Electronic Supplementary Information

A cyclometalated Pt(II)-Pt(II) Clamshell Dimer with a Triplet Emission at 887 nm

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1. Characterization

UV–Vis absorption. The photophysical rate constants for radiative decay (k_r), non-radiative decay (k_{nr})were calculated according to the literature equations[1]:

$$\Phi(PLQY) = k_r \times \tau; \qquad \tau = \frac{1}{k_r + k_{nr}}$$

PMMA film. 1 mg of sample and 49 mg of polymethyl methacrylate (PMMA) were dissolved in 10 ml of DCM solution. When mixed evenly, take a little of the above solution with a dropper and drop it evenly on the quartz plate. PMMA film containing samples can be obtained after drying to measure its photophysical properties.

X-ray data collection and structure determination. Single crystal analysis was performed using a Bruker SMART APEX II X-ray single crystal diffractometer equipped with a Kryo Flex low-temperature system. The structure was solved by ShelXS6, refined using Olex-2 software using full matrix least squares method, and optimized by ShelXL7. The thermal ellipsoids were drawn with a probability level of 30%. For clarity, hydrogen atoms were omitted. The CCDC reference numbers (CCDC: 2309303, 2309304, and 2309305) and data corresponding to each crystal can be obtained free of charge from the Cambridge crystallographic data center at www.ccdc.cam.ac.uk/. Their crystal data was listed in Table S1.

2. Photophysical Properties

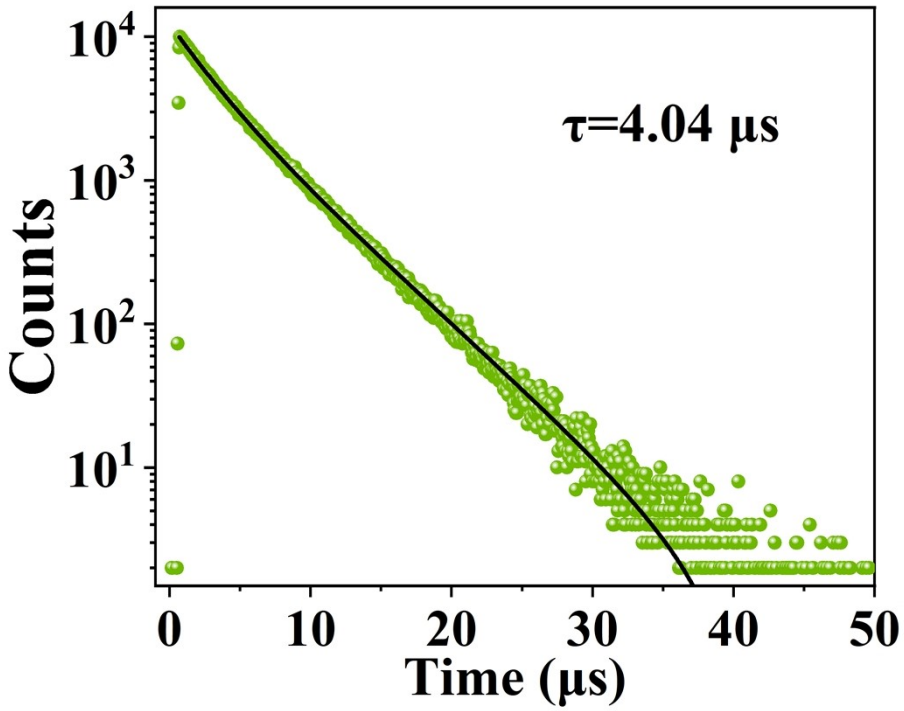


Figure S1. PL decay curves of complex **1a** in deoxygenated CH_2Cl_2.

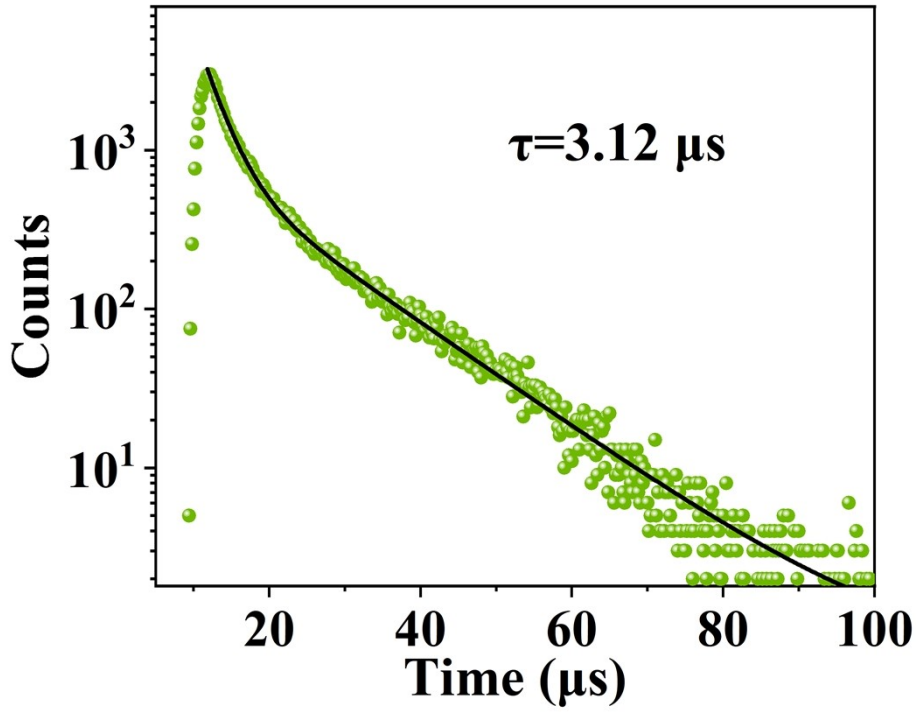


Figure S2. PL decay curves of complex **1a** in solid state.

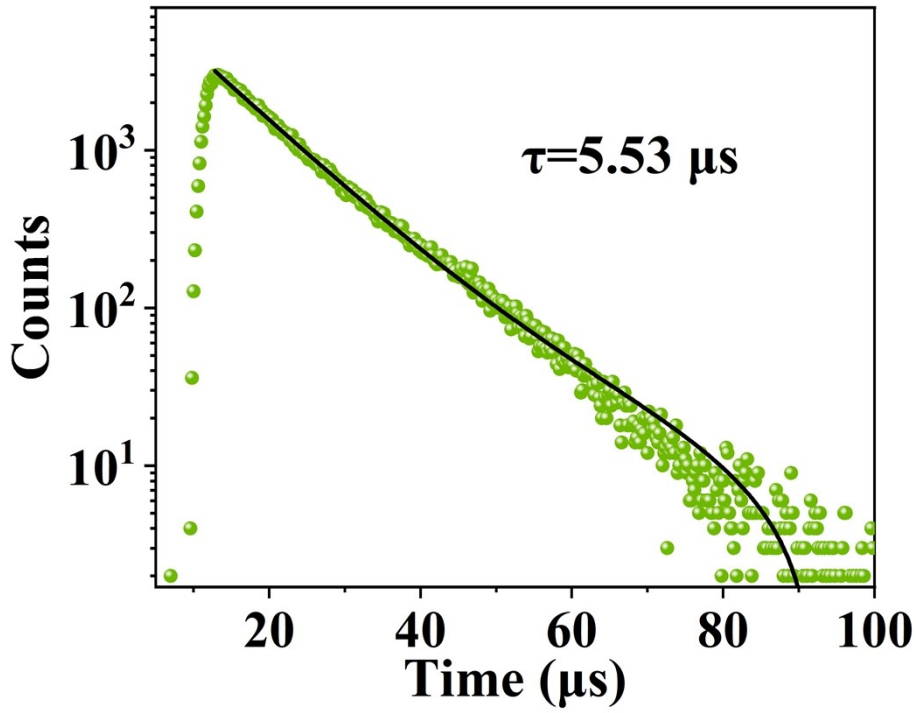


Figure S3. PL decay curves of complex **1a** in 2 wt% PMMA films.

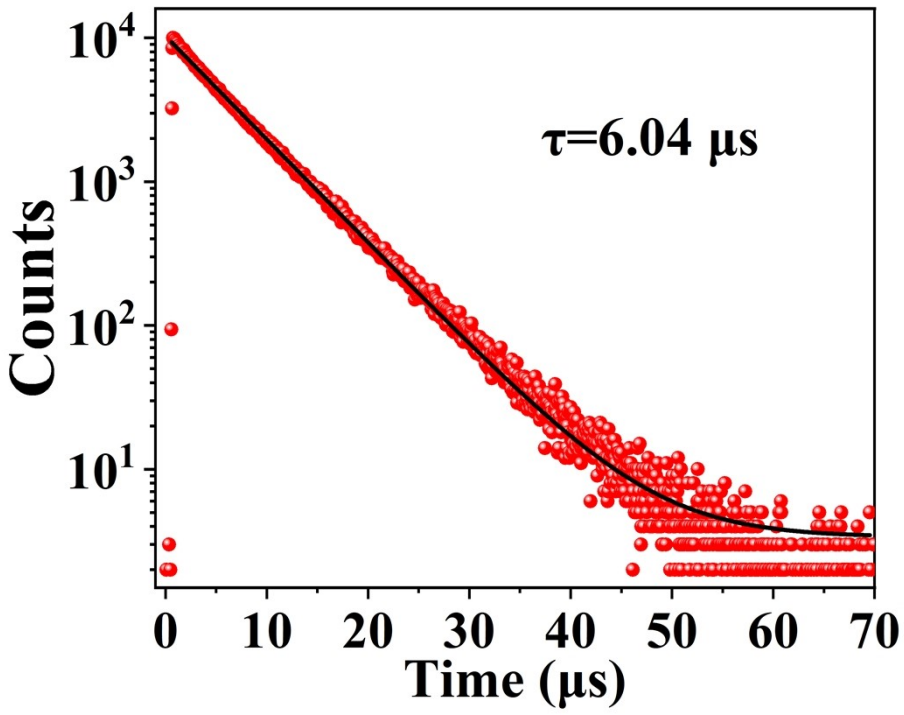


Figure S4. PL decay curves of complex **1b** in deoxygenated CH_2Cl_2.

