Supporting Information

(*E*)-4-Methyl-*N*-((Quinoline-2-yl)ethylidene)aniline as Ligand for IIB Supramolecular Complexes: Synthesis, Structure, Aggregation Induced Emission Enhancement and Application in PMMA-Doped Hybrid Material

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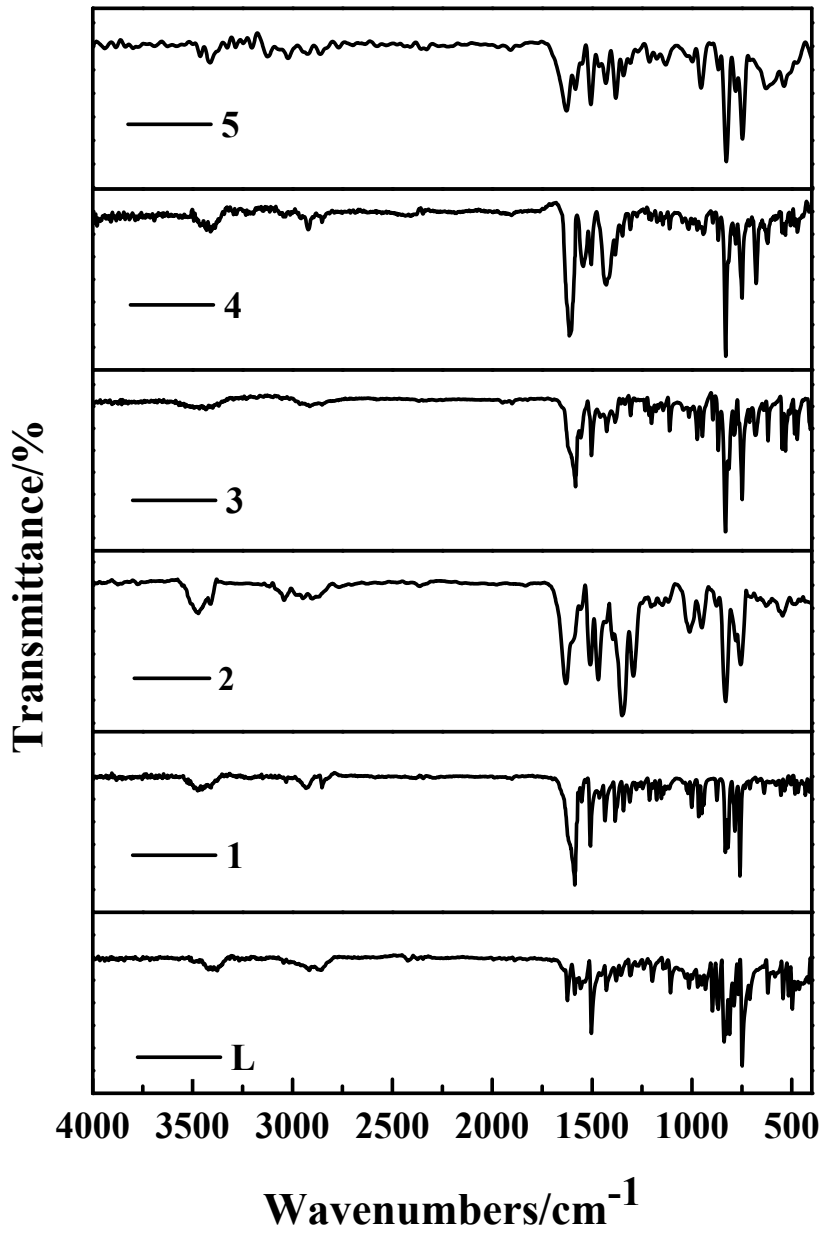

Fig. S1 Infrared spectra of ligand **L** and complexes **1**–**5** recorded from a KBr pellet.

