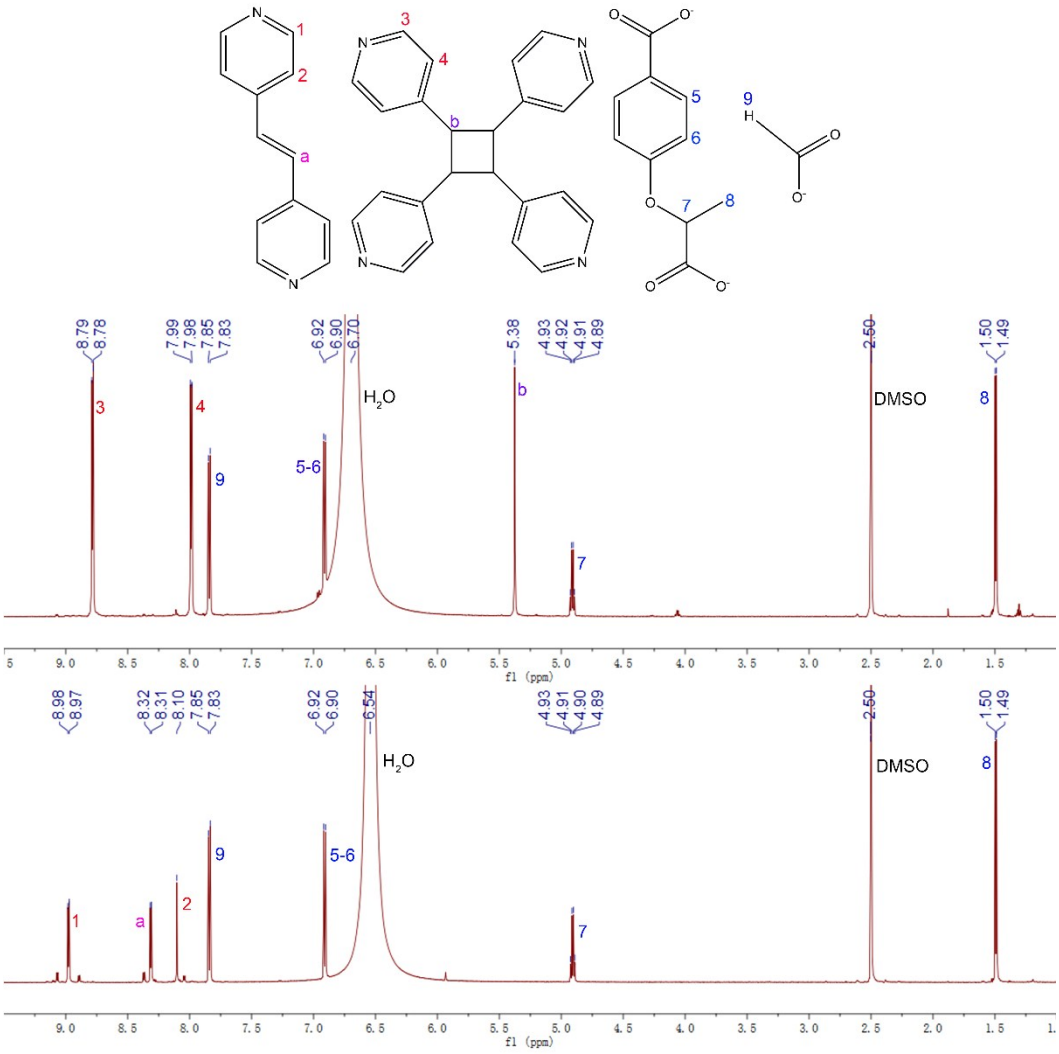

Fig. S5 ^{1}H NMR spectra of **1** (bottom) and **1a** (top) in DMSO-*d6* with 50 µL HNO_3 to dissolve the crystals (15 mg). The humps around 6.7 and 6.5 ppm is due to the protonated water.

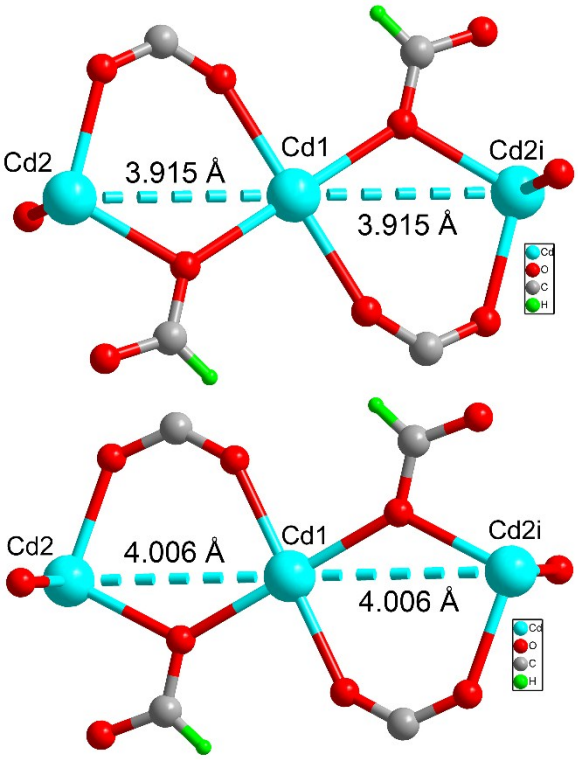

Fig. S6 The $[Cd_3(ceba)_2(fa)_2]$ unit in **1** (top) and **1a** (bottom).

