

Electronic Supplementary Information (ESI)

**Blue Phosphorescent *N*-Heterocyclic Carbene Chelated Platinum(II) Complexes
with α -Duryl- β -Diketonate Ancillary Ligand**

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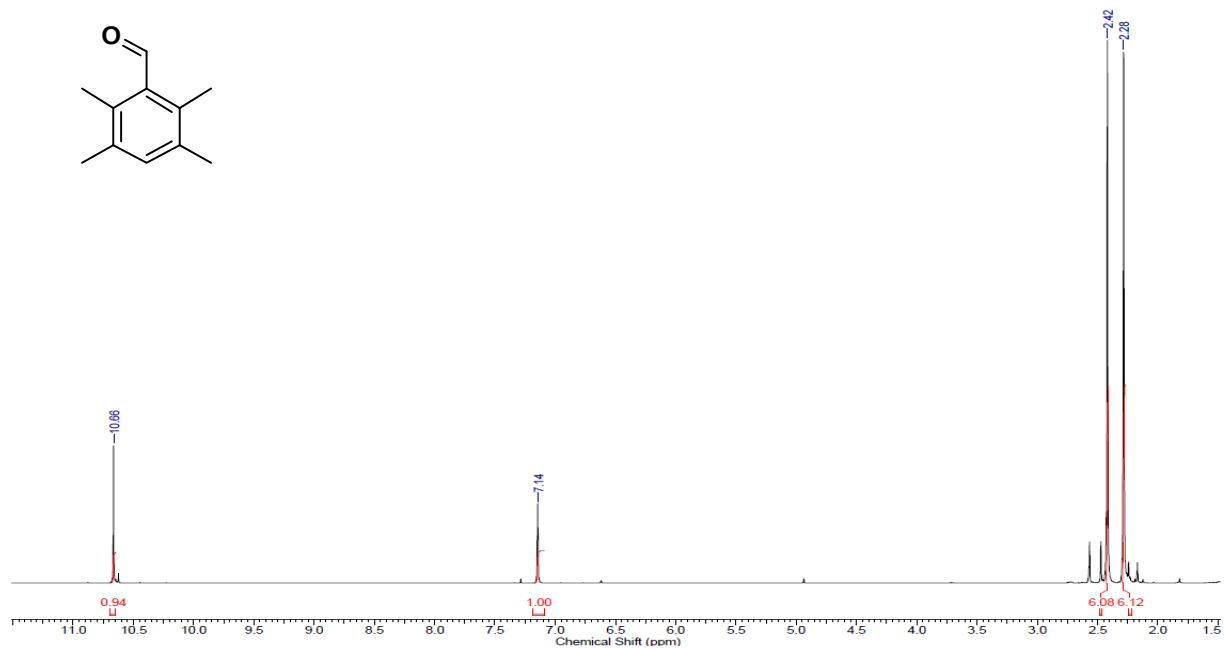
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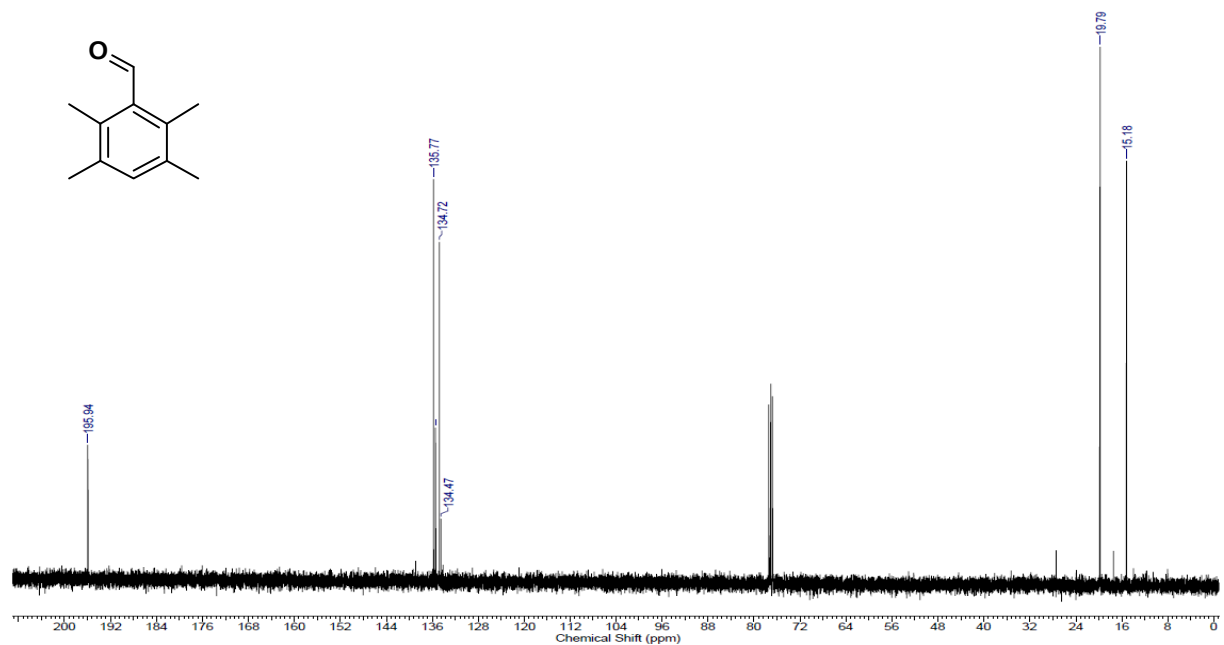
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I. ^1H & ^{13}C NMR Spectra

