Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.

A semi-conductive organic-inorganic hybrid emits pure white light with ultrahigh color rendering index

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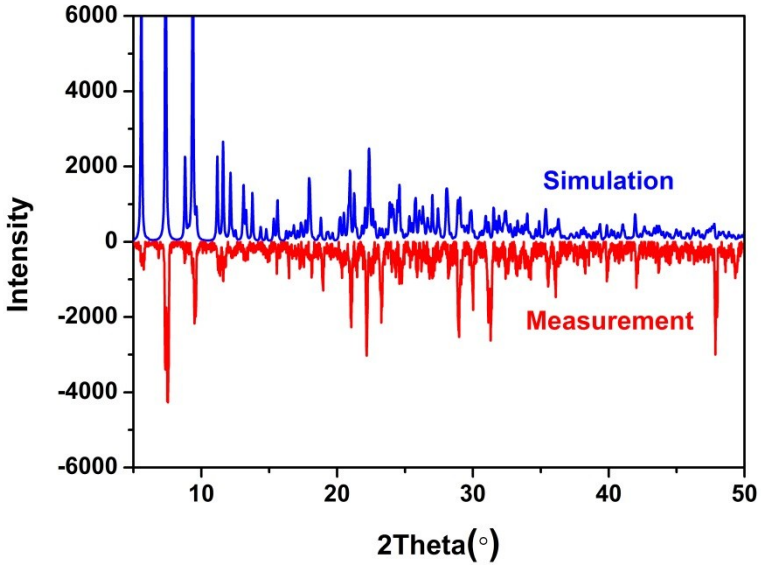


Figure S1. PXRD patterns of compound **1.**

Table S1. Crystallographic Data and Structure Refinement of 1.

Formula	$C_{60}H_{144}Br_{18}Cd_3N_{12}$
Formula weight (g/mol)	2809.30
Temperature (K)	293
Crystal system	triclinic
Space group	*P*-1
a (Å)	10.6818(3)
b (Å)	15.6189(4)
c (Å)	16.5803(5)
α (deg)	75.165(3)
β (deg)	76.833(3)
γ (deg)	72.093(3)
V (Å3)	2510.85(13)
Z	1
D_{calcd} (g/cm^3)	1.858
F (000)	1362.0
completeness (%)	99.7%
GOF (F^2)	1.042
R_1 (on F_o^2, I >2s(I))	0.0452
wR_2 (on F_o^2, I >2s(I))	0.1492

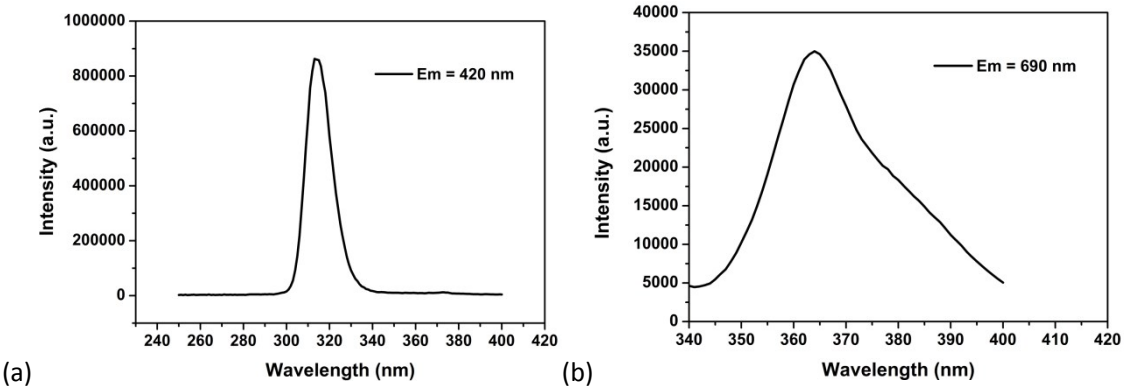
[a] $R_1 = \Sigma||F_0|-|F_c||/\Sigma|F_0|$, $\omega R_2 = [\Sigma[\omega(F_0^2-F_c^2)^2]/\Sigma[\omega(F_0^2)^2]]^{1/2}$

Table S2. Selected bond length (Å).

