Electronic Supplementary Information

Fabrication of blue organic light-emitting diode from novel uranium complexes: Synthesis, characterization, and electroluminescence studies of uranium anthracene-9-carboxylate complexes

Khodabakhsh Darzinezhad,[a] Mostafa M. Amini,[*a] Ezeddin Mohajerani,[c] Mahsa Armaghan,[b] Tim Oliver Knedel,[b] Afshin Abareghi,[c] Christoph Janiak,[*b]

Email addresses:

dordikeshemeykhoone@yahoo.com, m-pouramini@sbu.ac.ir, e-mohajerani@sbu.ac.ir, armaghan@uni-duesseldorf.de, tim-oliver.knedel@uni-duesseldorf.de, afabareghi@gmail.com, janiak@hhu.de

[a]*Department of Chemistry, ShahidBeheshti University, G.C., Tehran 1983963113, Iran*

[b]*Institut für Anorganische Chemie und Strukturchemie Heinrich-Heine Universität, D-40204 Düsseldorf, Germany*

[c]*Laser and Plasma Research Institute, Shahid Beheshti University, G.C., 1983963113, Tehran, Iran*

Table S1 Crystal data and structure refinement for **1**, **2** and **3**.

Complex	**1**	**2**	**3**
Empirical formula	$C_{38}H_{42}O_{10}U$	$C_{36}H_{40}O_{14}U_2$	$C_{62}H_{48}O_{16}U_2$
Formula weight (g mol^{-1})	896.75	1172.74	1525.06
T (K)	140	140	140
Wavelength λ (Å)	0.71073	0.71073	0.71073
Crystal system	monoclinic	triclinic	triclinic
Space group	$P2_1/c$	P-1	P-1
a (Å)	7.8016(8)	8.9252(7)	10.6301(6)
b (Å)	26.772(3)	9.2387(7)	11.9054(7)
c (Å)	17.7555(19)	12.1717(9)	11.9924(7)
α (º)	90	68.676(3)	110.639(3)
β (º)	93.142(5)	85.383(3)	100.789(3)
γ (º)	90	84.565(3)	98.333(3)
V ($Å^3$)	3702.9(7)	929.58(12)	1357.98(14)
Z	4	1	1
D_{calc} (mg m^{-3})	1.609	2.095	1.865
F(000)	1768.0	552.0	732.0
μ (mm^{-1})	4.439	8.767	6.028
Crystal size (mm^3)	0.328×0.346×0.679	0.05×0.1×0.2	0.05×0.05×0.1
θ range (º)	1.52-26.37	1.80-27.81	1.88-27.91
Reflections collected	106147	19539	24875
Unique reflection (R_{int})	7573 (0.033)	4370 (0.037)	6208 (0.025)
R_1, $wR_2{}^a[I > 2\sigma(I)]$	0.020, 0.045	0.018, 0.048	0.020, 0.037
R_1, $wR_2{}^a$ (all data)	0.022, 0.046	0.019, 0.049	0.017, 0.038

Goodness-of-fit (GOF) on F^2	1.10	1.04	1.03

[a] $R_1 = \Sigma||F_o|-|F_c||/\Sigma|F_o|$, $wR_2 = [\Sigma(w(F_o^2-F_c^2)^2)/\Sigma w(F_o^2)^2]^{1/2}$

Table S2 Selected band lengths (Å) and bond angles (º) for **1**.

U(1)–O(1)	1.747(2)	U(1)–O(5)	2.500(2)
U(1)–O(2)	1.750(2)	U(1)–O(6)	2.4931(19)
U(1)–O(3)	2.481(2)	U(1)–O(7)	2.433(2)
U(1)–O(4)	2.506(2)	U(1)–O(8)	2.4246(19)
O(1)–U(1)–O(2)	179.51(11)	O(3)–U(1)–O(6)	179.27(9)
O(1)–U(1)–O(8)	91.40(11)	O(1)–U(1)–O(5)	92.34(10)
O(2)–U(1)–O(8)	88.83(12)	O(2)–U(1)–O(5)	87.18(11)
O(1)–U(1)–O(7)	87.45(12)	O(8)–U(1)–O(5)	115.20(7)
O(2)–U(1)–O(7)	92.32(12)	O(7)–U(1)–O(5)	65.09(7)
O(8)–U(1)–O(7)	178.83(9)	O(3)– U(1)–O(5)	128.82(7)
O(1)–U(1)–O(3)	92.13(10)	O(6)–U(1)–O(5)	50.90(6)
O(2)–U(1)–O(3)	88.15(10)	O(1)–U(1)–O(4)	91.01(10)
O(8)–U(1)–O(3)	115.61(7)	O(2)–U(1)–O(4)	89.48(11)
O(7)–U(1)–O(3)	64.23(7)	O(8)–U(1)–O(4)	64.94(7)
O(1)–U(1)–O(6)	88.57(10)	O(7)– U(1)–O(4)	114.84(7)
O(2)–U(1)–O(6)	91.15(10)	O(3)–U(1)–O(4)	50.74(7)
O(8)–U(1)–O(6)	64.58(6)	O(6)–U(1)–O(4)	129.49(7)
O(7)–U(1)–O(6)	115.59(7)	O(5)–U(1)–O(4)	176.65(10)