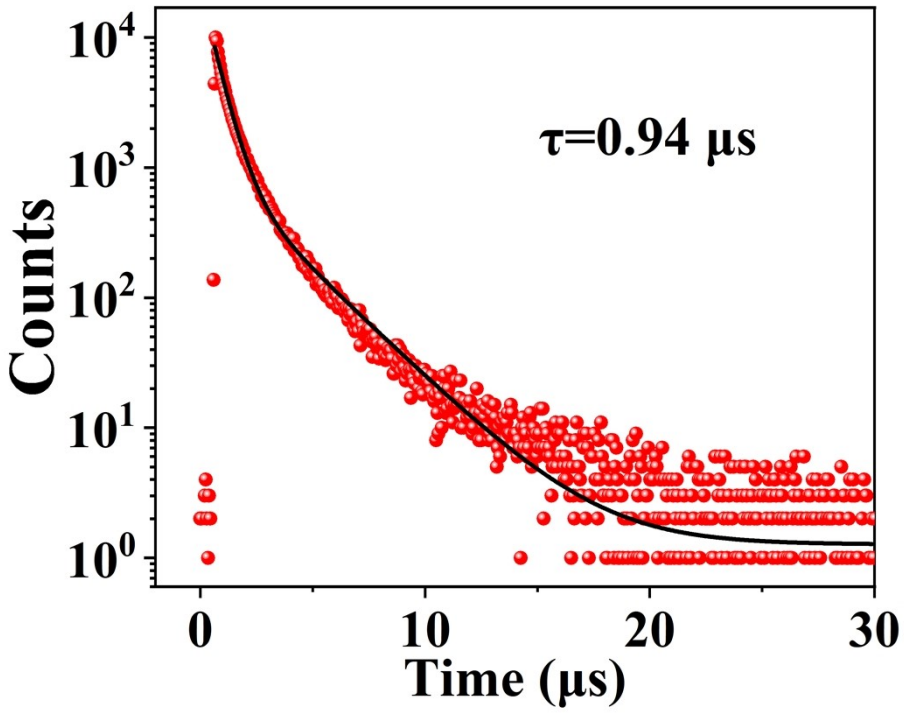


Figure S5. PL decay curves of complex **1b** in solid state.

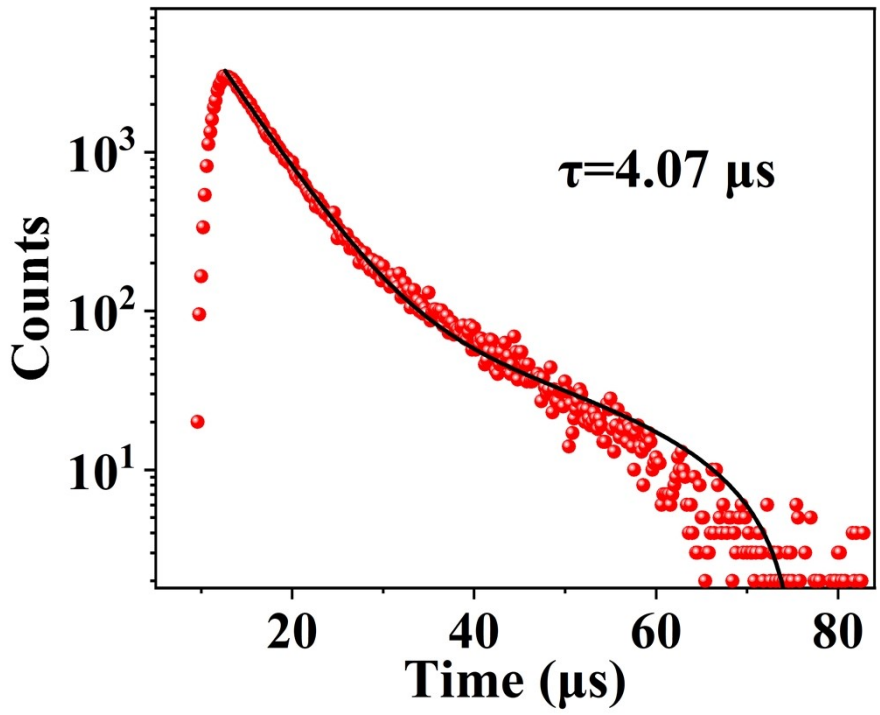


Figure S6. PL decay curves of complex **1b** in 2 wt% PMMA films.

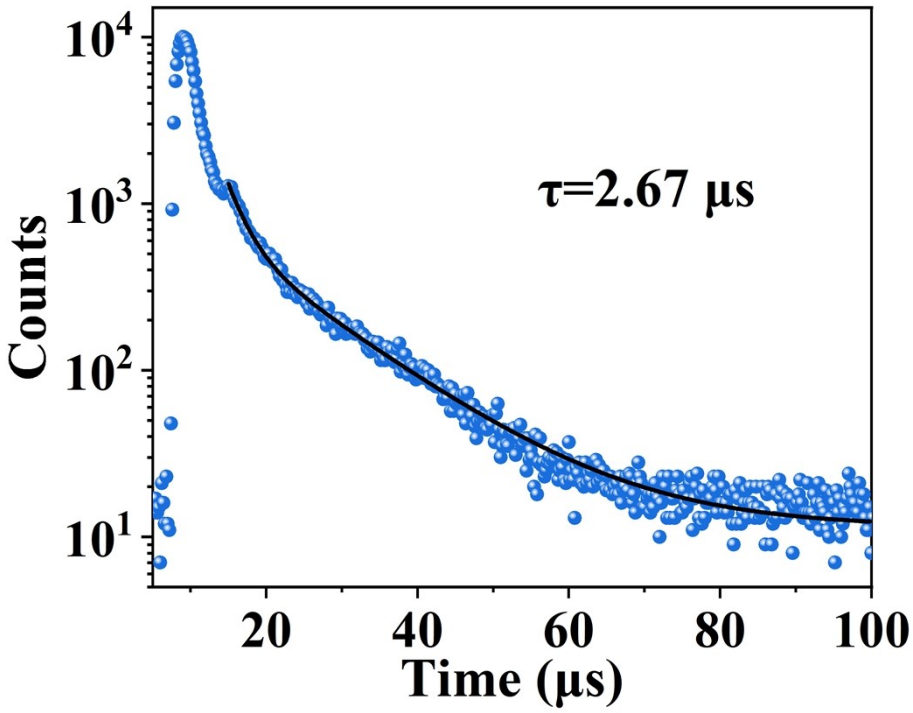


Figure S7. PL decay curves of complex **2** in solid state.

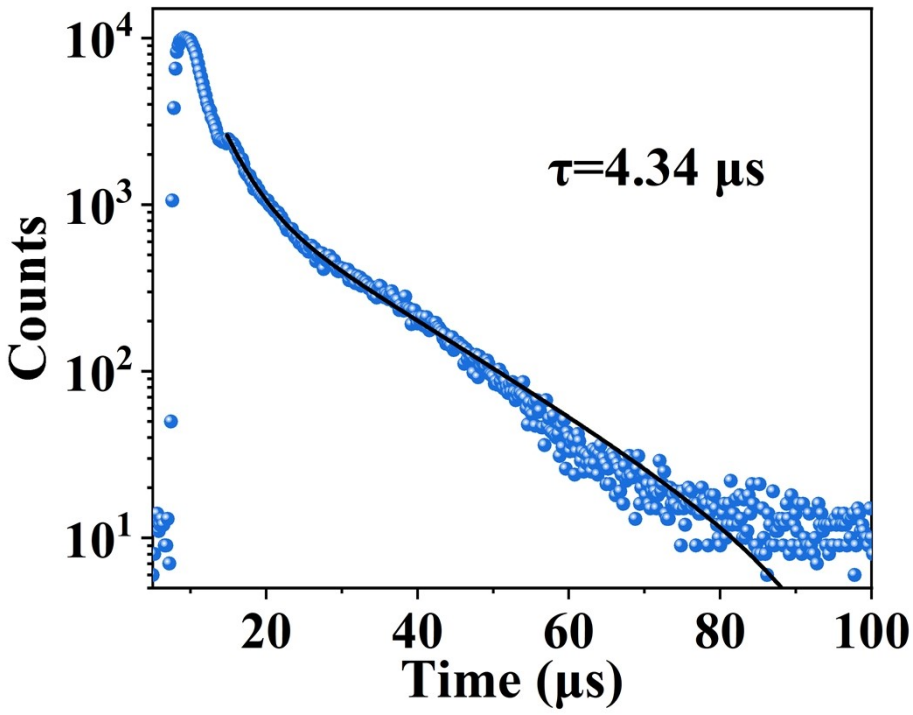


Figure S8. PL decay curves of complex **2** in 2 wt% PMMA films.

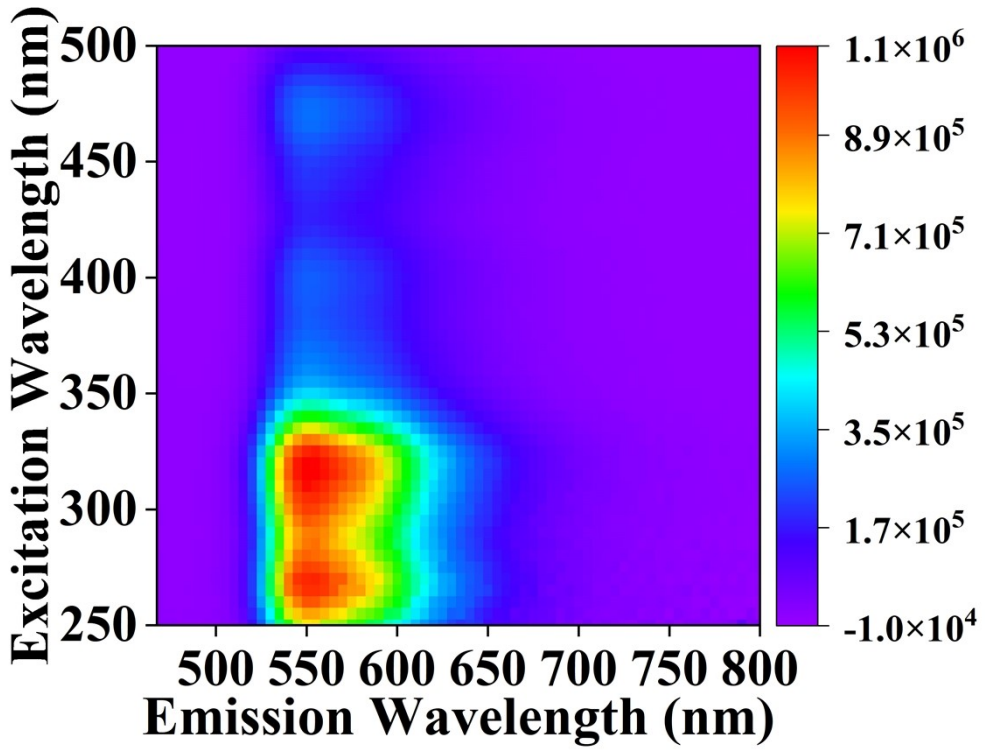


Figure S9. Two-dimension excitation-dependent emission spectra of **1a** in deoxygenated CH_2Cl_2.