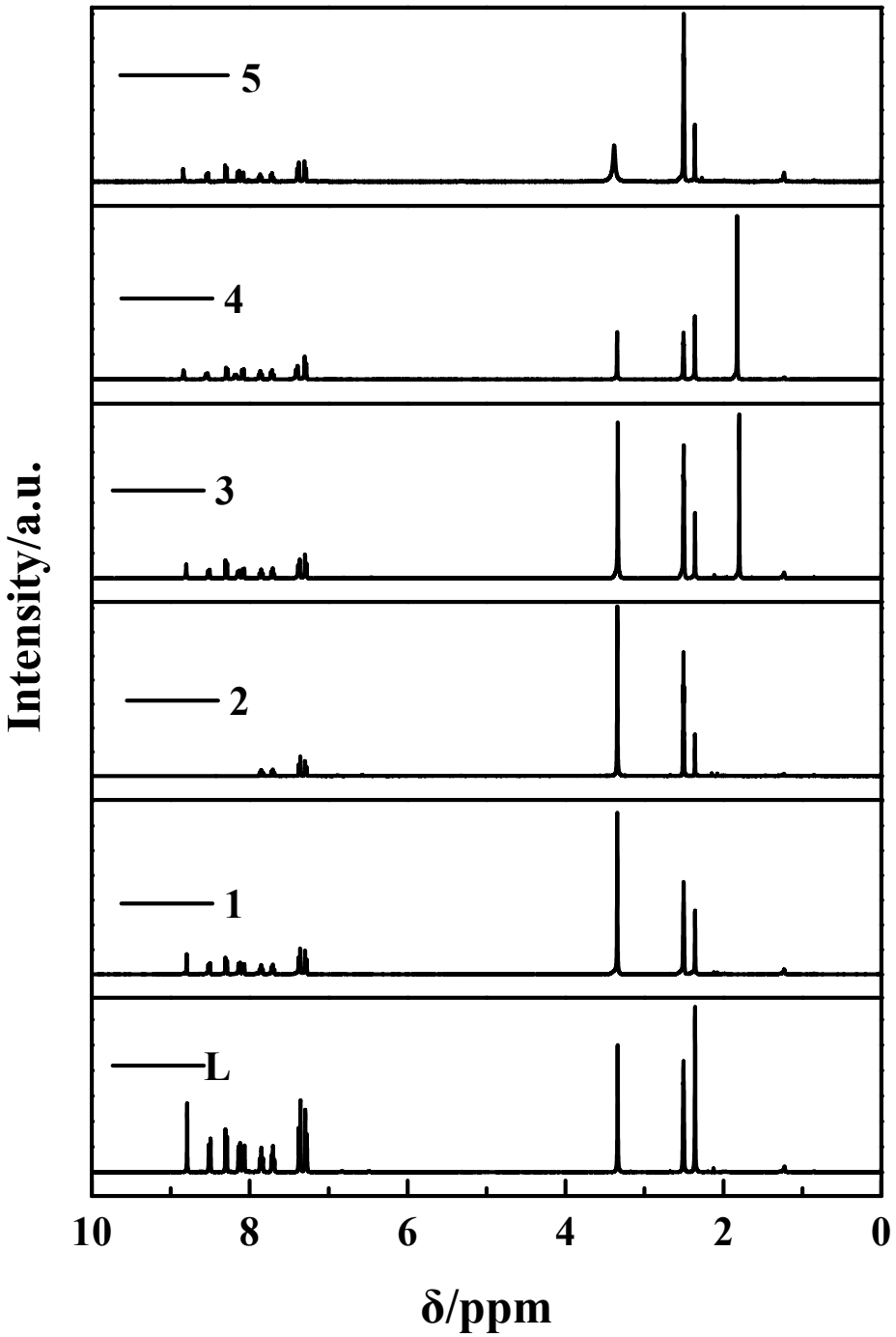

Fig. S2 ^{1}H NMR spectra of ligand **L** and complexes **1**–**5**.

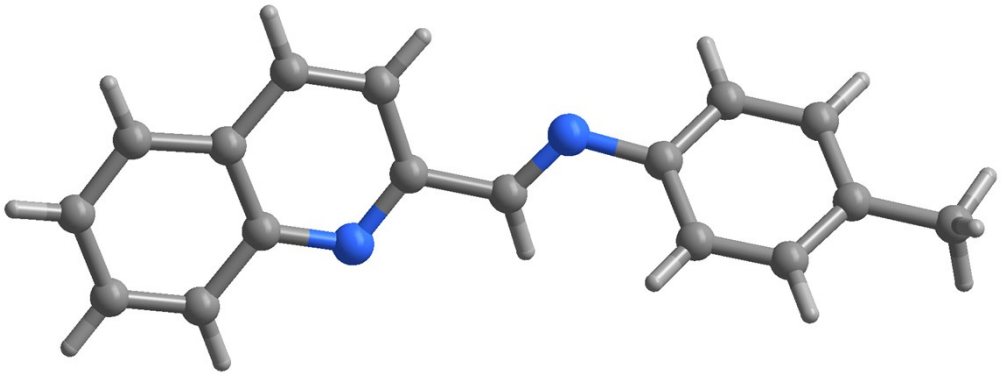

Fig. S3 Crystal structure of **L**.

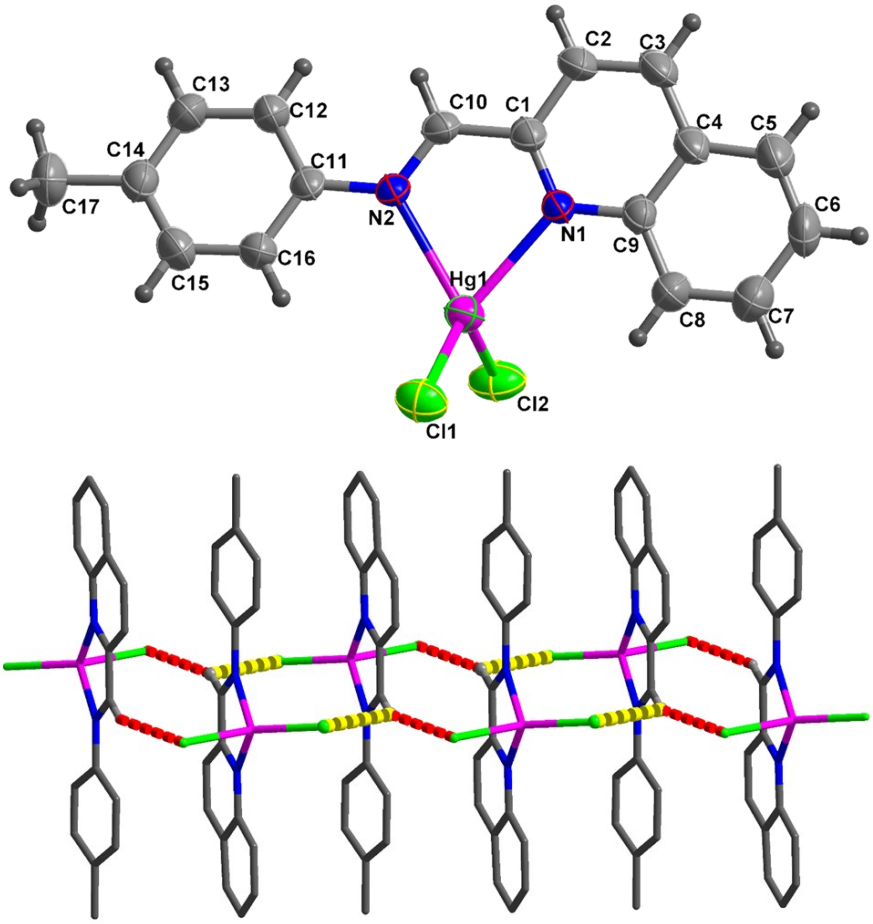

Fig. S4 View of the structure (1D chain) of complex **5**. Dotted lines represent the weak interactions.