Table S3 Selected band lengths (Å) and bond angles (º) for **2**.

U(1)–O(3)	1.769(2)	U(1)–O(2)	2.453(2)
U(1)–O(4)	1.766(2)	U(1)–O(1)	2.489(2)
U(1)–O(6)	2.3264(19)	U(1)–O(5)	2.400(2)
O(3)–U(1)–O(4)	176.73(9)	O(4)–U(1)–O(1)	90.68(9)
O(3)–U(1)–O(6)	92.43(9)	O(6)–U(1)–O(1)	159.51(7)
O(4)–U(1)–O(6)	93.14(9)	O(5)–U(1)–O(1)	73.16(7)
O(3)–U(1)–O(6)	90.12(9)	O(2)–U(1)–O(1)	52.64(7)
O(4)–U(1)–O(6)	93.14(9)	O(3)–U(1)–O(1)	87.31(9)
O(6)–U(1)–O(6)	70.67(8)	O(5)–U(1)–O(2)	125.80(7)
O(3)–U(1)–O(5)	88.53(9)	O(6)–U(1)–O(2)	77.22(7)
O(4)–U(1)–O(5)	88.43(9)	O(4)–U(1)–O(2)	91.79(9)
O(6)–U(1)–O(5)	86.35(7)	O(3)–U(1)–O(2)	89.03(9)

Table S4 Selected band lengths (Å) and bond angles (º) for **3**.

U(1)–O(4)	1.7621(16)	U(1)–O(7)	2.3619(16)
U(1)–O(3)	1.7622(16)	U(1)–O(2)	2.5091(17)
U(1)–O(5)	2.3769(18)	U(1)–O(1)	2.4139(19)
U(1)–O(6)	2.3154(18)		
O(4)–U(1)–O(3)	177.51(9)	O(7)–U(1)–O(2)	122.44(6)
O(4)–U(1)–O(5)	85.33(8)	O(4)–U(1)–O(1)	90.13(8)
O(3)–U(1)–O(5)	92.31(8)	O(3)–U(1)–O(1)	91.91(8)
O(4)–U(1)–O(6)	90.87(7)	O(5)–U(1)–O(1)	126.73(6)
O(3)–U(1)–O(6)	87.98(7)	O(6)–U(1)–O(1)	152.13(6)
O(5)–U(1)–O(6)	81.09(6)	O(7)–U(1)–O(1)	70.83(6)
O(4)–U(1)–O(7)	91.30(7)	O(2)–U(1)–O(1)	52.31(6)
O(3)–U(1)–O(7)	90.71(7)	O(6)–U(1)–O(2)	154.73(6)
O(5)–U(1)–O(7)	162.02(7)	O(5)–U(1)–O(2)	75.52(6)
O(6)–U(1)–O(7)	81.30(6)	O(3)–U(1)–O(2)	83.57(7)
O(4)–U(1)–O(2)	96.57(7)		

Table S5 Summary of short π–π ring-interactions in the crystal structures of complexes **2** and **3**.