Bond	(Å)	Bond	(Å)
Cd(1)–Br(1)	2.7349(5)	Cd(2)–Br(4)	2.5855(9)
Cd(1)–Br(2)	2.8371(8)	Cd(2)–Br(5)	2.5675(8)
Cd(1)–Br(3)	2.7980(6)	Cd(2)–Br(6)	2.5656(9)
		Cd(2)–Br(7)	2.6063(13)

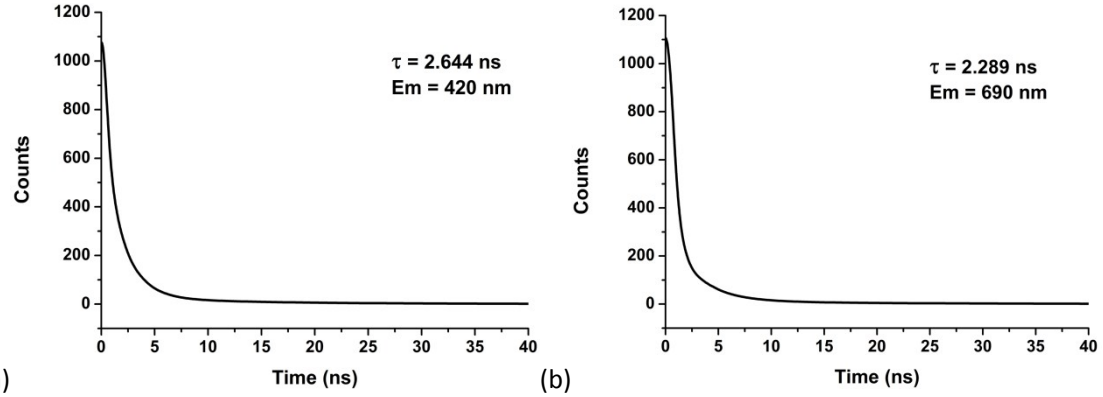
Table S3. The length of H-bonds of 1.

Bond	(Å)	Bond	(Å)
N1-H15A···Br2	2.626	N1-H15B···Br8	2.517
N2-H10B···Br2	2.665	N1-H15C···Br8	2.666
N2-H10C···Br5	2.607	N2-H10A···Br8	2.494
N5-H14C···Br6	2.481	N5-H14B···Br9	2.412
N6-H11A···Br7	2.629	N3-H6C···Br9	2.511
N3-H6B···Br8	2.521	N4-H18C···Br9	2.423



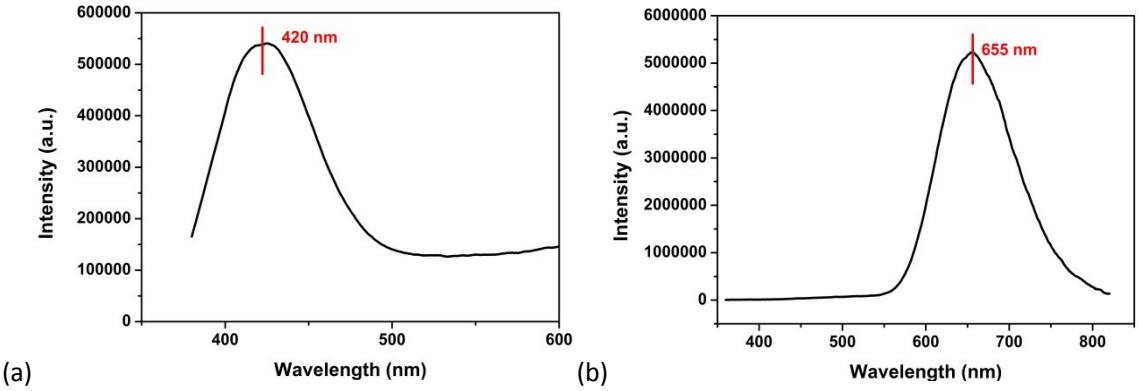
(a) (b)

Figure S2. Excitation spectrum of **1** at 420 nm (a) and 690 nm (b).