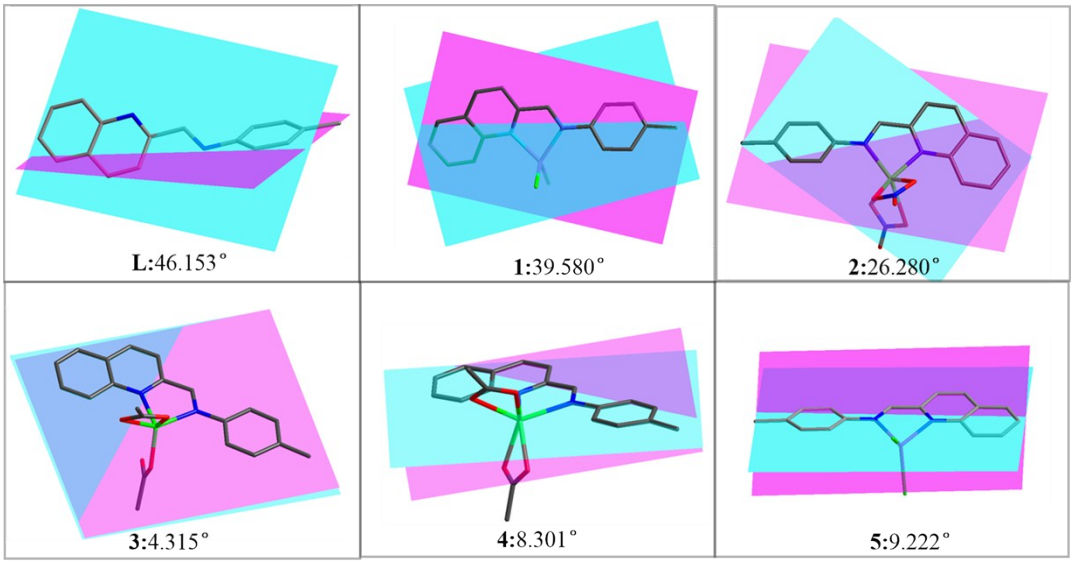

Fig. S5 Dihedral angles of **L** and complexes **1**–**5** between the quinoline and benzene rings.

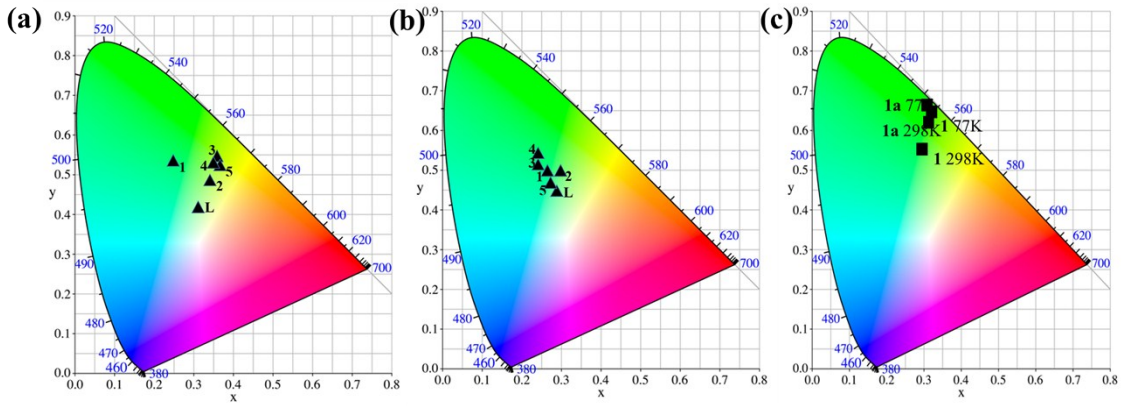

Fig. S6 CIE chromaticity diagram (1931 CIE standard) for **L** and complexes **1**–**5** (a) in the crystal state at 298 K (b) acetonitrile solution at 298K (c) in the crystal state and powder state at 77 K and 298 K.

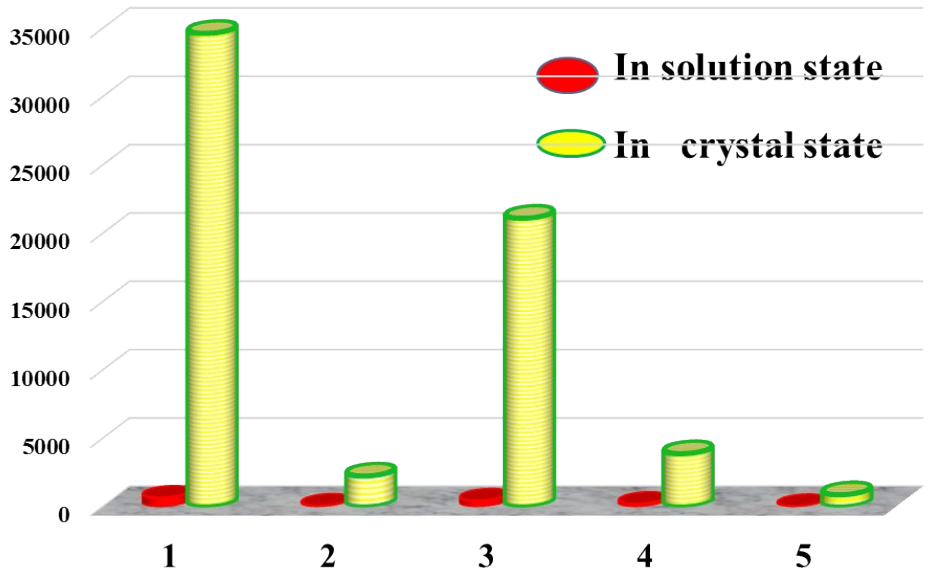

Fig. S7 The comparison of emission spectra of the complexes 1–5 in CH3CN solution and crystal state at 298K, upon excitation with 365 nm.