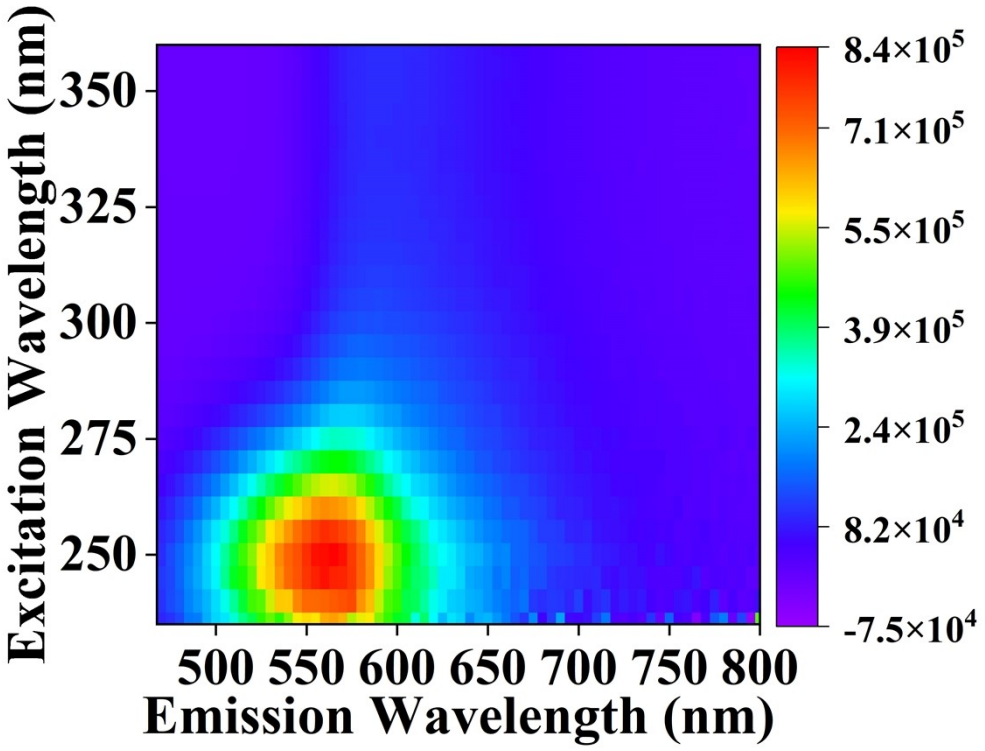


Figure S10. Two-dimension excitation-dependent emission spectra of **1a** in solid state.

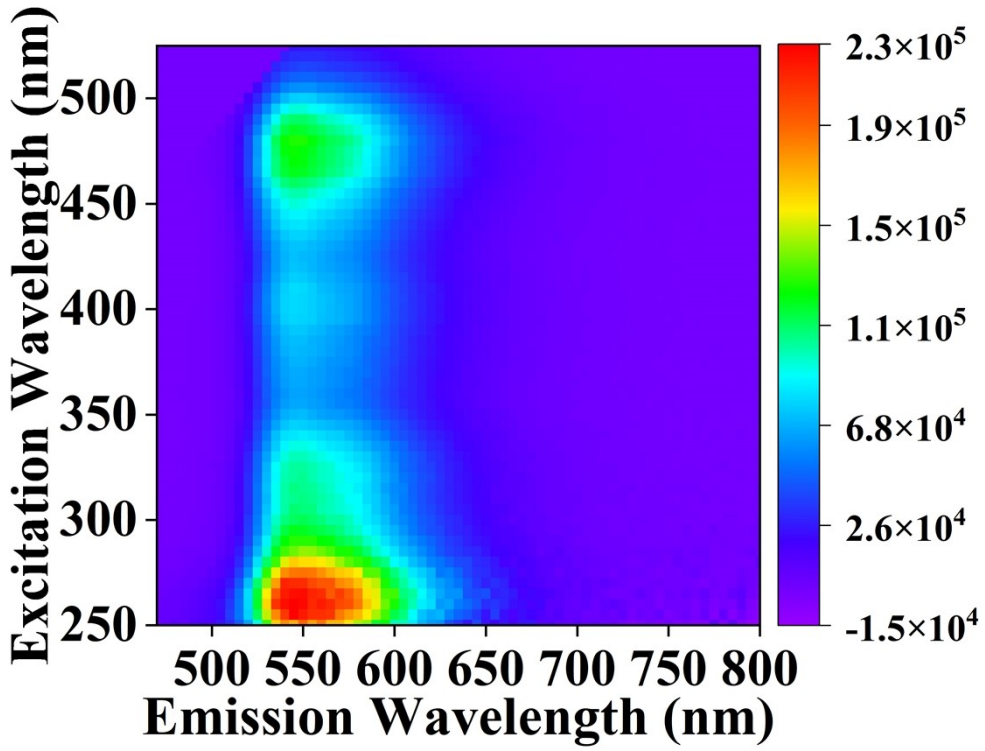


Figure S11. Two-dimension excitation-dependent emission spectra of **1a** in 2 wt% PMMA films.

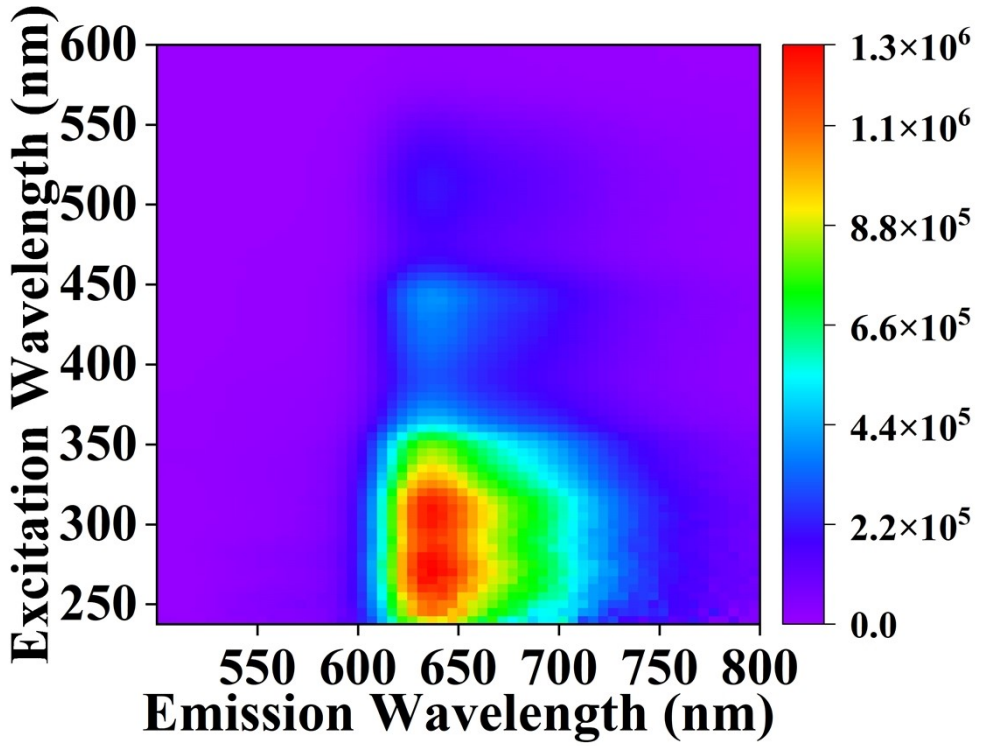


Figure S12. Two-dimension excitation-dependent emission spectra of **1b** in deoxygenated CH_2Cl_2.

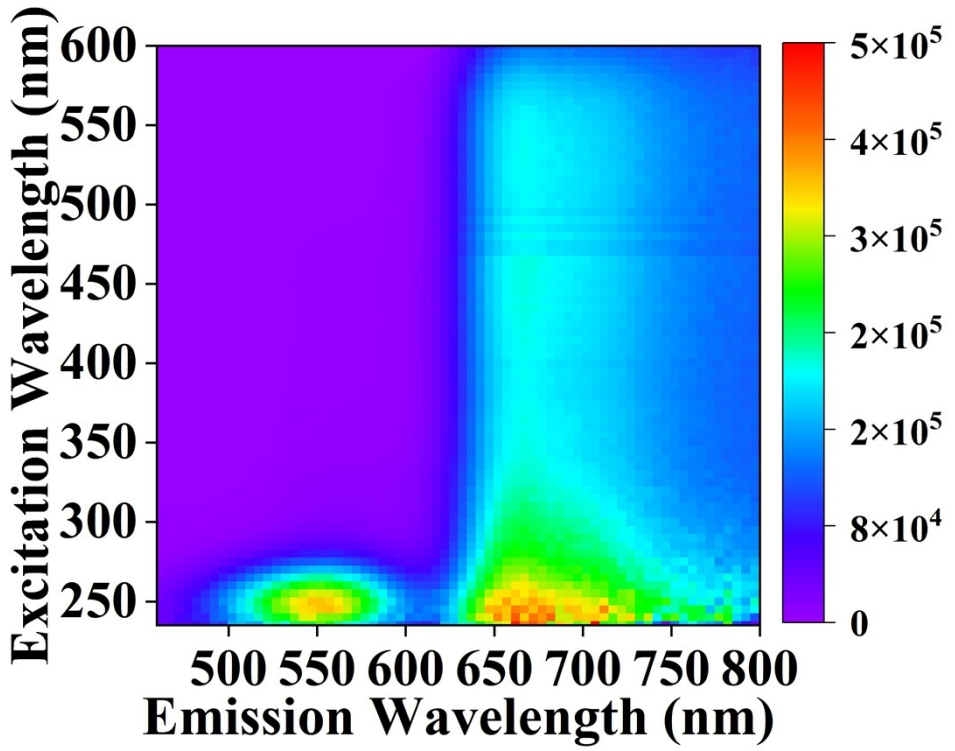


Figure S13. Two-dimension excitation-dependent emission spectra of **1b** in solid state.

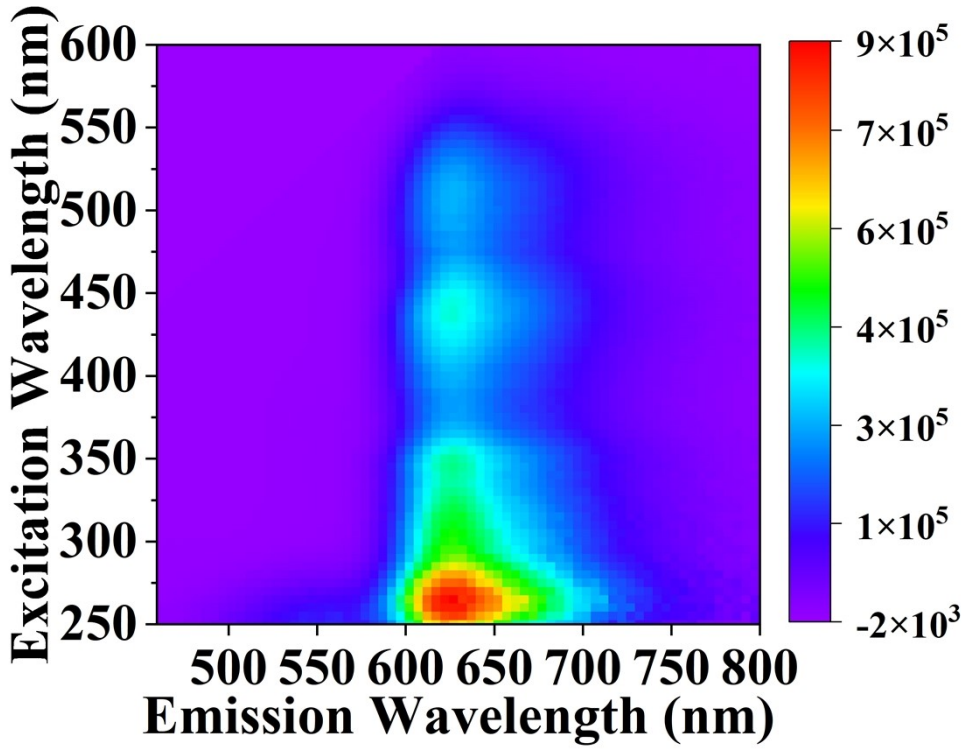


Figure S14. Two-dimension excitation-dependent emission spectra of **1b** in 2 wt% PMMA films.