Cg(I)···Cg(J)	**Cg···Cg (Å)**	**α (◦)**	**β (◦)**	**γ(◦)**	**Slippage (Å)**	**Symmetry operation on Cg(J)**
2						
Cg1-Cg1	3.7136(19)	0.00(15)	21.5	21.5	1.359	2-x,1-y,-y
Cg1-Cg3	3.664(2)	1.11(17)	18.7	19.2	1.174	2-x,1-y,-z
Cg2-Cg3	3.747(2)	1.92(18)	22.2	20.3	1.414	2-x,1-y,-z
Cg1 (C2, C3, C8, C9, C10, C15), Cg2 (C3>C8), Cg3 (C10>C15)						
3						
Cg1- Cg1	3.8469 (13)	0.03(10)	17.6	17.6	1.160	-x, -y, -z
Cg1- Cg3	3.9136 (14)	0.61(11)	20.8	20.2	1.390	-x, -y, -z
Cg3- Cg2	3.8181 (14)	2.15(11)	17.0	18.4	1.114	-x, -y, -z
Cg1 (C2, C3, C8, C9, C10, C15), Cg2 (C3>C8), Cg3 (C10>C15) Cg is the centroid of the ring α=Dihedral angle between Planes Cg β=Angle between Cg(I)→ Cg(J) vector and normal to plane I γ=Angle between Cg → Cg vector and normal to plane J						

Table S6 Summary of intermolecular X-H·· π interactions in the crystal structures of complexes **1**, **2**, and **3**.

X-H	**Cg**	**H···Cg(Å)**	**X ··Cg(Å)**	**γ (◦)**	**X-H···Cg (◦)**
1					
C17-H17	Cg (C4-C6, C11-C13)	2.83	3.3906(4)	12.76	119
C19-H19	Cg (C1-C4, C13-C14)	2.86	3.5220(4)	7.22	127
C35-H35B	Cg (C18-C20, C25-C27)	2.76	3.6936(4)	7.35	156
C37-H37B	Cg (C4-C6, C11-C13)	2.87	3.7345(4)	14.10	147
2					
C17-H17	Cg (C10>C15)	2.72	3.437(4)	8.59	131
3					
O8-H8B	(C26>C31)	2.68(4)	3.324(3)	18.77	135(4)
C25-H25	(C10>C15)	2.92	3.746(2)	6.11	146
C27-H27	Cg (C2-C3, C8-C10, C15)	2.60	3.350(2)	15.58	136
γ = Angle between Cg → H vector and ring Cg normal					

Table S7 Photophysical data of complexes, anthracene-9-carboxylic acid and uranyl acetate dihydrate.

	absorption		emission	
	λ_{max} (nm)	ε (L/mol cm)×10^3	λ_{max} (nm)	FWHM (nm)
Complex **1**	250, 368	2599, 363	440	75
Complex **2**	256, 368	1113, 64	443	70
Complex **3**	255, 367	2151, 700	443	75
Anthracene-9-carboxylic acid	252, 364	2.62, 1.64	441	75
Uranyl acetate dihydrate	239	0.80	615	72