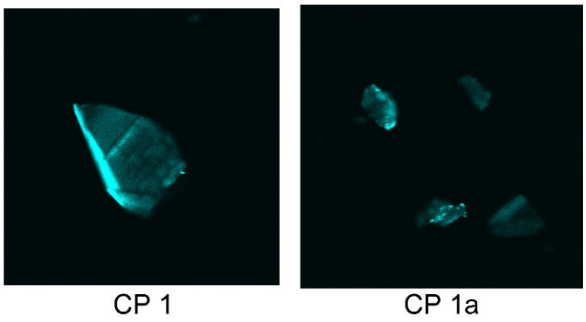

Fig. S7 Confocal fluorescence microscopy images for single crystals of CP **1** and **1a**. All samples were excited at 352 nm with an Ar ion laser.

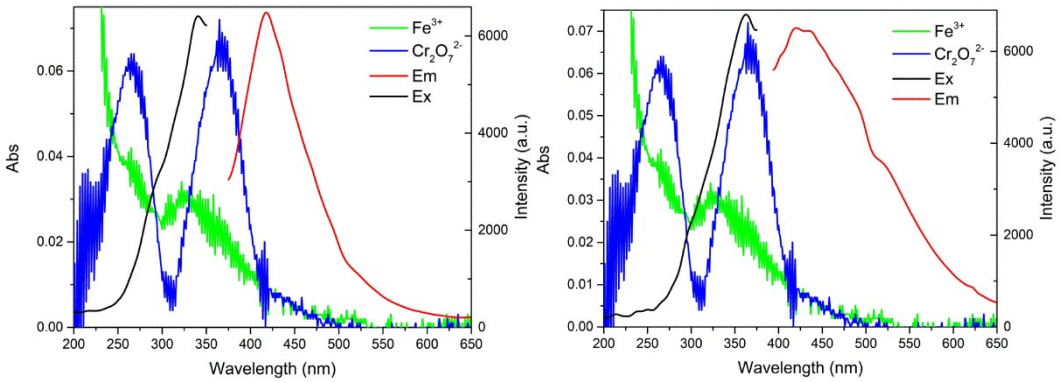

Fig. S8 Photoluminescence of CPs **1** (left) and **1a** (right) and UV-vis absorption spectra of Fe^{3+} and $Cr_2O_7^{2-}$ ions.

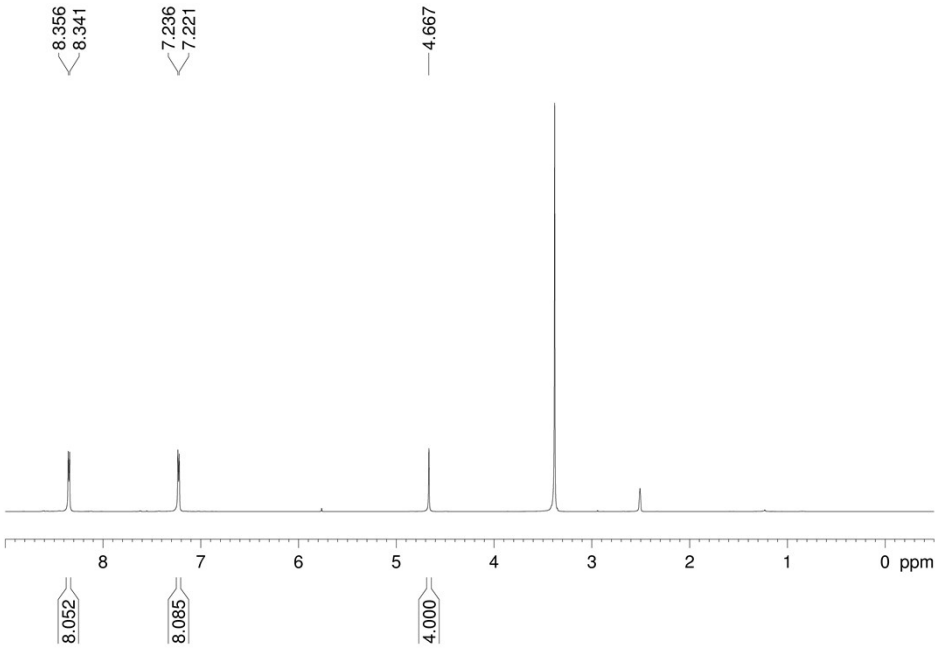

Fig. S9 The ^{1}HNMR spectrum of *rctt*-tpcb in DMSO-d_6.

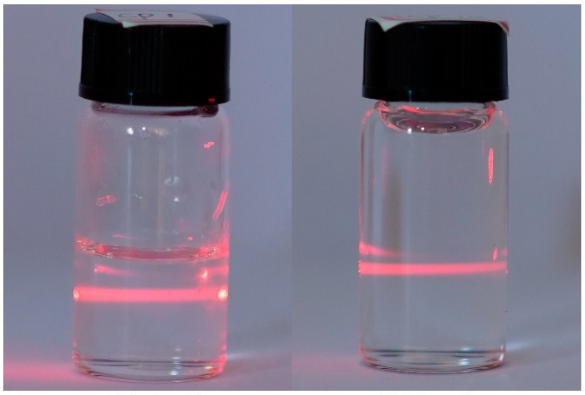

Fig. S10 Tyndall effect of the colloidal suspension of **1** and **1a** in the DMF**.**