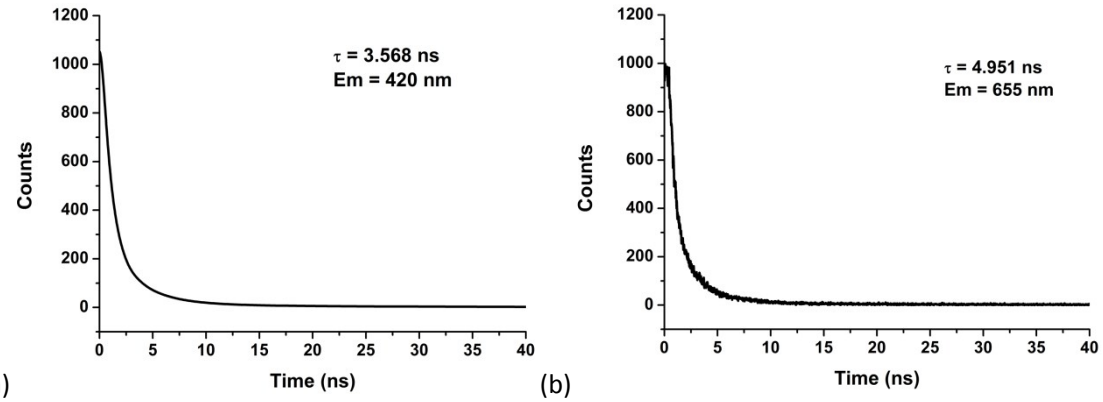
(a) (b)

Figure S3. Luminescence decay data of **1** at 420 nm (a) and 690 nm (b).



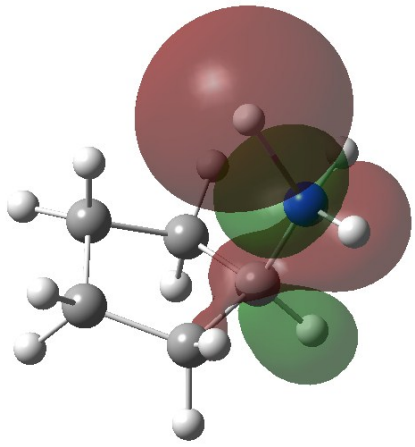
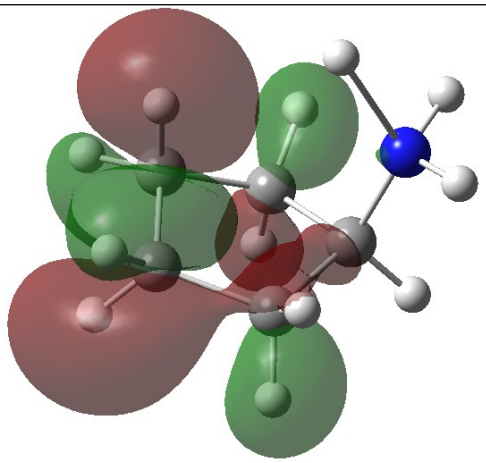
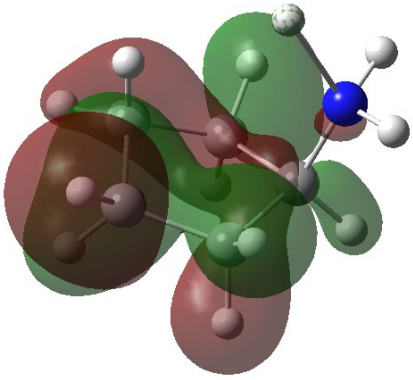
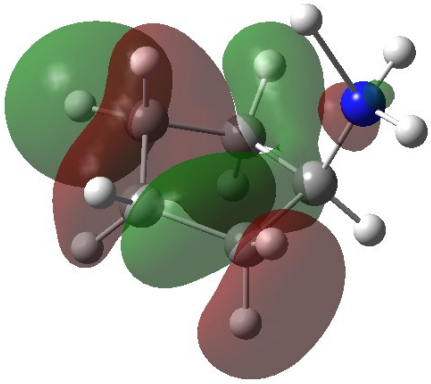
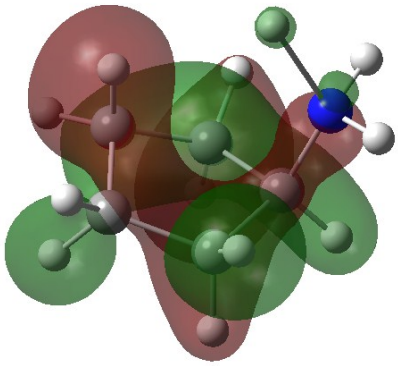
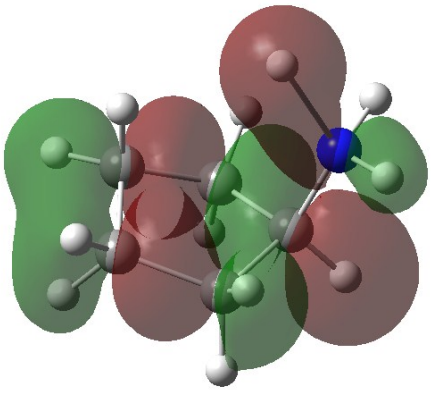
(a) (b)