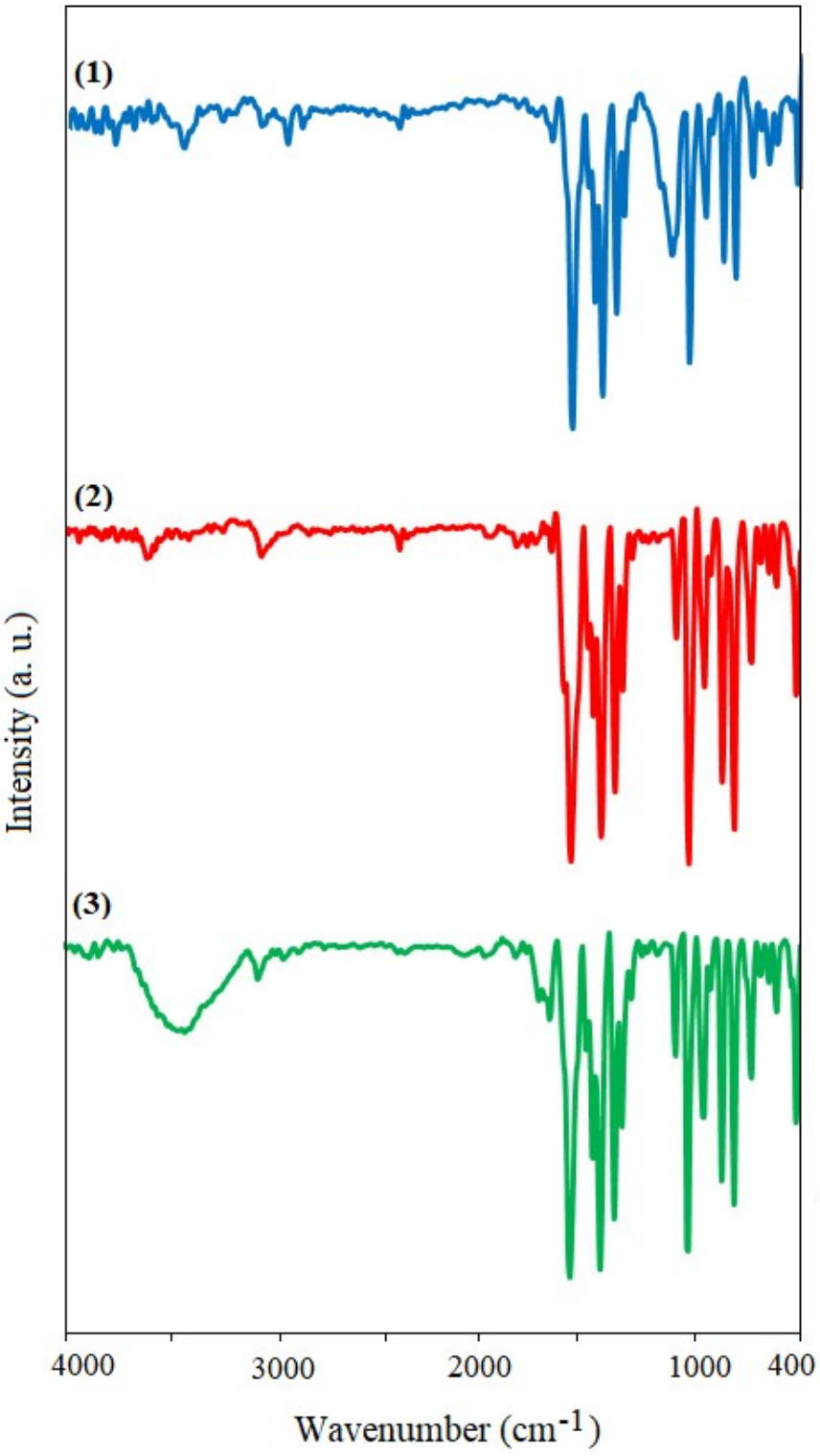


Figure S1 Infrared spectra of compounds **1**, **2** and **3**.