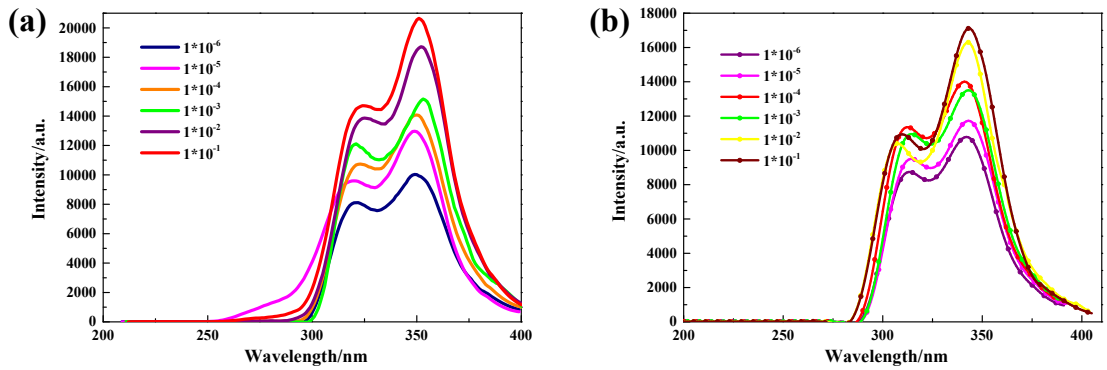

Fig. S8 The excitation spectra of **1** and **3** in different concentrations of CH_3CN.

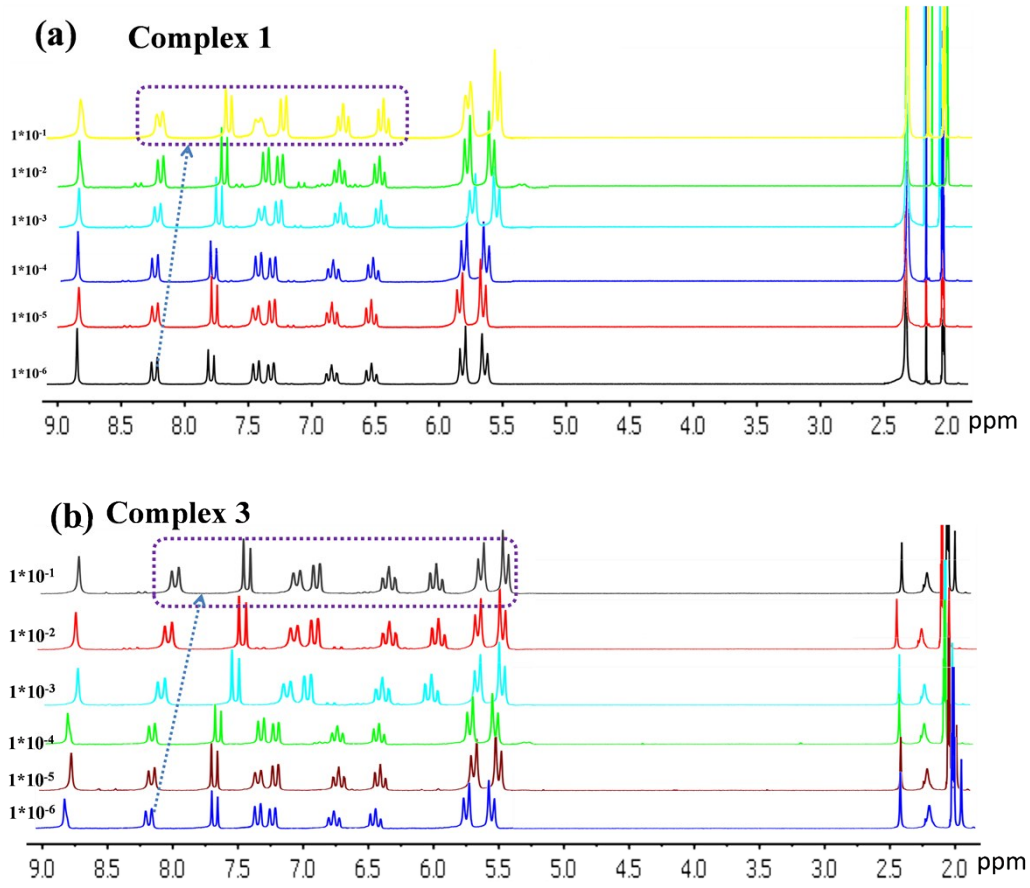

Fig. S9 ^{1}H NMR study of (a) complex **1** (b) **3** at varying concentrations (CD_3CN, 298 K).

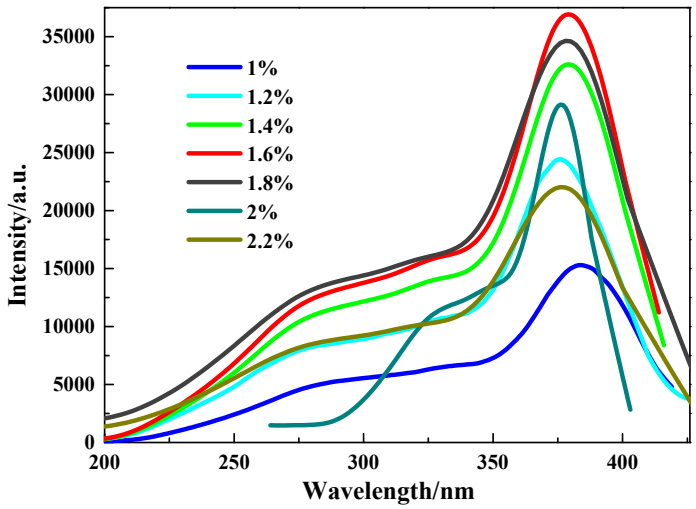

Fig. S10 Excitation spectra of these **1**-PMMA films in different dopant concentrations.

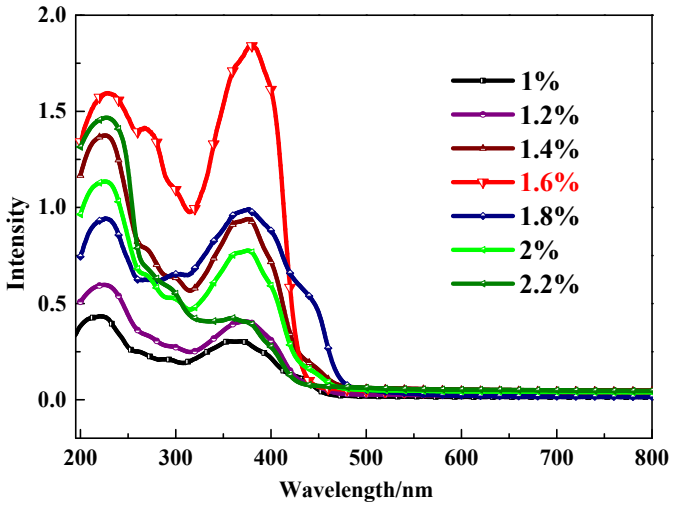

Fig. S11 UV−vis absorption spectra of the **1**-PMMA films in different dopant concentrations in the solid state at room temperature.