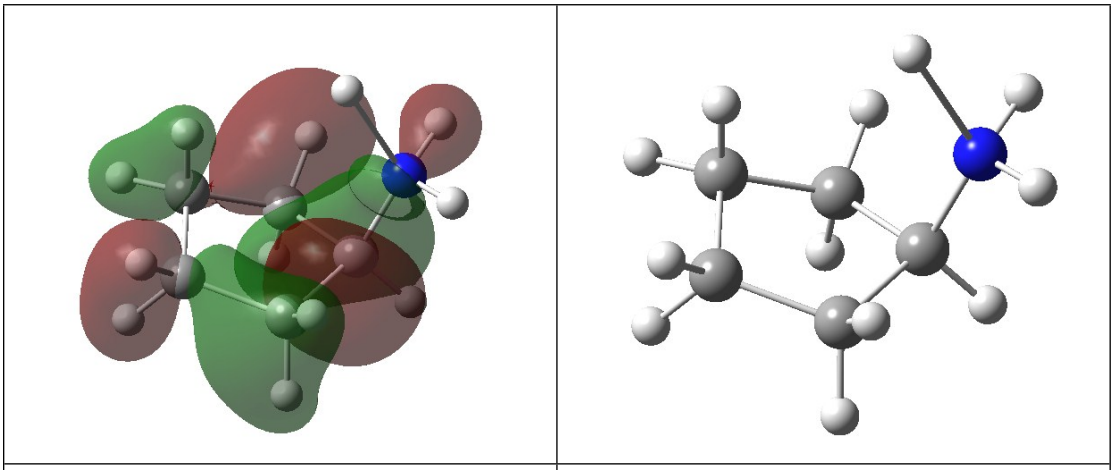
Figure S4. Emission spectrum of $[C_5H_9NH_3]^+Br^-$ (a) and $CdBr_2$ (b).



(a) (b)

Figure S5. Luminescence decay data of $[C_5H_9NH_3]^+Br^-$ (a) and $CdBr_2$ (b).

	
LUMO (E = -9.48 eV) 6.55/93.45	HOMO (E = -11.08 eV) 99.55/0.45
	
HOMO-1 (E = -13.92 eV) 97.86/2.14	HOMO-2 (E = -14.11 eV) 97.83/2.17
	
HOMO-3 (E = -14.23 eV) 95.14/4.86	HOMO-4 (E = -14.40 eV) 87.95/12.05



HOMO-5 (E = -14.63 eV) 94.49/5.51	**S_1**-optimized structure

Figure S6. Plots of the frontier molecular orbitals involved in the emission transitions of cation part calculated by TD-DFT method at the PBE1PBE level (isovalue = 0.03) combined with the partial molecular orbital compositions (%, C5/NH_3) and the optimized structure in the **S_1** state.