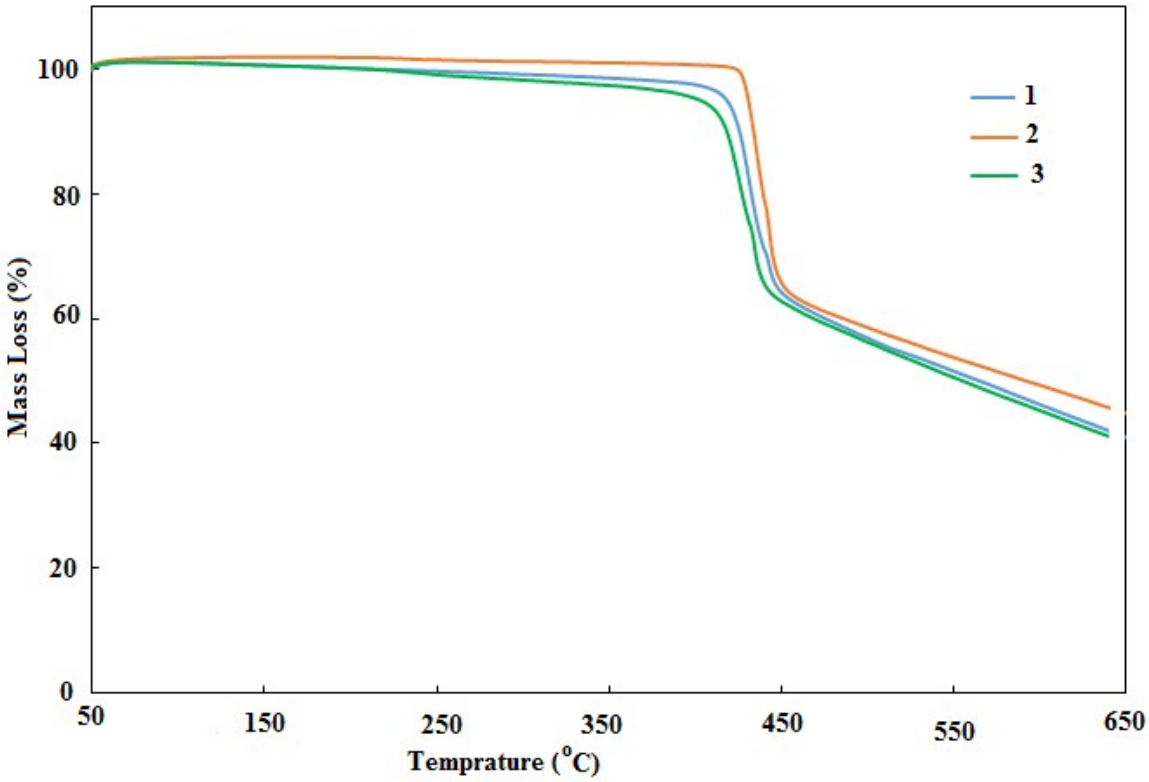


Figure S2 TGA diagrams of compounds **1**, **2** and **3**.

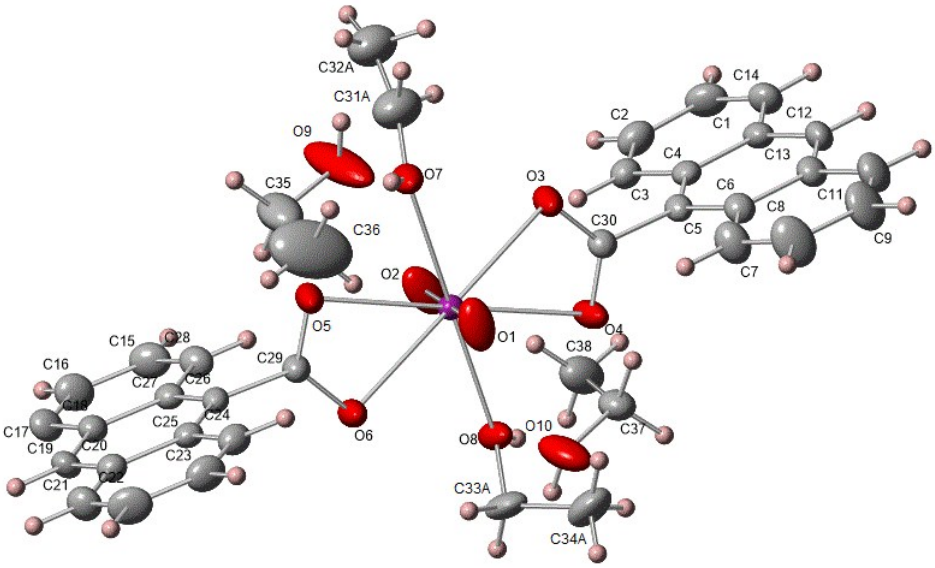


Figure S3 X-ray molecular structure for $[UO_2(C_{15}H_9O_2)_2(CH_3CH_2OH)_2]\cdot 2CH_3CH_2OH$ (**1**) with the atom-labeling scheme. Displacement ellipsoids are drawn at the 50% probability level.