3. NMR and ESI-Mass spectra

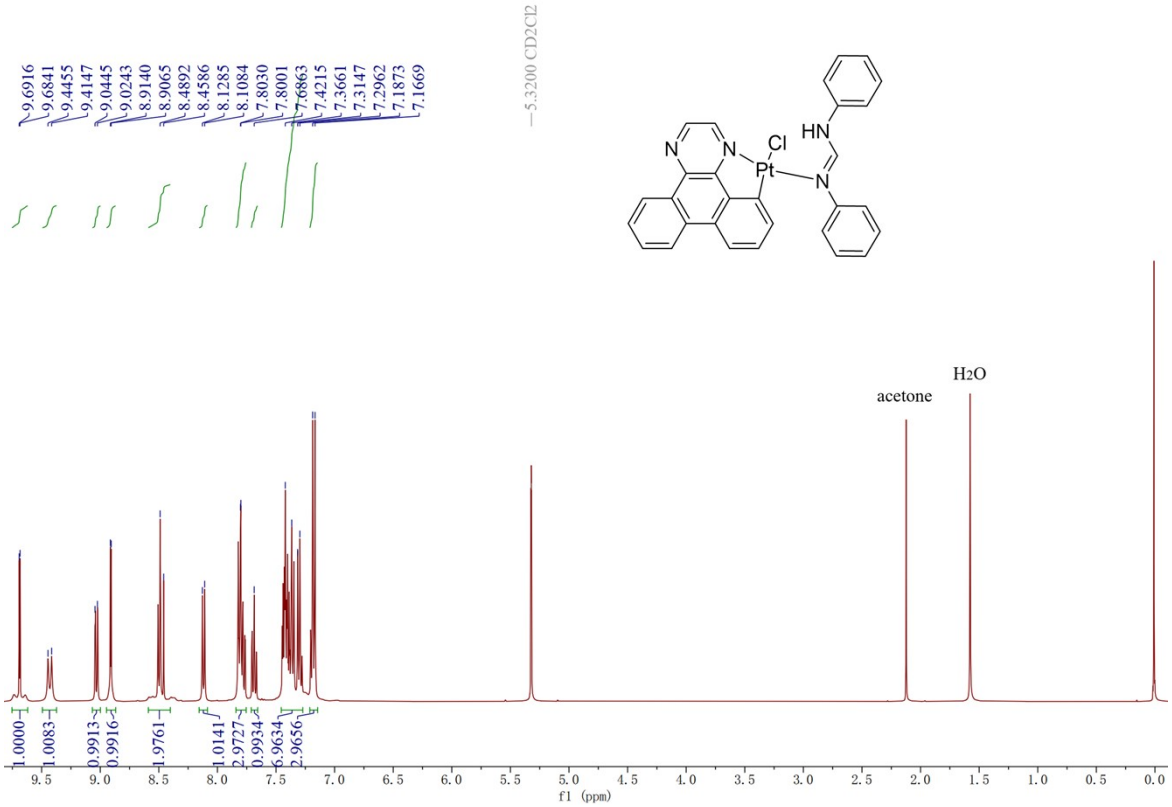


Figure S15. ^{1}H NMR spectrum of **1a** in CD_2Cl_2.

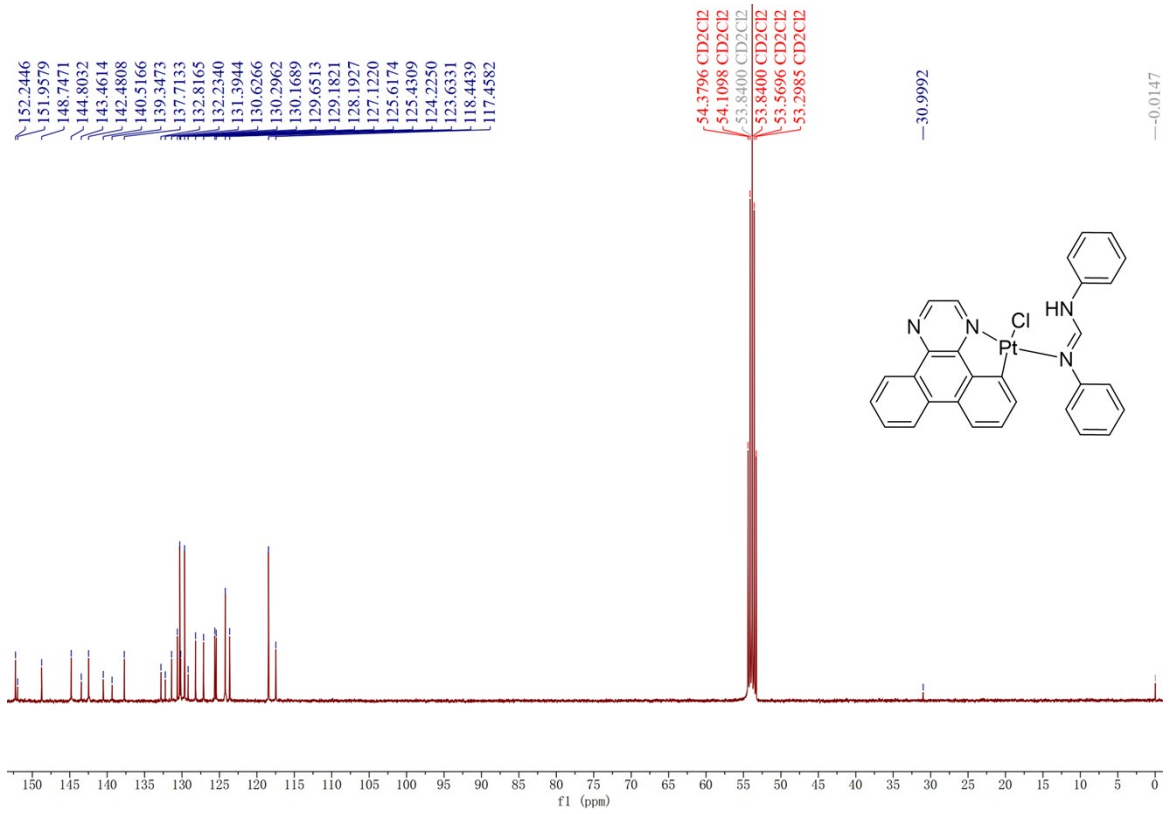


Figure S16. ^{13}C NMR spectrum of **1a** in CD_2Cl_2.

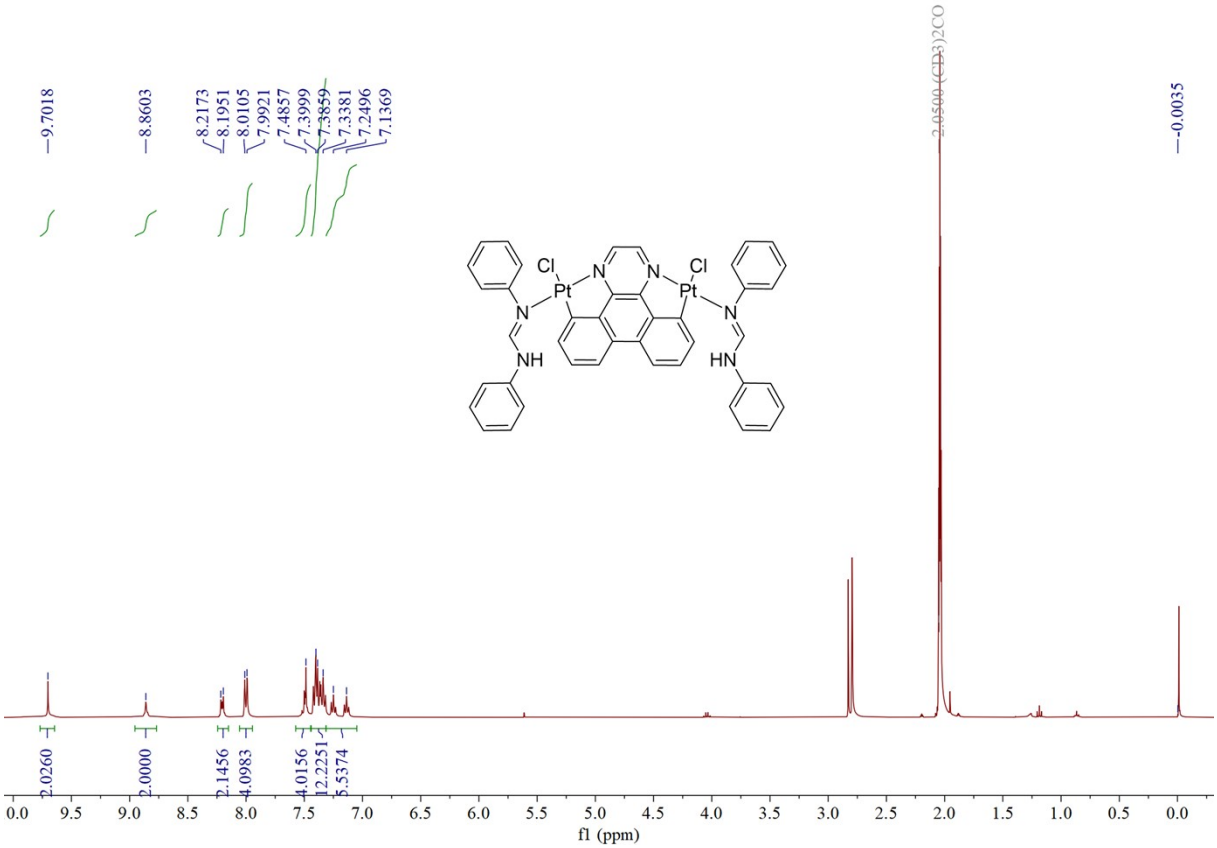


Figure S17. ^{1}H NMR spectrum of **1b** in acetone-d_6.