Table S4 The optimized geometrical coordinates (unit: angstroms) of the cation part in the lowest singlet excited state **S_1** by TD-DFT method at the PBE1PBE level.

Center number	Atomic type	Coordinates		
		X	Y	Z
1	C	0.798076	0.010115	0.619822
2	H	1.285797	0.02473	1.592079
3	C	-0.13478	1.228509	0.430003
4	H	-0.43476	1.63982	1.407998
5	H	0.350168	2.041897	-0.10954
6	C	-0.13692	-1.20954	0.500312
7	H	0.359544	-2.11794	0.135097
8	H	-0.55098	-1.48107	1.479739
9	C	-1.24334	-0.8213	-0.44024
10	H	-0.93843	-0.66291	-1.51597
11	H	-2.1403	-1.44322	-0.45695
12	C	-1.38968	0.770651	-0.27896
13	H	-1.74839	1.379229	-1.11249
14	H	-2.3234	0.594458	0.346089
15	H	2.331253	-0.86135	-0.54316
16	N	1.788975	-0.0019	-0.49441
17	H	2.431433	0.786845	-0.45408
18	H	1.49508	0.242223	-2.29363

Table S5. The emission transitions for the cation part in the solid state by TD-DFT method at the PBE1PBE level.

States	*E*, nm (eV)	O.S.	Transition (contri.)	Assignment
S_1	364	0.0033	HOMO-1→LUMO (96%)	
S_2	348	0.0005	HOMO-2→LUMO (97%)	
S_3	343	0.0003	HOMO-3→LUMO (87%) HOMO-4→LUMO (10%)	C5→NH_3
S_4	317	0.0030	HOMO-5→LUMO (81%) HOMO-4→LUMO (11%)	

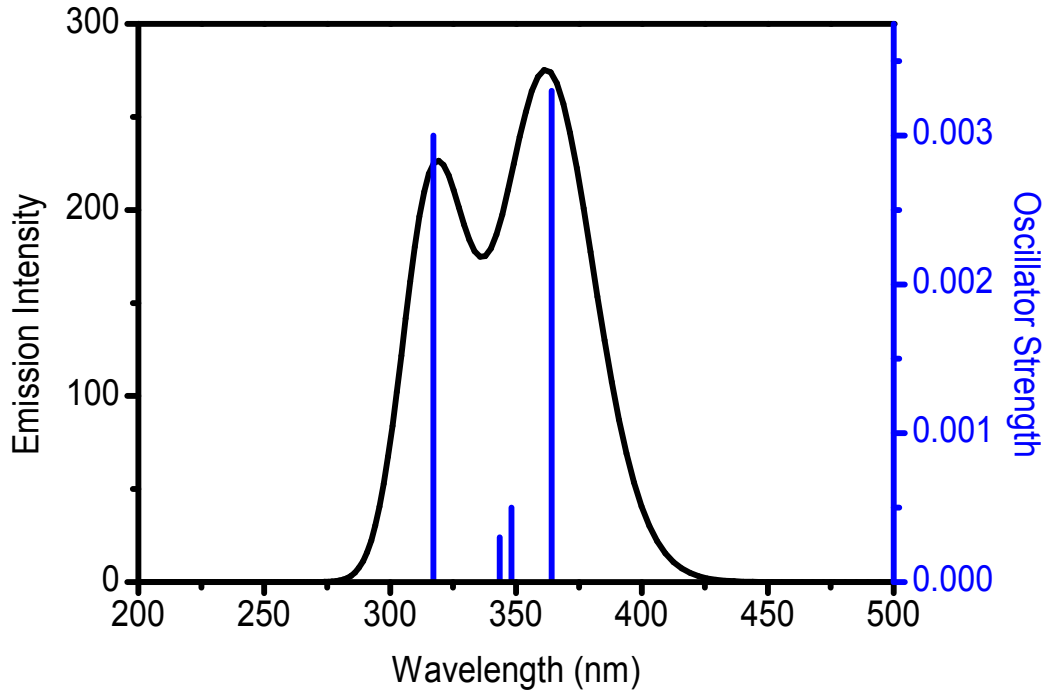


Figure S7. The calculated (blue vertical bars) and simulated (black line, implemented by GaussSum) emission spectra of the cation part at ambient temperature calculated by TD-DFT method at the PBE1PBE level.