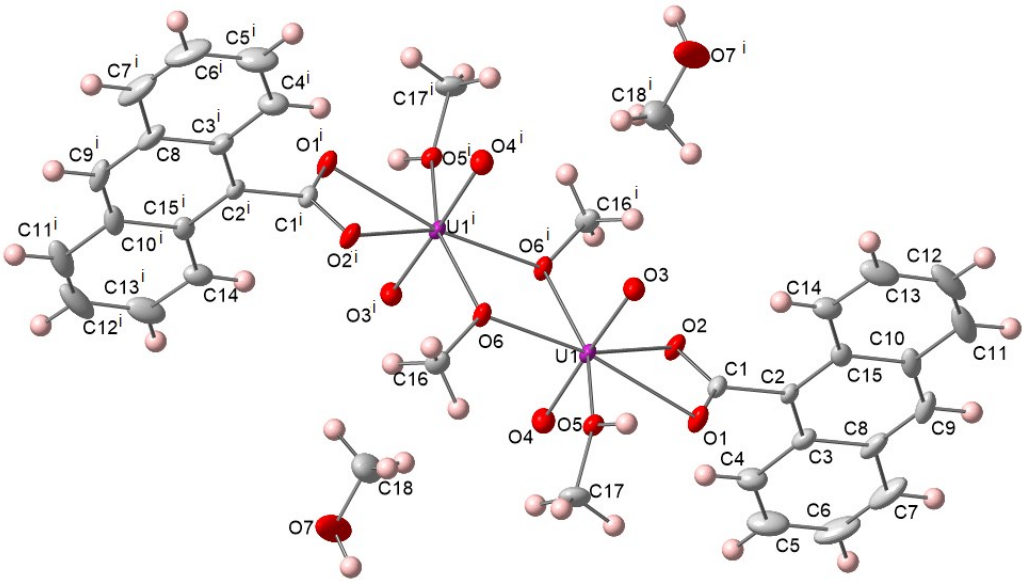


Figure S4 X-ray molecular structure for $[U_2O_4(C_{15}H_9O_2)_2(CH_3O)_2(CH_3OH)_2]\cdot 2CH_3OH$ (**2**) with the atom-labeling scheme. Displacement ellipsoids are drawn at the 50% probability level. Symmetry transformation i = 1-x, 1-y, 1-z.

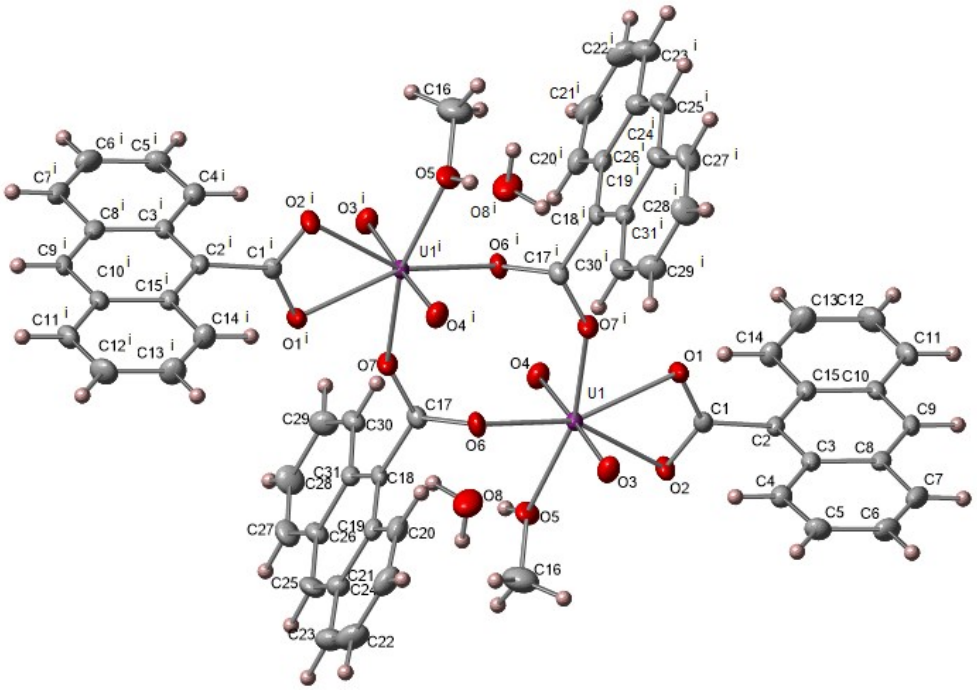


Figure S5 X-ray molecular structure for $[U_2O_4(C_{15}H_9O_2)_4(CH_3OH)_2]\cdot 2H_2O$ (**3**) with the atom-labeling scheme. Displacement ellipsoids are drawn at the 50% probability level. Symmetry transformation i = 1-x, 1-y, -z.