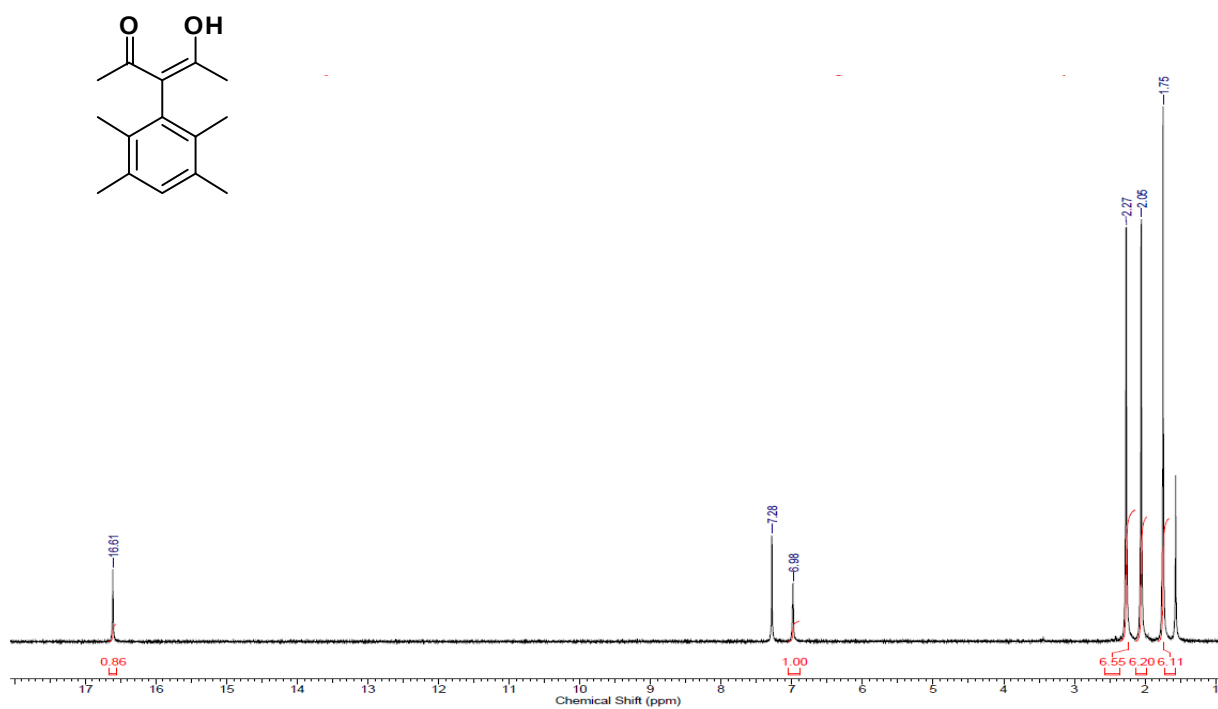
i) ^1H NMR spectra of **1** in CDCl_3



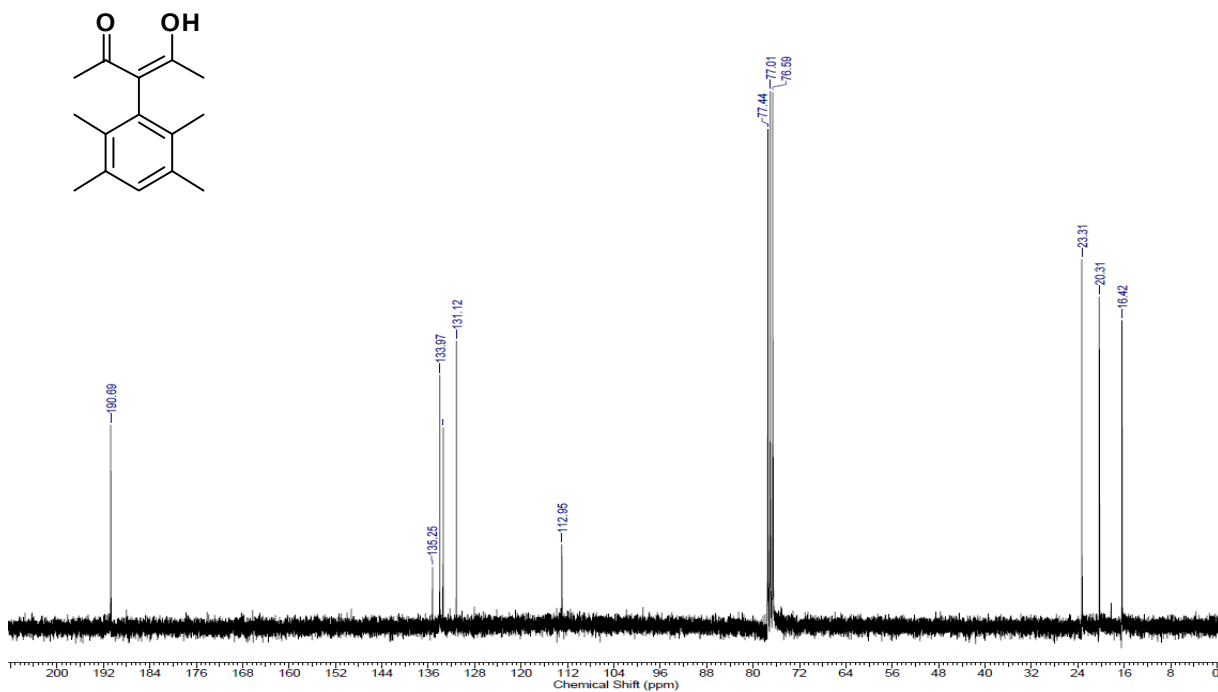