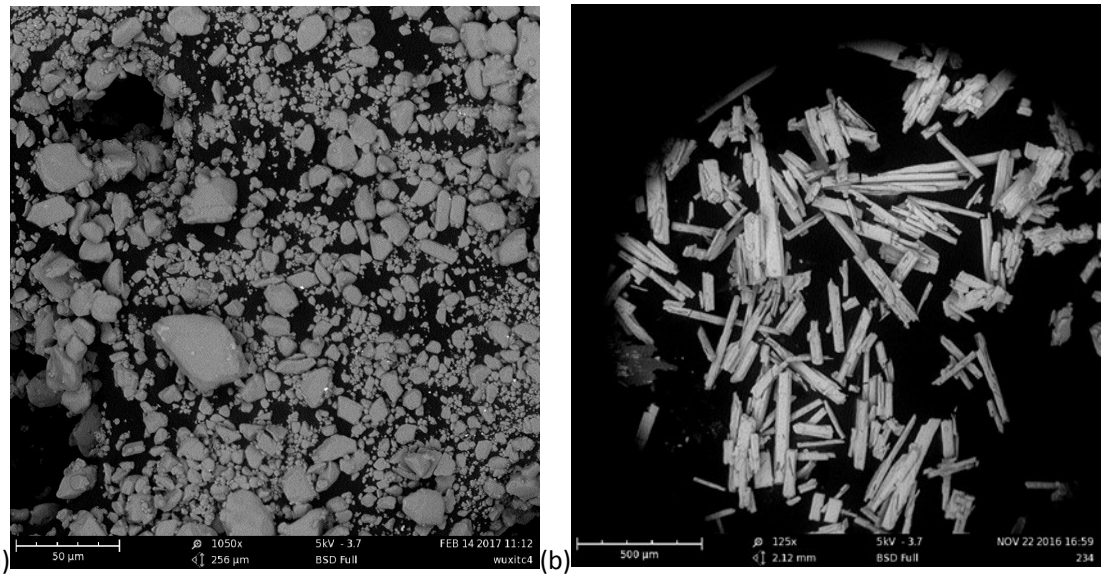


Figure S8. SEM images of (a) hand grinded powders and (b) crystals.

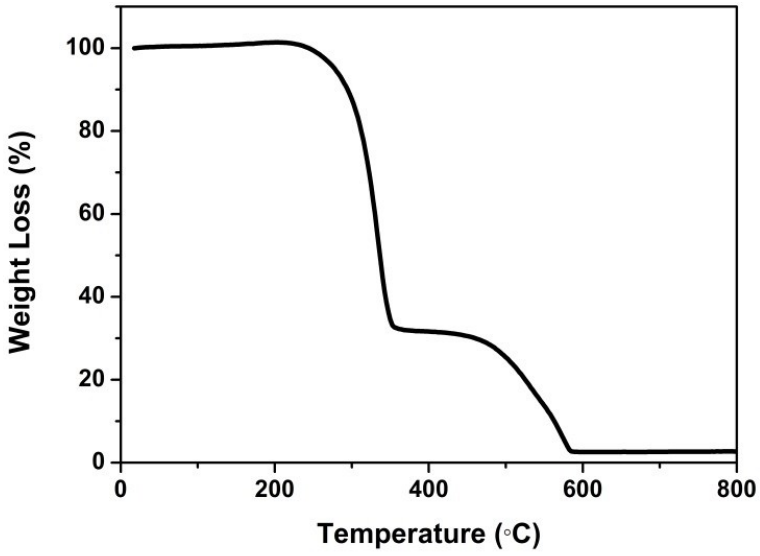


Figure S9. TG curve of compound **1**.