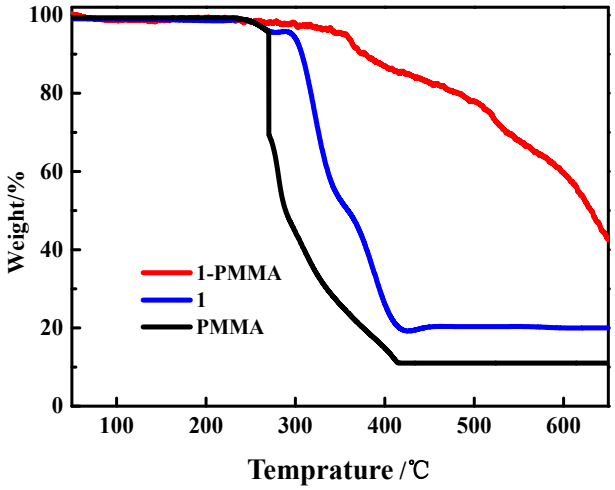

Fig. S12 The comparison TG curves of pure **1**, PMMA, and **1**-PMMA

Table S1. Selected bond distances (Å) and angles (°) for complexes **1** and **5**.

Parameter	**1**	Parameter	**5**
Zn(1)-N(1)	2.056(9)	Hg(1)-N(1)	2.334(5)
Zn(1)-N(2)	2.070(9)	Hg(1)-N(2)	2.369(5)
Zn(1)-Cl(1)	2.199(4)	Hg(1)-Cl(1)	2.3678(19)
Zn(1)-Cl(2)	2.188(4)	Hg(1)-Cl(2)	2.4239(19)
N(2)-C(10)	1.286(13)	N(2)-C(10)	1.283(8)
N(1)-Zn(1)-N(2)	79.8(3)	N(1)-Hg(1)-N(2)	72.34(18)
N(1)-Zn(1)-Cl(2)	119.0(3)	N(1)-Hg(1)-Cl(1)	125.43(14)
N(1)-Zn(1)-Cl(1)	108.4(3)	N(1)-Hg(1)-Cl(2)	105.26(14)
N(2)-Zn(1)-Cl(2)	118.0(3)	N(2)-Hg(1)-Cl(2)	110.46(13)
N(2)-Zn(1)-Cl(1)	110.4(3)	N(2)-Hg(1)-Cl(1)	119.29(14)
Cl(2)-Zn(1)-Cl(1)	115.86(16)	Cl(1)-Hg(1)-Cl(2)	116.23(7)

C(1)-N(1)-Zn(1)	114.2(7)	C(1)-N(1)-Hg(1)	113.6(4)
C(9)-N(1)-Zn(1)	127.0(7)	C(9)-N(1)-Hg(1)	126.1(4)
C(10)-N(2)-Zn(1)	112.2(7)	C(10)-N(2)-Hg(1)	112.8(4)
C(11)-N(2)-Zn(1)	126.6(7)	C(11)-N(2)-Hg(1)	125.3(4)

Table S2. Selected bond distances (Å) and angles (°) for **2**, **3** and **4**.

2			
Parameter		Parameter	
N(2)-C(10)	1.274(3)	N(2)-Zn(1)-O(6)	148.03(8)
Zn(1)-N(1)	2.0702(17)	O(2)-Zn(1)-O(6)	84.81(9)
Zn(1)-O(5)	2.082(2)	O(3)-Zn(1)-O(6)	90.88(9)
Zn(1)-N(2)	2.0968(19)	N(1)-Zn(1)-N(3)	119.80(7)
Zn(1)-O(2)	2.127(2)	O(5)-Zn(1)-N(3)	121.80(7)
Zn(1)-O(3)	2.248(3)	N(2)-Zn(1)-N(3)	117.62(7)
Zn(1)-O(6)	2.345(3)	O(2)-Zn(1)-N(3)	29.06(7)
Zn(1)-N(3)	2.602(2)	O(3)-Zn(1)-N(3)	28.58(7)
Zn(1)-N(4)	2.620(2)	O(6)-Zn(1)-N(3)	87.08(8)
N(1)-Zn(1)-O(5)	113.08(8)	N(1)-Zn(1)-N(4)	112.45(7)
N(1)-Zn(1)-N(2)	81.22(7)	O(5)-Zn(1)-N(4)	28.20(7)
O(5)-Zn(1)-N(2)	91.99(8)	N(2)-Zn(1)-N(4)	120.13(7)
N(1)-Zn(1)-O(2)	148.15(8)	O(2)-Zn(1)-N(4)	90.57(8)
O(5)-Zn(1)-O(2)	97.67(9)	O(3)-Zn(1)-N(4)	117.01(9)
N(2)-Zn(1)-O(2)	106.73(8)	O(6)-Zn(1)-N(4)	28.30(7)
N(1)-Zn(1)-O(3)	91.46(7)	N(3)-Zn(1)-N(4)	105.04(6)
O(5)-Zn(1)-O(3)	142.43(8)	N(3)-O(2)-Zn(1)	96.64(16)
N(2)-Zn(1)-O(3)	120.65(9)	N(3)-O(3)-Zn(1)	91.69(17)
O(2)-Zn(1)-O(3)	57.64(8)	N(4)-O(5)-Zn(1)	100.38(16)
N(1)-Zn(1)-O(6)	104.85(8)	N(4)-O(6)-Zn(1)	88.22(17)
O(1)-Zn(1)-N(2)	94.02(12)	N(4)-Zn(2)-C(41)	123.11(13)
C(9)-N(1)-Zn(1)	129.61(15)	C(11)-N(2)-Zn(1)	127.68(14)
C(10)-N(2)-Zn(1)	110.43(15)	O(1)-N(3)-Zn(1)	175.3(2)
O(2)-N(3)-Zn(1)	54.30(13)	O(3)-N(3)-Zn(1)	59.73(14)
O(4)-N(4)-Zn(1)	171.9(2)	O(6)-N(4)-Zn(1)	63.47(16)
O(5)-N(4)-Zn(1)	51.41(12)		
3			
Parameter		Parameter	
N(2)-C(10)	1.270(4)	C(20)-O(3)-Zn(1)	115.1(3)
O(12)-Zn(3)	2.324(4)	C(39)-O(5)-Zn(2)	111.4(3)
O(11)-Zn(3)	2.037(3)	O(8)-C(41)-Zn(2)	70.5(3)
O(10)-Zn(3)	1.925(3)	O(7)-C(41)-Zn(2)	50.8(2)
C(62)-Zn(3)	2.529(5)	C(43)-N(5)-Zn(3)	112.3(2)
O(8)-Zn(2)	2.435(4)	C(51)-N(5)-Zn(3)	128.7(2)
O(7)-Zn(2)	2.014(3)	C(53)-N(6)-Zn(3)	127.8(2)
Zn(1)-O(3)	1.921(3)	C(52)-N(6)-Zn(3)	111.4(2)