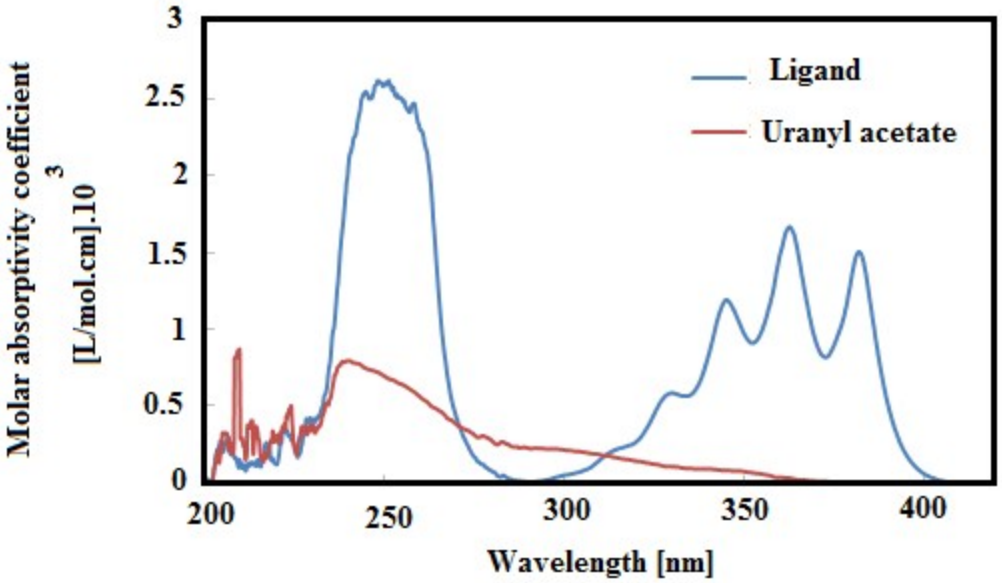


Figure S6 UV spectra of anthracene-9-carboxylic acid (non-deprotonated ligand) and uranyl acetate dihydrate.

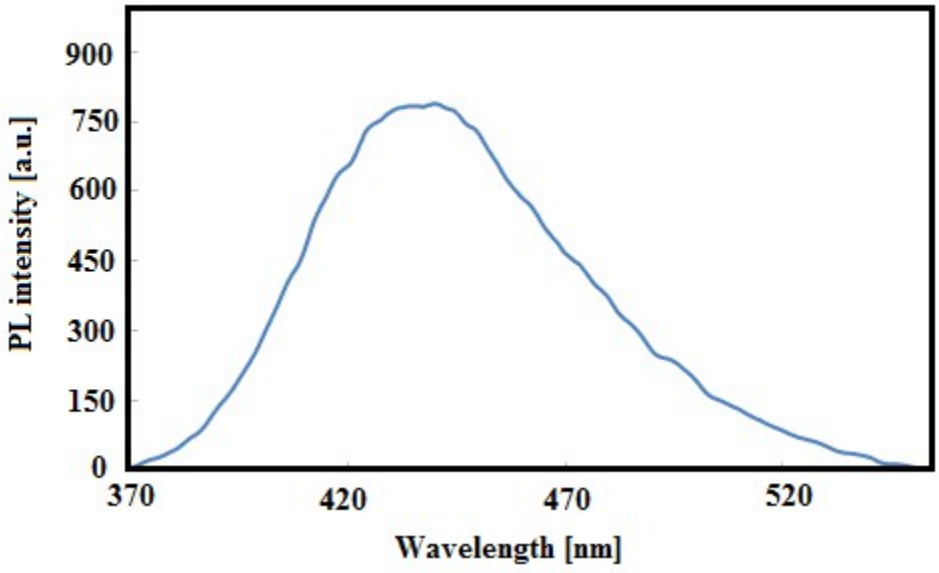


Figure S7 PL spectrum of anthracene-9-carboxylic acid at an excitation wavelength of 270 nm.

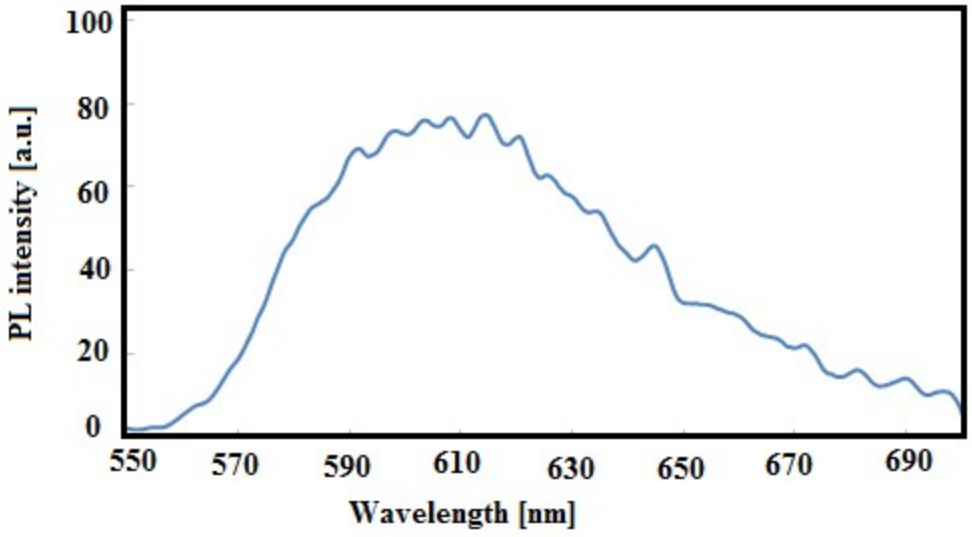
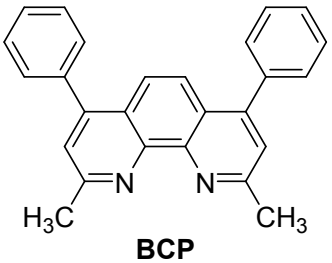
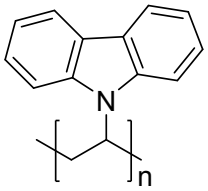