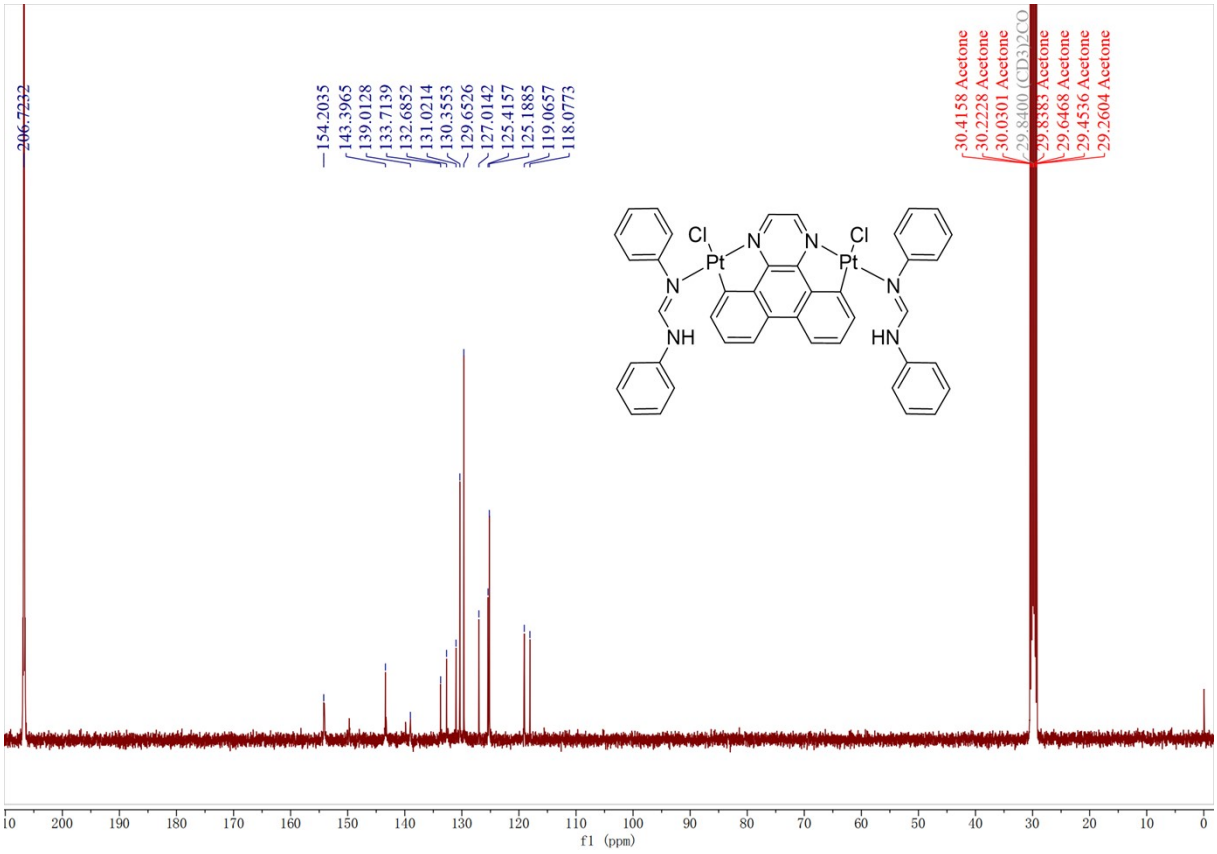


Figure S18. ^{13}C NMR spectrum of **1b** in acetone-d_6.

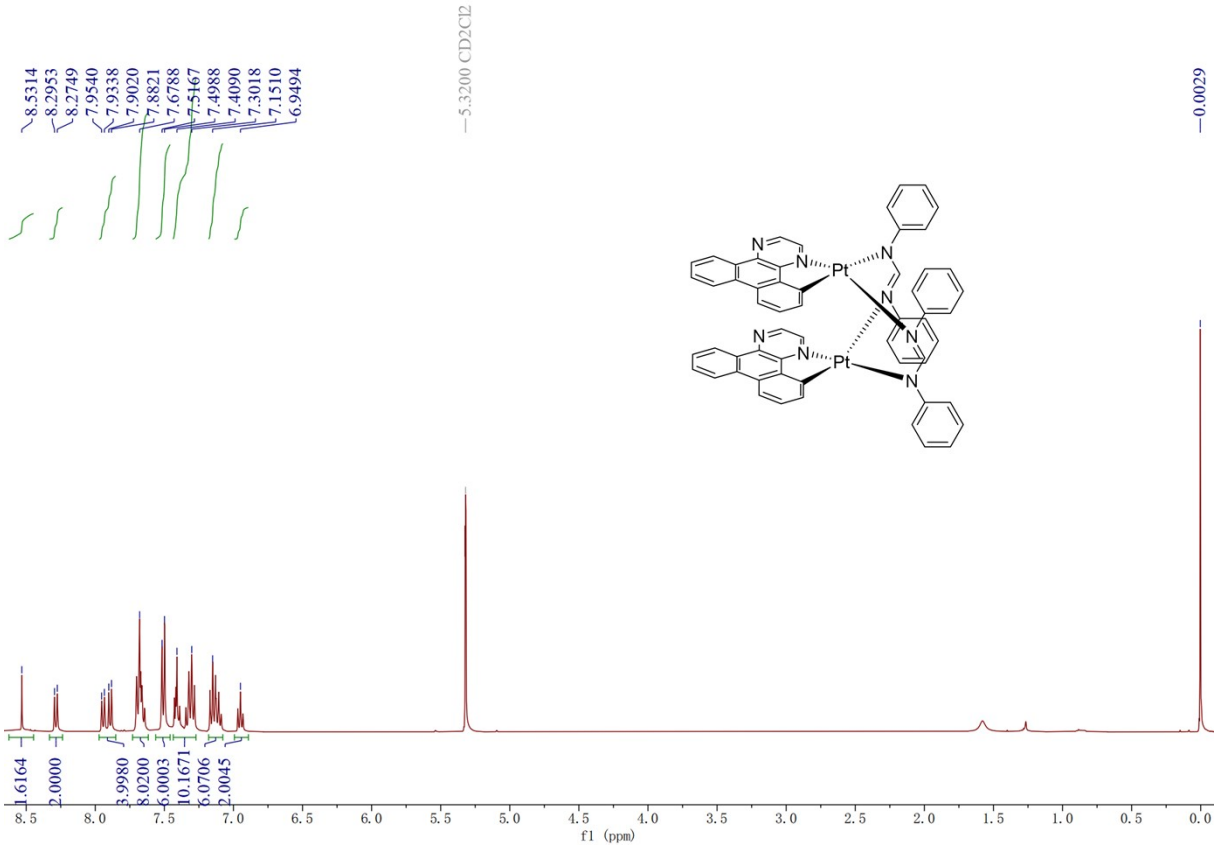


Figure S19. ^{1}H NMR spectrum of **2** in CD_2Cl_2.

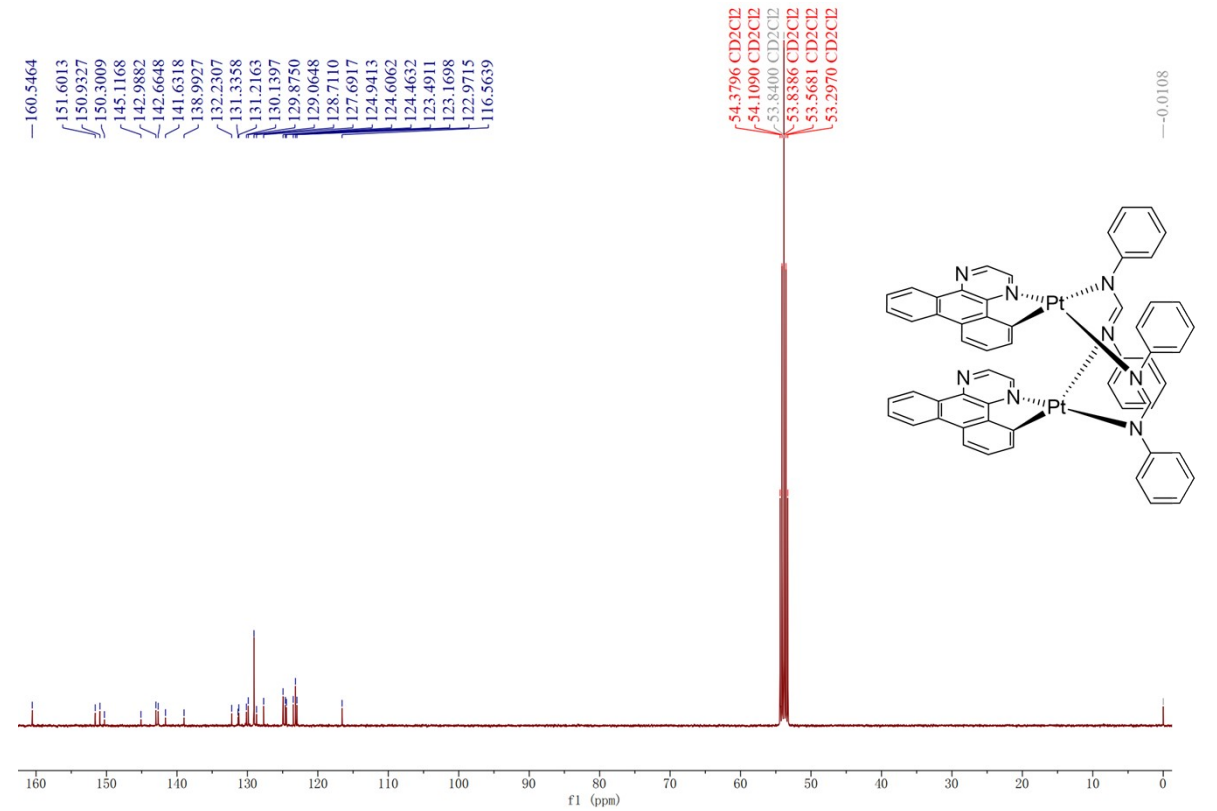


Figure S20. ^{13}C NMR spectrum of **2** in CD_2Cl_2.

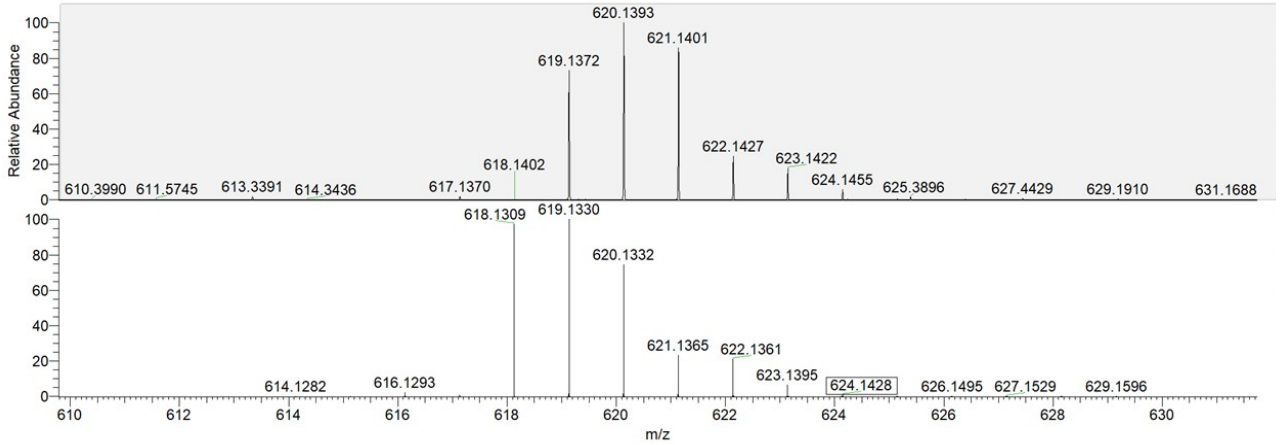


Figure S21. HR-MS spectra for **1a**.