Zn(1)-O(1)	2.056(3)	C(18)-O(2)-Zn(1)	85.8(3)
Zn(1)-N(1)	2.087(3)	C(32)-N(4)-Zn(2)	127.5(2)
Zn(1)-N(2)	2.142(3)	O(5)-Zn(2)-N(3)	133.05(13)
Zn(1)-O(2)	2.311(4)	O(7)-Zn(2)-N(3)	118.33(13)
Zn(1)-C(18)	2.534(4)	O(5)-Zn(2)-N(4)	110.50(16)
Zn(2)-O(5)	1.939(3)	O(7)-Zn(2)-N(4)	96.42(12)
Zn(2)-N(3)	2.092(3)	N(3)-Zn(2)-N(4)	79.45(12)
Zn(2)-N(4)	2.134(3)	O(5)-Zn(2)-O(8)	96.32(17)
Zn(2)-C(41)	2.554(5)	O(7)-Zn(2)-O(8)	56.50(12)
Zn(3)-N(5)	2.085(3)	N(3)-Zn(2)-O(8)	96.40(13)
Zn(3)-N(6)	2.134(3)	N(4)-Zn(2)-O(8)	146.98(13)
O(3)-Zn(1)-N(1)	129.23(14)	O(5)-Zn(2)-C(41)	102.13(15)
O(1)-Zn(1)-N(1)	120.29(12)	O(7)-Zn(2)-C(41)	28.48(13)
O(3)-Zn(1)-N(2)	113.73(16)	N(3)-Zn(2)-C(41)	109.94(14)
O(1)-Zn(1)-N(2)	94.02(12)	N(4)-Zn(2)-C(41)	123.11(13)
N(1)-Zn(1)-N(2)	79.46(12)	O(8)-Zn(2)-C(41)	28.04(12)
O(3)-Zn(1)-O(2)	95.79(17)	O(10)-Zn(3)-O(11)	105.34(13)
O(1)-Zn(1)-O(2)	58.14(12)	O(10)-Zn(3)-N(5)	130.90(12)
N(1)-Zn(1)-O(2)	96.30(13)	O(11)-Zn(3)-N(5)	122.08(12)
N(2)-Zn(1)-O(2)	145.24(12)	O(10)-Zn(3)-N(6)	109.33(14)
O(3)-Zn(1)-C(18)	103.15(14)	O(11)-Zn(3)-N(6)	95.99(12)
O(1)-Zn(1)-C(18)	29.39(12)	N(5)-Zn(3)-N(6)	79.48(11)
N(1)-Zn(1)-C(18)	110.68(13)	O(10)-Zn(3)-O(12)	97.23(16)
N(2)-Zn(1)-C(18)	121.07(12)	O(11)-Zn(3)-O(12)	58.08(12)
N(6)-Zn(3)-O(12)	147.50(13)	N(5)-Zn(3)-O(12)	97.34(12)
O(10)-Zn(3)-C(62)	102.75(13)	C(1)-N(1)-Zn(1)	112.3(2)
O(11)-Zn(3)-C(62)	29.34(13)	C(9)-N(1)-Zn(1)	128.5(3)
N(5)-Zn(3)-C(62)	112.09(12)	C(42)-C(41)-Zn(2)	169.1(4)
N(6)-Zn(3)-C(62)	123.14(13)	C(10)-N(2)-Zn(1)	111.2(3)
O(12)-Zn(3)-C(62)	28.74(12)	C(11)-N(2)-Zn(1)	127.3(2)
C(18)-O(1)-Zn(1)	97.0(3)	C(31)-N(4)-Zn(2)	111.5(3)

4

Parameter		Parameter	
N(2)-C(10)	1.292(10)	O(5)-C(39)-Cd(2)	58.7(5)
Cd(1)-O(3)	2.283(6)	O(6)-C(39)-Cd(2)	60.5(5)
Cd(1)-O(1)	2.291(7)	C(40)-C(39)-Cd(2)	175.9(6)
Cd(1)-N(1)	2.313(7)	O(12)-C(62)-Cd(3)	62.4(5)
Cd(1)-N(2)	2.338(7)	O(11)-C(62)-Cd(3)	58.3(4)
Cd(1)-O(2)	2.364(6)	C(63)-C(62)-Cd(3)	172.4(7)
Cd(1)-O(4)	2.372(7)	O(3)-Cd(1)-O(1)	99.2(2)
Cd(2)-O(7)	2.281(7)	O(3)-Cd(1)-N(1)	140.8(2)
Cd(2)-O(5)	2.303(6)	O(1)-Cd(1)-N(1)	120.0(2)
Cd(2)-N(3)	2.333(7)	O(3)-Cd(1)-N(2)	106.8(2)