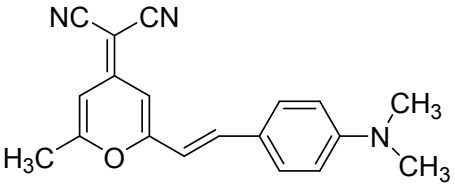
Figure S8 PL spectrum of uranyl acetate dihydrate at an excitation wavelength of 270 nm.



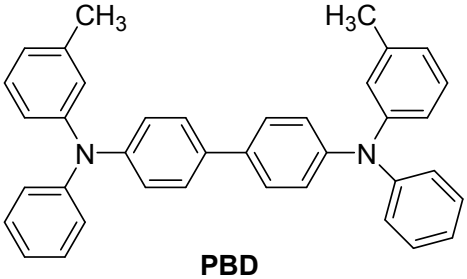
BCP



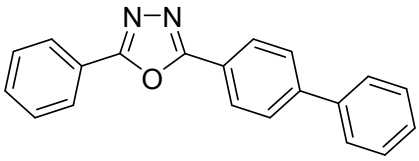
PVK



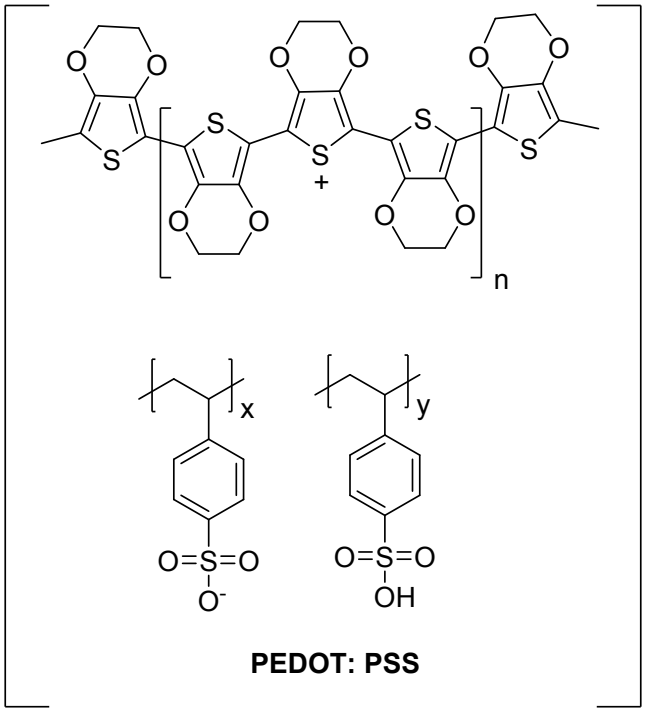
DCM



PBD



TPD



PEDOT: PSS

Scheme S1 Formulae of materials used to fabricate the BOLED: 2,9-dimethyl-4,7-diphenyl-1,10-phenanthroline (BCP), poly(9-vinylcarbazole) (PVK), 4-(dicyanomethylene)-2-methyl-6-(4-dimethylaminostyryl)-4*H*-pyran (DCM), *N,N*′-bis(3-methylphenyl)-*N,N*′-diphenylbenzidine (TPD), 2-phenyl-5-(4-biphenylyl)-1,3,4-oxadiazole (PBD), poly(3,4-ethylenedioxythiophene) poly(styrenesulfonate) (PEDOT:PSS.)