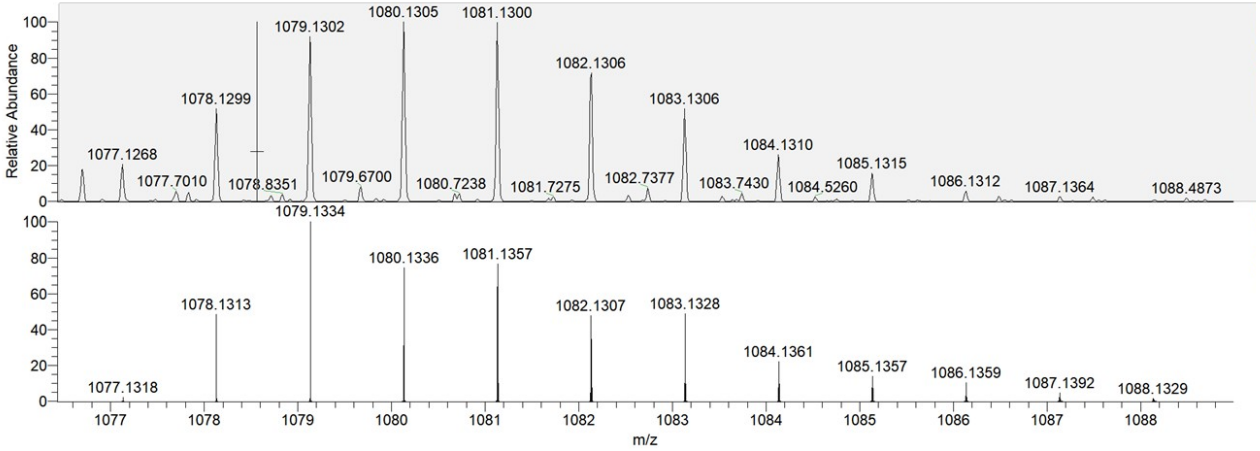


Figure S22. HR-MS spectra for **1b**.

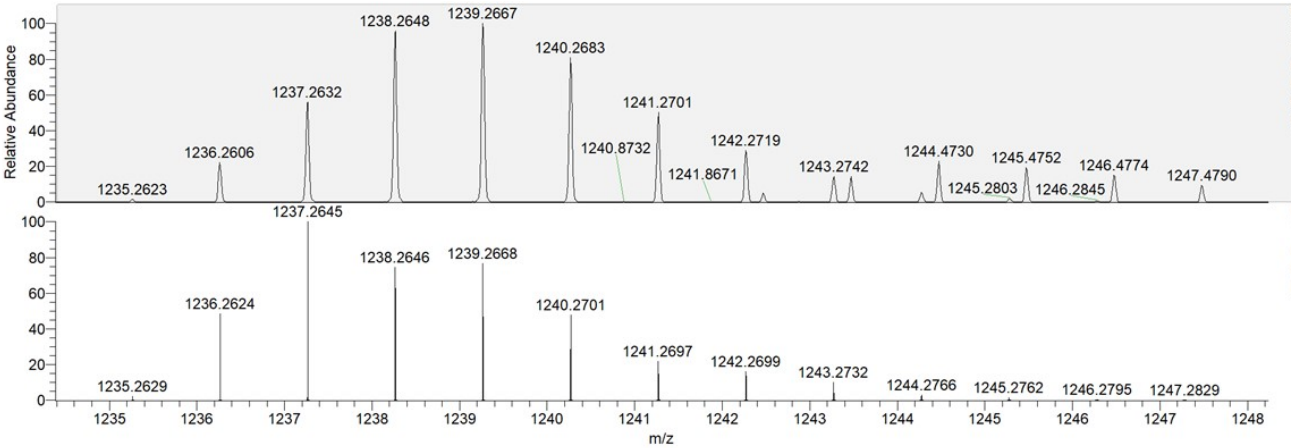


Figure S23. HR-MS spectra for **2**.

4. Crystal data

Table S1. Summary of the crystal data of **1a**,**1b** and **2**.

	1a	**1b**	**2**
CCDC number	2309303	2309304	2309305
Empirical formula	$C_{29}H_{21}ClN_4Pt$	$C_{45}H_{38}Cl_2N_6OPt_2$	$C_{58}H_{40}N_8Pt_2$
Formula weight	656.04	1139.89	1239.16
Temperature/K	213.00 K	213.00 K	173.00 K
Crystal system	Monoclinic	Triclinic	Triclinic
Space group	$P2_1/c$	P-1	P-1
a/Å	11.3936(3)	9.8009(2)	15.2393(15)
b/Å	14.8792(4)	14.1903(2)	17.0218(15)
c/Å	42.2998(10)	16.5817(3)	21.676(2)
α/°	90	83.3520(10)	87.771(5)
β/°	94.0900(10)	84.872(2)	85.211(6)
γ/°	90	73.3060(10)	72.665(5)
Volume/Å^3	7152.7(3)	2190.27(8)	5348.0(9)
z	12	2	4
ρcalcmg/mm^3	1.828	1.728	1.539
m/mm^{-1}	8.384	9.056	9.979
F(000)	3816.0	1096.0	2400.0
Crystal size/mm^3	0.09 × 0.07 × 0.05	0.07 x 0.07 x 0.05	0.12 × 0.11 × 0.1
2Θ range for data collection	5.48 to 109.938°	7.012 to 109.858	4.09 to 159.829
Index ranges	-13 ≤ h ≤ 13, -18 ≤ k ≤ 17, -50 ≤ l ≤ 51	-11 ≤ h ≤11, -17 ≤ k ≤17, -20 ≤ l ≤ 20	-18 ≤ h ≤ 19, -21 ≤ k ≤ 21, -23 ≤ l ≤ 26
Reflections collected	142743	26819	50654
Independent reflections	13545 [$R_{(int)}$ =0.0677, R_{sigma} =0.0335]	8113 [R(int) = 0.0557, R_{sigma} = 0.0563]	21592 [Rint = 0.0771, R_{sigma} =0.0874]
Data/restraints/parameters	13545/0/946	8113/36/507	21592/1299/1129
Goodness-of-fit on F^2	1.070	1.062	0.998
Final R indexes [I>=2σ (I)]	R_1 = 0.0420, wR2 = 0.1059	R_1 = 0.0440, wR_2 = 0.1084	R1 = 0.1357, wR2 = 0.3196
Final R indexes [all data]	R_1 = 0.0502, wR2 = 0.1105	R_1 = 0.0567, wR_2 = 0.1164	R1 = 0.1624, wR2 = 0.3335
Largest diff. peak/hole / e Å^{-3}	2.47/-2.42	2.32/-2.20	2.05/-2.46

Table S2. Bond lengths [Å] and angles [°] for **1a**.

Pt1-Cl1	2.3658(17)	C22-C23	1.401(9)
Pt1-N1	2.033(5)	C23-C24	1.387(10)
Pt1-N3	2.003(5)	C24-C25	1.381(11)
Pt1-C22	1.984(6)	C26-C27	1.350(10)
N1-C1	1.442(8)	C27-C28	1.400(11)
N1-C7	1.282(8)	C28-C29	1.394(11)
N2-C7	1.324(8)	Pt2-Cl2	2.3893(17)
N2-C8	1.421(7)	Pt2-N5	2.008(5)
N3-C14	1.369(8)	Pt2-N7	2.017(5)
N3-C17	1.339(8)	Pt2-C51	1.953(6)
N4-C15	1.352(8)	N5-C30	1.443(8)
N4-C16	1.315(8)	N5-C36	1.297(8)
C1-C2	1.383(9)	N6-C36	1.336(8)
C1-C6	1.394(10)	N6-C37	1.417(8)
C2-C3	1.404(10)	N7-C43	1.354(8)
C3-C4	1.371(12)	N7-C46	1.338(8)
C4-C5	1.398(12)	N8-C44	1.353(8)
C5-C6	1.375(11)	N8-C45	1.303(9)
C8-C9	1.377(8)	C30-C31	1.367(10)
C8-C13	1.396(9)	C30-C35	1.381(10)
C9-C10	1.366(9)	C31-C32	1.379(11)
C10-C11	1.373(9)	C32-C33	1.365(13)
C11-C12	1.362(9)	C33-C34	1.382(14)
C12-C13	1.377(9)	C34-C35	1.384(11)
C14-C15	1.389(8)	C37-C38	1.367(9)
C14-C21	1.423(8)	C37-C42	1.368(10)
C15-C18	1.461(9)	C38-C39	1.384(10)
C16-C17	1.390(9)	C39-C40	1.349(12)
C18-C19	1.414(9)	C40-C41	1.364(14)
C18-C29	1.415(9)	C41-C42	1.387(13)
C19-C20	1.469(9)	C43-C44	1.391(8)
C19-C26	1.403(9)	C43-C50	1.431(8)
C20-C21	1.400(9)	C44-C47	1.465(10)
C20-C25	1.411(9)	C45-C46	1.388(9)
C21-C22	1.423(8)	C47-C48	1.407(10)

C47-C58	1.411(9)	C73-C76	1.457(8)
C48-C49	1.458(9)	C74-C75	1.379(9)
C48-C55	1.403(10)	C76-C77	1.428(9)
C49-C50	1.394(9)	C76-C87	1.404(9)
C49-C54	1.403(9)	C77-C78	1.461(9)
C50-C51	1.455(8)	C77-C84	1.407(9)
C51-C52	1.383(8)	C78-C79	1.402(8)
C52-C53	1.387(9)	C78-C83	1.400(9)
C53-C54	1.386(10)	C79-C80	1.420(8)
C55-C56	1.395(11)	C80-C81	1.370(8)
C56-C57	1.361(13)	C81-C82	1.403(9)
C57-C58	1.370(12)	C82-C83	1.379(10)
Pt3-Cl3	2.4001(16)	C84-C85	1.362(10)
Pt3-N9	2.034(5)	C85-C86	1.381(11)
Pt3-N11	2.026(5)	C86-C87	1.368(10)
Pt3-C80	1.992(6)		
N9-C59	1.423(8)	N1-Pt1-Cl1	87.44(15)
N9-C65	1.302(8)	N3-Pt1-Cl1	91.97(14)
N10-C65	1.326(9)	N3-Pt1-N1	179.0(2)
N10-C66	1.420(9)	C22-Pt1-Cl1	173.25(18)
N11-C72	1.351(7)	C22-Pt1-N1	98.2(2)
N11-C75	1.326(8)	C22-Pt1-N3	82.4(2)
N12-C73	1.348(7)	C1-N1-Pt1	117.3(4)
N12-C74	1.332(8)	C7-N1-Pt1	125.2(4)
C59-C60	1.389(10)	C7-N1-C1	115.8(5)
C59-C64	1.401(9)	C7-N2-C8	125.0(5)
C60-C61	1.393(10)	C14-N3-Pt1	114.6(4)
C61-C62	1.359(12)	C17-N3-Pt1	127.8(4)
C62-C63	1.389(13)	C17-N3-C14	117.6(5)
C63-C64	1.366(11)	C16-N4-C15	116.1(5)
C66-C67	1.399(12)	C2-C1-N1	119.7(6)
C66-C71	1.361(12)	C2-C1-C6	119.8(6)
C67-C68	1.379(12)	C6-C1-N1	120.4(6)
C68-C69	1.367(16)	C1-C2-C3	120.0(7)
C69-C70	1.387(17)	C4-C3-C2	119.7(7)
C70-C71	1.374(13)	C3-C4-C5	120.1(7)
C72-C73	1.393(8)	C6-C5-C4	120.3(8)
C72-C79	1.429(8)	C5-C6-C1	120.0(8)