Cd(2)-O(6)	2.341(6)	O(1)-Cd(1)-N(2)	94.6(2)
Cd(2)-N(4)	2.355(7)	N(1)-Cd(1)-N(2)	72.5(2)
Cd(2)-O(8)	2.368(8)	O(3)-Cd(1)-O(2)	106.8(3)
Cd(3)-O(11)	2.284(6)	O(1)-Cd(1)-O(2)	55.1(2)
Cd(3)-O(9)	2.303(6)	N(1)-Cd(1)-O(2)	96.3(2)
Cd(3)-N(5)	2.309(6)	N(2)-Cd(1)-O(2)	137.7(3)
Cd(3)-N(6)	2.347(6)	O(3)-Cd(1)-O(4)	55.0(2)
Cd(3)-O(10)	2.348(6)	O(1)-Cd(1)-O(4)	145.0(3)
Cd(3)-O(12)	2.375(6)	N(1)-Cd(1)-O(4)	88.7(2)
O(4)-Cd(1)-C(18)	128.3(3)	N(2)-Cd(1)-O(4)	114.2(2)
O(3)-Cd(1)-C(20)	27.8(2)	O(2)-Cd(1)-O(4)	105.9(3)
O(1)-Cd(1)-C(20)	122.7(3)	O(3)-Cd(1)-C(18)	105.2(3)
N(1)-Cd(1)-C(20)	115.4(3)	O(1)-Cd(1)-C(18)	27.7(2)
N(2)-Cd(1)-C(20)	115.3(2)	N(1)-Cd(1)-C(18)	109.6(2)
C(18)-Cd(1)-C(20)	118.1(3)	O(7)-Cd(2)-O(8)	53.8(2)
O(7)-Cd(2)-O(5)	103.5(3)	O(5)-Cd(2)-O(8)	151.5(3)
O(7)-Cd(2)-N(3)	141.1(3)	N(3)-Cd(2)-O(8)	89.0(2)
O(5)-Cd(2)-N(3)	115.4(2)	O(6)-Cd(2)-O(8)	109.1(3)
O(7)-Cd(2)-O(6)	103.9(3)	N(4)-Cd(2)-O(8)	109.5(3)
O(5)-Cd(2)-O(6)	55.3(2)	O(7)-Cd(2)-C(39)	106.2(3)
N(3)-Cd(2)-O(6)	98.2(2)	O(5)-Cd(2)-C(39)	27.4(2)
O(7)-Cd(2)-N(4)	107.2(3)	N(3)-Cd(2)-C(39)	108.2(2)
O(5)-Cd(2)-N(4)	92.8(2)	O(6)-Cd(2)-C(39)	27.9(2)
N(3)-Cd(2)-N(4)	72.1(2)	N(4)-Cd(2)-C(39)	116.8(2)
O(6)-Cd(2)-N(4)	139.9(2)	O(8)-Cd(2)-C(39)	133.5(3)
O(7)-Cd(2)-C(41)	26.9(2)	O(10)-Cd(3)-O(12)	104.6(2)
O(5)-Cd(2)-C(41)	128.2(3)	O(11)-Cd(3)-C(60)	105.3(3)
N(3)-Cd(2)-C(41)	115.4(3)	O(9)-Cd(3)-C(60)	27.6(2)
O(6)-Cd(2)-C(41)	107.5(3)	N(5)-Cd(3)-C(60)	112.0(2)
N(4)-Cd(2)-C(41)	111.7(2)	N(6)-Cd(3)-C(60)	118.7(2)
O(8)-Cd(2)-C(41)	26.8(2)	O(10)-Cd(3)-C(60)	27.9(2)
C(60)-O(9)-Cd(3)	93.2(5)	O(12)-Cd(3)-C(60)	126.4(2)
C(62)-O(12)-Cd(3)	90.2(5)	O(11)-Cd(3)-C(62)	28.1(2)
C(62)-O(11)-Cd(3)	93.7(5)	O(9)-Cd(3)-C(62)	121.3(3)
C(53)-N(6)-Cd(3)	124.0(5)	N(5)-Cd(3)-C(62)	115.0(3)
C(10)-N(2)-Cd(1)	114.4(5)	N(6)-Cd(3)-C(62)	112.8(2)
C(11)-N(2)-Cd(1)	124.8(5)	O(10)-Cd(3)-C(62)	107.5(2)
O(4)-Cd(1)-C(20)	27.3(2)	O(12)-Cd(3)-C(62)	27.5(2)
C(22)-N(3)-Cd(2)	114.7(5)	C(60)-Cd(3)-C(62)	117.7(3)
C(30)-N(3)-Cd(2)	126.4(5)	C(18)-O(1)-Cd(1)	93.6(5)
O(2)-Cd(1)-C(18)	27.4(2)	C(18)-O(2)-Cd(1)	90.5(6)
C(31)-N(4)-Cd(2)	113.4(5)	C(20)-O(3)-Cd(1)	93.8(5)
C(32)-N(4)-Cd(2)	123.8(5)	C(20)-O(4)-Cd(1)	90.3(6)
C(53)-N(6)-Cd(3)	124.0(5)	C(39)-O(5)-Cd(2)	93.9(5)

C(43)-N(5)-Cd(3)	115.1(5)	C(39)-O(6)-Cd(2)	91.6(5)
C(60)-O(10)-Cd(3)	90.8(5)	C(41)-O(8)-Cd(2)	91.9(6)
C(52)-N(6)-Cd(3)	113.6(5)		

Table S3. The geometrical parameters of C–H···O/Cl hydrogen bonding and π···π stacking interactions for complexes **1**–**5**.