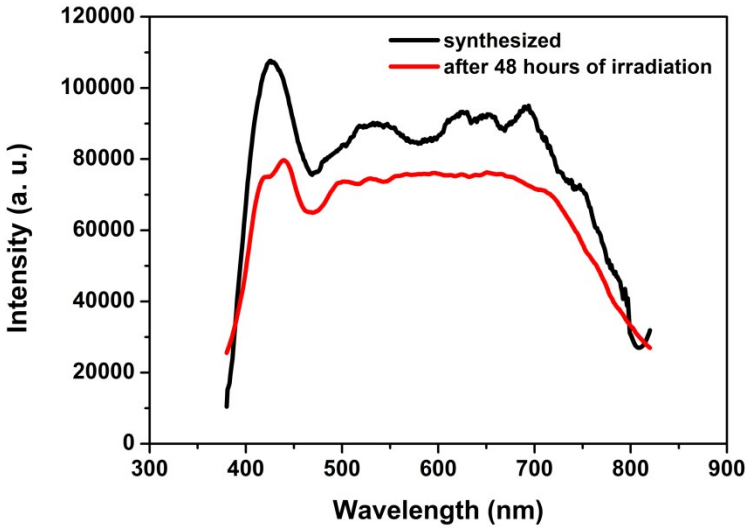


Figure S10. Photoluminescence spectrum of **1** before and after irradiated for 48 hours.

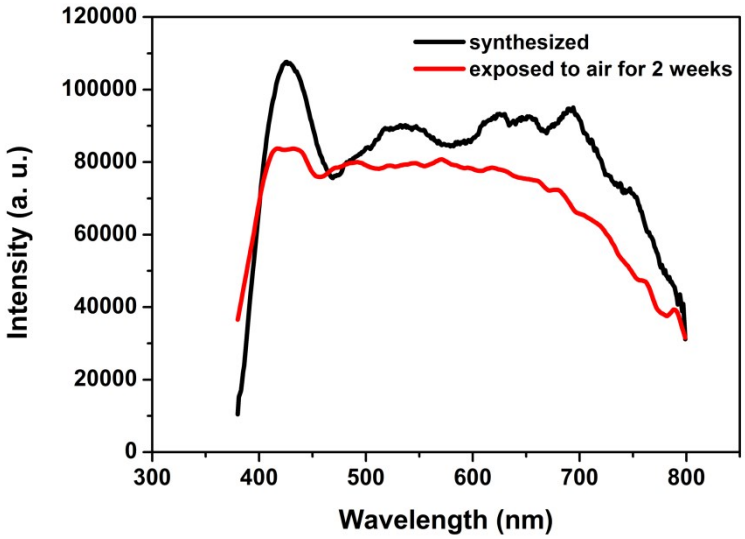


Figure S11. Photoluminescence spectrum of **1** before and after exposed to ambient conditions for two weeks.

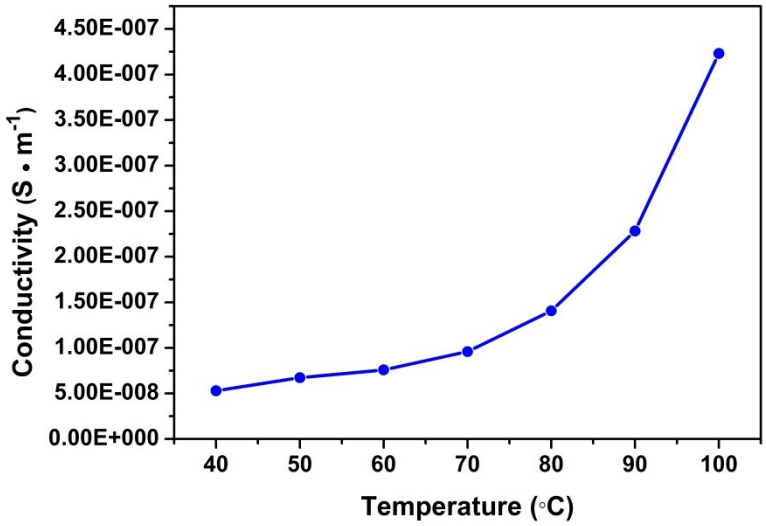


Figure S12. Temperature-dependent conductivity of **1**.