N1-C7-N2	124.9(6)	C28-C29-C18	119.1(7)
C9-C8-N2	118.8(5)	N5-Pt2-Cl2	91.12(15)
C9-C8-C13	119.1(6)	N5-Pt2-N7	174.02(19)
C13-C8-N2	122.1(5)	N7-Pt2-Cl2	93.42(15)
C10-C9-C8	120.7(6)	C51-Pt2-Cl2	175.74(18)
C9-C10-C11	120.4(6)	C51-Pt2-N5	92.5(2)
C12-C11-C10	119.4(6)	C51-Pt2-N7	83.1(2)
C11-C12-C13	121.4(6)	C30-N5-Pt2	118.3(4)
C12-C13-C8	119.0(6)	C36-N5-Pt2	124.2(4)
N3-C14-C15	121.1(6)	C36-N5-C30	117.4(5)
N3-C14-C21	114.5(5)	C36-N6-C37	125.3(5)
C15-C14-C21	124.4(6)	C43-N7-Pt2	113.6(4)
N4-C15-C14	121.1(6)	C46-N7-Pt2	128.9(4)
N4-C15-C18	121.4(6)	C46-N7-C43	117.5(5)
C14-C15-C18	117.5(6)	C45-N8-C44	116.0(6)
N4-C16-C17	125.1(6)	C31-C30-N5	119.3(6)
N3-C17-C16	119.0(6)	C31-C30-C35	120.9(7)
C19-C18-C15	119.9(6)	C35-C30-N5	119.8(6)
C19-C18-C29	120.7(6)	C30-C31-C32	119.9(8)
C29-C18-C15	119.4(6)	C33-C32-C31	120.6(9)
C18-C19-C20	120.1(6)	C32-C33-C34	119.2(8)
C26-C19-C18	117.2(6)	C35-C34-C33	121.1(9)
C26-C19-C20	122.7(6)	C30-C35-C34	118.4(8)
C21-C20-C19	119.7(6)	N5-C36-N6	123.2(6)
C21-C20-C25	116.7(6)	C38-C37-N6	119.3(6)
C25-C20-C19	123.6(6)	C38-C37-C42	119.6(7)
C20-C21-C14	118.5(6)	C42-C37-N6	121.0(6)
C20-C21-C22	124.9(6)	C37-C38-C39	120.3(7)
C22-C21-C14	116.5(6)	C40-C39-C38	120.1(8)
C21-C22-Pt1	112.0(4)	C39-C40-C41	120.0(8)
C23-C22-Pt1	132.1(5)	C40-C41-C42	120.5(9)
C23-C22-C21	115.9(6)	C37-C42-C41	119.3(9)
C24-C23-C22	119.7(7)	N7-C43-C44	120.6(6)
C25-C24-C23	123.8(7)	N7-C43-C50	116.0(5)
C24-C25-C20	119.0(6)	C44-C43-C50	123.4(6)
C27-C26-C19	122.7(7)	N8-C44-C43	121.6(6)
C26-C27-C28	120.3(7)	N8-C44-C47	120.6(6)
C29-C28-C27	120.0(7)	C43-C44-C47	117.7(6)

N8-C45-C46	124.3(6)	C60-C59-N9	118.4(6)
N7-C46-C45	119.9(6)	C60-C59-C64	119.0(6)
C48-C47-C44	119.4(6)	C64-C59-N9	122.5(6)
C48-C47-C58	120.6(7)	C61-C60-C59	119.1(7)
C58-C47-C44	120.0(7)	C62-C61-C60	121.5(9)
C47-C48-C49	121.0(6)	C61-C62-C63	119.4(8)
C55-C48-C47	117.6(6)	C64-C63-C62	120.3(8)
C55-C48-C49	121.4(7)	C63-C64-C59	120.6(8)
C50-C49-C48	119.2(6)	N9-C65-N10	121.5(6)
C50-C49-C54	116.0(6)	C67-C66-N10	119.8(8)
C54-C49-C48	124.9(6)	C71-C66-N10	120.7(8)
C43-C50-C51	114.7(5)	C71-C66-C67	119.5(8)
C49-C50-C43	119.2(5)	C68-C67-C66	120.8(10)
C49-C50-C51	126.0(6)	C69-C68-C67	118.2(11)
C50-C51-Pt2	112.4(4)	C68-C69-C70	121.9(10)
C52-C51-Pt2	134.1(5)	C71-C70-C69	119.0(11)
C52-C51-C50	113.5(6)	C66-C71-C70	120.6(10)
C51-C52-C53	122.2(6)	N11-C72-C73	121.0(5)
C52-C53-C54	122.3(6)	N11-C72-C79	116.0(5)
C53-C54-C49	120.0(6)	C73-C72-C79	123.0(5)
C56-C55-C48	120.1(8)	N12-C73-C72	120.8(5)
C57-C56-C55	121.8(8)	N12-C73-C76	120.7(5)
C56-C57-C58	119.7(7)	C72-C73-C76	118.5(5)
C57-C58-C47	120.2(8)	N12-C74-C75	123.6(6)
N9-Pt3-Cl3	88.30(15)	N11-C75-C74	120.0(6)
N11-Pt3-Cl3	94.49(14)	C77-C76-C73	119.2(5)
N11-Pt3-N9	174.4(2)	C87-C76-C73	120.6(6)
C80-Pt3-Cl3	174.79(18)	C87-C76-C77	120.2(6)
C80-Pt3-N9	95.0(2)	C76-C77-C78	120.6(5)
C80-Pt3-N11	81.9(2)	C84-C77-C76	116.8(6)
C59-N9-Pt3	123.3(4)	C84-C77-C78	122.5(6)
C65-N9-Pt3	118.7(4)	C79-C78-C77	118.9(5)
C65-N9-C59	117.9(5)	C83-C78-C77	124.9(6)
C65-N10-C66	124.7(6)	C83-C78-C79	116.2(6)
C72-N11-Pt3	113.8(4)	C78-C79-C72	119.8(5)
C75-N11-Pt3	127.9(4)	C78-C79-C80	124.7(5)
C75-N11-C72	118.1(5)	C80-C79-C72	115.6(5)
C74-N12-C73	116.3(5)	C79-C80-Pt3	112.5(4)

C81-C80-Pt3	131.1(5)	C85-C84-C77	122.0(7)
C81-C80-C79	116.3(6)	C84-C85-C86	120.3(7)
C80-C81-C82	120.7(6)	C87-C86-C85	120.7(7)
C83-C82-C81	121.7(6)	C86-C87-C76	119.9(7)
C82-C83-C78	120.4(6)		

Table S3. Bond lengths [Å] and angles [°] for **1b**.

Pt1-Cl1	2.3846(18)	C7-C8	1.412(9)
Pt1-N1	2.019(5)	C7-C11	1.391(9)
Pt1-N3	2.019(5)	C8-C9	1.372(10)
Pt1-C1	2.005(6)	C9-C10	1.381(10)
Pt2-Cl2	2.3863(17)	C11-C12	1.449(9)
Pt2-N2	2.049(5)	C12-C13	1.415(9)
Pt2-N4	2.043(6)	C13-C14	1.426(8)
Pt2-C2	1.980(7)	C15-C16	1.386(9)
N1-C13	1.346(8)	C17-C18	1.392(9)
N1-C15	1.333(8)	C17-C22	1.373(9)
N2-C12	1.328(8)	C18-C19	1.396(10)
N2-C16	1.327(8)	C19-C20	1.365(10)
N3-C17	1.434(8)	C20-C21	1.405(11)
N3-C23	1.281(8)	C21-C22	1.367(10)
N4-C30	1.429(9)	C24-C25	1.339(12)
N4-C36	1.298(10)	C24-C29	1.347(11)
N5-C23	1.328(9)	C25-C26	1.429(13)
N5-C24	1.431(9)	C26-C27	1.398(14)
N6-C36	1.323(10)	C27-C28	1.331(12)
N6-C37	1.429(9)	C28-C29	1.376(11)
C1-C3	1.385(9)	C30-C31	1.346(11)
C1-C14	1.401(9)	C30-C35	1.409(10)
C2-C10	1.406(9)	C31-C32	1.395(11)
C2-C11	1.415(9)	C32-C33	1.411(12)
C3-C4	1.427(10)	C33-C34	1.357(12)
C4-C5	1.372(10)	C34-C35	1.379(11)
C5-C6	1.407(9)	C37-C38	1.357(12)
C6-C7	1.483(9)	C37-C42	1.365(12)
C6-C14	1.387(9)	C38-C39	1.402(14)

C39-C40	1.362(16)	C4-C5-C6	120.1(7)
C40-C41	1.376(15)	C5-C-6C7	123.6(6)
C41-C42	1.380(13)	C14-C6-C5	117.5(6)
		C14-C6-C7	118.9(6)
N1-Pt1-Cl1	95.05(15)	C8-C7-C6	125.0(6)
N3-Pt1-Cl1	91.43(16)	C11-C7-C6	119.9(6)
N3-Pt1-N1	173.5(2)	C11-C7-C8	115.1(6)
C1-Pt1-Cl1	177.22(19)	C9-C8-C7	120.2(6)
C1-Pt1-N1	82.3(2)	C8-C9-C10	122.5(6)
C1-Pt1-N3	91.3(2)	C9-C10-C2	121.2(6)
N2-Pt2-Cl2	91.87(15)	C2-C11-C12	112.8(6)
N4-Pt2-Cl2	92.74(16)	C7-C11-C2	127.1(6)
N4-Pt2-N2	175.4(2)	C7-C11-C12	120.1(6)
C2-Pt2-Cl2	173.96(18)	N2-C12-C11	119.2(6)
C2-Pt2-N2	82.2(2)	N2-C12-C13	121.0(6)
C2-Pt2-N4	93.2(2)	C13-C12-C11	119.6(6)
C13-N1-Pt1	111.9(4)	N1-C13-C12	121.0(6)
C15-N1-Pt1	131.6(4)	N1-C13-C14	118.9(5)
C15-N1-C13	116.5(5)	C12-C13-C14	120.1(6)
C12-N2-Pt2	111.6(4)	C1-C14-C13	114.0(6)
C16-N2-Pt2	130.8(4)	C6-C14-C1	124.7(6)
C16-N2-C12	117.6(5)	C6-C14-C13	121.3(6)
C17-N3-Pt1	120.1(4)	N1-C15-C16	122.2(6)
C23-N3-Pt1	120.5(5)	N2-C16-C15	121.6(6)
C23-N3-C17	119.1(6)	C18-C17-N3	118.0(5)
C30-N4-Pt2	120.2(5)	C22-C17-N3	123.7(6)
C36-N4-Pt2	121.1(5)	C22-C17-C18	118.3(6)
C36-N4-C30	118.7(6)	C17-C18-C19	119.9(7)
C23-N5-C24	125.0(6)	C20-C19-C18	121.1(7)
C36-N6-C37	127.0(7)	C19-C20-C21	118.8(7)
C3-C1-Pt1	130.8(5)	C22-C21-C20	119.7(7)
C3-C1-C14	116.2(6)	C21-C22-C17	122.2(7)
C14-C1-Pt1	112.9(5)	N3-C23-N5	123.4(6)
C10-C2-Pt2	132.2(5)	C25-C24-N5	116.7(8)
C10-C2-C11	113.8(6)	C25-C24-C29	120.8(8)
C11-C2-Pt2	114.0(4)	C29-C24-N5	122.5(7)
C1-C3-C4	120.8(6)	C24-C25-C26	119.3(10)
C5-C4-C3	120.6(6)	C27-C26-C25	118.9(10)

C28-C27-C26	118.7(9)	C34-C35-C30	118.7(8)
C27-C28-C29	121.9(8)	N4-C36-N6	123.2(7)
C24-C29-C28	120.4(8)	C38-C37-N6	122.3(8)
C31-C30-N4	121.6(7)	C38-C37-C42	119.8(8)
C31-C30-C35	119.2(8)	C42-C37-N6	117.9(8)
C35-C30-N4	119.1(7)	C37-C38-C39	120.3(10)
C30-C31-C32	122.7(8)	C40-C39-C38	119.8(11)
C31-C32-C33	117.7(8)	C39-C40-C41	119.2(10)
C34-C33-C32	119.4(8)	C40-C41-C42	120.7(10)
C33-C34-C35	122.3(8)	C37-C42-C41	120.0(10)

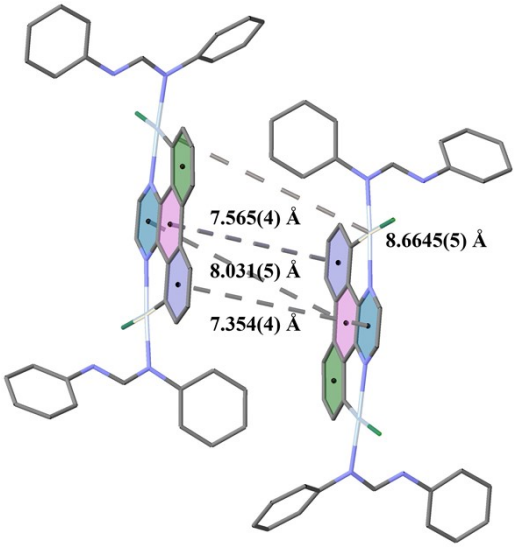
Table S4. Bond lengths [Å] and angles [°] for **2**.