	coordination geometry	dihedral angle (deg)[a]	D–H···A	D–H/Å	H···A/Å	D···A/Å	D–H···A/°	dimension
1	tetrahedral	39.6	C5–H5A···Cl1	0.930	2.943	3.786	151.539(2)	3D
			C10–H10A···Cl1	0.930	2.590	3.450	154.121(2)	
			$\pi_{Cg1}\cdots\pi_{Cg1}$			3.718		
2	octahedral	29.3	C2–H2A···O4	0.930	2.608	3.259	127.517(4)	2D
			C10–H10A···O4	0.930	2.670	3.433	139.724(1)	
			C5–H5A···O3	0.930	2.654	3.455	144.709(1)	
			$\pi_{Cg1}\cdots\pi_{Cg1}$			3.615		
3	trigonal bipyramidal	4.3	C3–H3A···O1	0.9305	2.619	3.380	139.467	3D
			C10–H10A···O6	0.9312	2.3622	3.2508	159.777	
			C12–H12A···O6	0.9290	2.6259	3.5139	159.908	
			C17–H17A···O8	0.9278	2.6870	3.5907	157.070	
			C19–H19A···O7	0.9302	2.6804	3.4668	139.486	
			C33–H33A···O4	0.9326	2.4680	3.3881	170.200	
			C38–H38A···O5	0.9236	2.6753	3.5796	157.185	
			C49–H49A···O2	0.9308	2.4930	3.3223	148.586	
			C54–H54A···O9	0.9310	2.5630	3.4460	157.364	
			C63–H63C···O11	0.9300	2.5954	3.3825	13.399	
			$\pi_{Cg1}\cdots\pi_{Cg1}$			3.619		
4	octahedral	8.3	C3–H3A···O9	0.9305	2.5682	3.509	142.236	3D

				C12–H12A···O1	0.9326	2.6346	3.3910	138.629		
				C13–H13A···O3	0.9311	2.5600	3.3974	149.940		
				C16–H16A···O8	0.9303	2.6061	3.5328	173.768		
				C19–H19C···O5	0.9611	2.5828	3.5238	166.273		
				C21–H21B···O10	0.9300	2.6777	3.5080	145.003		
				C34–H34A···O11	0.9229	2.6098	3.3880	141.571		
				C49–H49A···O6	0.9277	2.4813	3.3492	155.691		
				C12–H58A···O12	0.9309	2.6493	3.5463	162.090		
				$\pi_{Cg1}\cdots\pi_{Cg1}$			3.712			
5	tetrahedral		9.2	C10–H10A···Cl2	0.930	2.7864	3.6377	152.670	1D	
				C10–H10A···Cl1	0.930	2.8274	3.3080	113.346		
				$\pi_{Cg1}\cdots\pi_{Cg1}$			3.735			

a Between the quinoline ring and benzene ring; C_{g1} = quinoline ring; C_{g2} = benzene ring;

Table S4. The luminescence data of ligand **L** and complexes **1**–**5** in different state.

Complex	λ_{em} (nm)	FWHM (nm)	CIE (x, y)	Conditions
L	521	141.81	0.30 0.40	crystal-298K
	515	97.80	0.27 0.43	CH_3CN-298K
1	518	78.3	0.25 0.51	crystal-298K
	520	67.0	0.32 0.62	powder-298K
	507	77.32	0.26 0.49	CH_3CN-298K
	537	51.4	0.34 0.64	powder-77K
	532	61.0	0.34 0.65	crystal -77K
2	521	101.28	0.33 0.45	crystal-298K
	517	92.03	0.26 0.49	CH_3CN-298K
3	524	98.74	0.35 0.53	crystal-298K
	507	61.37	0.25 0.48	CH_3CN-298K
4	522	87.56	0.35 0.52	crystal-298K
	516	77.48	0.28 0.52	CH_3CN-298K
5	519	77.29	0.32 0.51	crystal-298K
	515	113.51	0.27 0.43	CH_3CN-298K

Table S5. The luminescence lifetimes of ligand **L** and complexes **1**–**5** in the solid state and acetonitrile solution at 298 K and 77 K.

Complex	τ_1 (μs)	A_1 (%)	τ_2 (μs)	A_2 (%)	τ^a (μs)	Conditions
L	1.15	55.09	9.38	44.91	8.30	crystal-298K
	1.05	61.28	7.78	38.72	6.60	CH_3CN-298K
1	1.19	57.57	10.78	42.43	9.53	crystal-298K
	1.28	55.91	10.87	44.09	9.62	powder-298K
	1.18	47.24	9.84	52.76	9.00	CH_3CN-298K
	1.07	22.52	11.76	77.48	11.48	powder-77K
	0.96	32.14	11.54	67.86	11.26	crystal-77K
2	1.05	55.82	10.49	44.18	9.43	crystal-298K
	1.04	65.99	8.11	34.01	6.70	CH_3CN-298K
3	1.01	53.84	9.41	46.16	8.48	crystal-298K
	1.09	61.18	8.36	38.82	7.12	CH_3CN-298K
4	1.13	56.05	9.50	43.95	8.40	crystal-298K
	1.08	59.09	8.18	40.91	7.04	CH_3CN-298K
5	1.18	56.33	9.66	43.67	8.51	cyrstal-298K
	0.87	67.88	6.80	32.12	5.54	CH_3CN-298K

$^a\ \tau = \dfrac{\tau_1^2 A_1\% + \tau_2^2 A_2\%}{\tau_1 A_1\% + \tau_2 A_2\%}$

Table S6. Luminescence data for **1** in different state.

Complex	λem (nm)	Intensity	τ (μs)	FWHM (nm)	CIE (x, y)	Conditions
	518	34590	9.53	78.3	0.25 0.51	crystal-298K
	520	49384	9.62	67.0	0.32 0.62	powder-298K
1	532	76306	11.26	61.0	0.34 0.65	crystal-77K
	537	95065	11.48	51.4	0.34 0.64	powder-77K

Table S7. Luminescence data for **1** and **1**-PMMA.

	Excitation (λ, nm)	Emission (λ_{max}, nm)	Intensity	Lifetimes (μs)				
				τ_1 (μs)	A_1 (%)	τ_2 (μs)	A_2 (%)	τ^a (μs)
1	365	497	49384	1.19	57.57	10.78	42.43	9.53
1-1%PMMA	365	520	31589	1.39	50.91	10.45	49.09	9.35
1-1.2%PMMA	365	521	132602	1.12	29.90	10.63	70.10	10.22
1-1.4%PMMA	365	509	358185	0.96	42.14	11.54	57.86	10.94
1-1.6%PMMA	365	520	973106	0.99	51.74	12.87	48.26	11.96
1-1.8%PMMA	365	520	729941	1.40	56.80	11.19	43.20	9.81
1-2%PMMA	365	520	182758	1.49	55.31	10.83	44.69	9.47
1-2.2%PMMA	365	521	31589	1.24	51.97	10.51	48.03	9.46