Pt1-N2	1.93(2)	C4-C5	1.36(3)
Pt1-N3	2.064(18)	C6-C5	1.446(9)
Pt1-N7	2.07(2)	C6-C7	1.446(9)
Pt1-C6	1.935(17)	C8-C7	1.446(9)
Pt2-Pt1	2.8439(15)	C9-C8	1.446(9)
Pt2-N4	2.023(19)	C9-C10	1.446(9)
Pt2-N5	2.04(2)	C10-C5	1.446(9)
Pt2-N8	2.112(18)	C10-C11	1.40(3)
Pt2-C21	2.07(2)	C11-C12	1.405(10)
N1-C2	1.42(3)	C13-C12	1.405(10)
N1-C3	1.35(3)	C14-C13	1.405(10)
N2-C1	1.35(3)	C14-C15	1.405(10)
N2-C4	1.35(3)	C16-C11	1.405(10)
N3-C46	1.435(19)	C16-C15	1.405(10)
N3-C52	1.42(3)	C17-N5	1.34(3)
N4-C52	1.19(2)	C17-C18	1.40(3)
N7-C39	1.24(3)	C18-N6	1.41(3)
N7-C40	1.45(2)	C19-N5	1.42(3)
N8-C33	1.39(2)	C19-C32	1.36(3)
N8-C39	1.41(3)	C20-C19	1.54(3)
C1-C2	1.47(4)	C20-C25	1.32(3)
C3-C16	1.47(3)	C21-C20	1.23(3)
C4-C3	1.50(4)	C21-C22	1.31(3)

C22-C23	1.45(3)	N2-Pt1-Pt2	97.7(6)
C24-C23	1.28(3)	N2-Pt1-N3	95.1(8)
C25-C24	1.49(3)	N2-Pt1-N7	174.5(7)
C25-C26	1.46(3)	N2-Pt1-C6	81.6(7)
C27-C26	1.406(9)	N3-Pt1-Pt2	80.5(5)
C27-C28	1.406(9)	N3-Pt1-N7	89.9(8)
C29-C28	1.406(9)	N7-Pt1-Pt2	80.8(5)
C29-C30	1.406(9)	C6-Pt1-Pt2	98.6(5)
C31-C26	1.406(9)	C6-Pt1-N3	176.5(7)
C31-C30	1.406(9)	C6-Pt1-N7	93.3(6)
C31-C32	1.44(3)	N4-Pt2-Pt1	82.6(6)
C32-N6	1.52(3)	N4-Pt2-N5	91.7(7)
C34-C33	1.3900	N4-Pt2-N8	90.3(7)
C35-C34	1.3900	N4-Pt2-C21	171.6(8)
C36-C35	1.3900	N5-Pt2-Pt1	98.7(8)
C37-C36	1.3900	N5-Pt2-N8	177.7(8)
C38-C33	1.3900	N5-Pt2-C21	81.1(9)
C38-C37	1.3900	N8-Pt2-Pt1	82.6(5)
C40-C45	1.3900	C21-Pt2-Pt1	94.2(7)
C41-C40	1.3900	C21-Pt2-N8	96.9(8)
C42-C41	1.3900	C3-N1-C2	114(2)
C43-C42	1.3900	C1-N2-Pt1	129.0(18)
C43-C44	1.3900	C4-N2-Pt1	115.4(16)
C45-C44	1.3900	C4-N2-C1	115(2)
C46-C47	1.3900	C46-N3-Pt1	124.0(14)
C47-C48	1.3900	C52-N3-Pt1	119.3(13)
C48-C49	1.3900	C52-N3-C46	116.4(16)
C50-C49	1.3900	C52-N4-Pt2	123.6(19)
C50-C51	1.3900	C52-N4-C53	118(2)
C51-C46	1.3900	C53-N4-Pt2	117.5(12)
C53-N4	1.51(2)	C17-N5-Pt2	126.6(18)
C54-C53	1.3900	C17-N5-C19	122(2)
C54-C55	1.3900	C19-N5-Pt2	111.0(15)
C55-C56	1.3900	C18-N6-C32	114(2)
C56-C57	1.3900	C39-N7-Pt1	127.0(17)
C57-C58	1.3900	C39-N7-C40	117(2)
C58-C53	1.3900	C40-N7-Pt1	115.9(14)
		C33-N8-Pt2	125.6(13)

C33-N8-C39	115.3(17)	C21-C20-C25	131(2)
C39-N8-Pt2	119.1(14)	C25-C20-C19	113(2)
N2-C1-C2	122(2)	C20-C21-Pt2	116.3(17)
N1-C2-C1	122(2)	C20-C21-C22	119(2)
N1-C3-C4	121(2)	C22-C21-Pt2	124.6(19)
N1-C3-C16	122(2)	C21-C22-C23	117(2)
C16-C3-C4	116(2)	C24-C23-C22	124(2)
N2-C4-C3	124(2)	C23-C24-C25	115(2)
N2-C4-C5	116(2)	C20-C25-C24	114(2)
C5-C4-C3	120(2)	C20-C25-C26	128(2)
C4-C5-C6	113.7(15)	C26-C25-C24	117.3(19)
C4-C5-C10	120.8(16)	C27-C26-C25	122.8(15)
C10-C5-C6	125.4(16)	C31-C26-C25	117.7(15)
C5-C6-Pt1	112.8(10)	C31-C26-C27	119.1(18)
C7-C6-Pt1	132.4(11)	C28-C27-C26	120.7(18)
C7-C6-C5	114.7(15)	C27-C28-C29	116.6(18)
C8-C7-C6	117.8(17)	C28-C29-C30	125.4(19)
C9-C8-C7	128.7(19)	C31-C30-C29	114.0(19)
C8-C9-C10	111.2(18)	C26-C31-C32	116.7(15)
C9-C10-C5	121.1(18)	C30-C31-C26	122.6(18)
C11-C10-C5	121.6(14)	C30-C31-C32	119.8(16)
C11-C10-C9	117.0(12)	C19-C32-N6	115(2)
C10-C11-C12	120.3(15)	C19-C32-C31	124(2)
C10-C11-C16	118.9(13)	C31-C32-N6	121(2)
C16-C11-C12	120(2)	N8-C33-C34	115.2(13)
C13-C12-C11	114(2)	N8-C33-C38	124.7(13)
C12-C13-C14	130(2)	C34-C33-C38	120.0
C15-C14-C13	111(2)	C35-C34-C33	120.0
C14-C15-C16	123.5(19)	C34-C35-C36	120.0
C11-C16-C3	121.7(17)	C35-C36-C37	120.0
C11-C16-C15	120(2)	C36-C37-C38	120.0
C15-C16-C3	117.4(17)	C37-C38-C33	120.0
N5-C17-C18	115(2)	N7-C39-N8	123(2)
C17-C18-N6	128(2)	C41-C40-N7	120.3(15)
N5-C19-C20	115(2)	C41-C40-C45	120.0
C32-C19-N5	125(2)	C45-C40-N7	119.7(15)
C32-C19-C20	120(2)	C42-C41-C40	120.0
C21-C20-C19	116(2)	C43-C42-C41	120.0

C42-C43-C44	120.0	C46-C51-C50	120.0
C45-C44-C43	120.0	N4-C52-N3	127(2)
C44-C45-C40	120.0	C54-C53-N4	119.5(14)
C47-C46-N3	116.7(13)	C58-C53-N4	119.9(14)
C51-C46-N3	122.8(13)	C58-C53-C54	120.0
C51-C46-C47	120.0	C55-C54-C53	120.0
C46-C47-C48	120.0	C56-C55-C54	120.0
C49-C48-C47	120.0	C55-C56-C57	120.0
C48-C49-C50	120.0	C56-C57-C58	120.0
C51-C50-C49	120.0	C53-C58-C57	120.0



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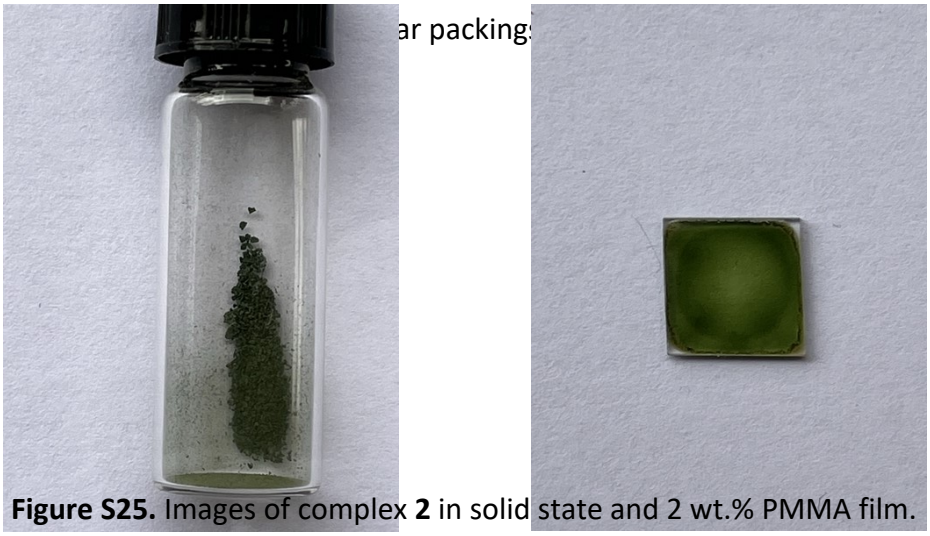

Figure S25. Images of complex **2** in solid state and 2 wt.% PMMA film.

5. References

1. B. An, Z. G. Wang, L. C. Yang and X. P. Li, *Journal of Applied Spectroscopy*, 2017, **84**, 555-559.