ii) ^{13}C NMR spectra of **1** in CDCl_3



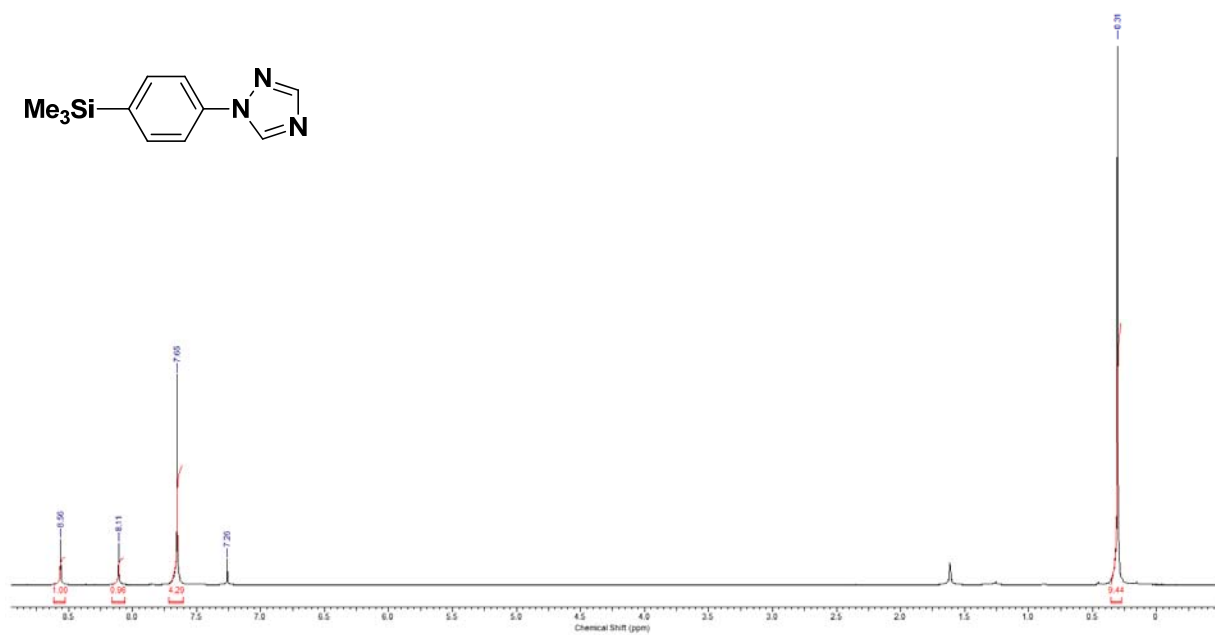
iii) ^1H NMR spectra of **2** in CDCl_3



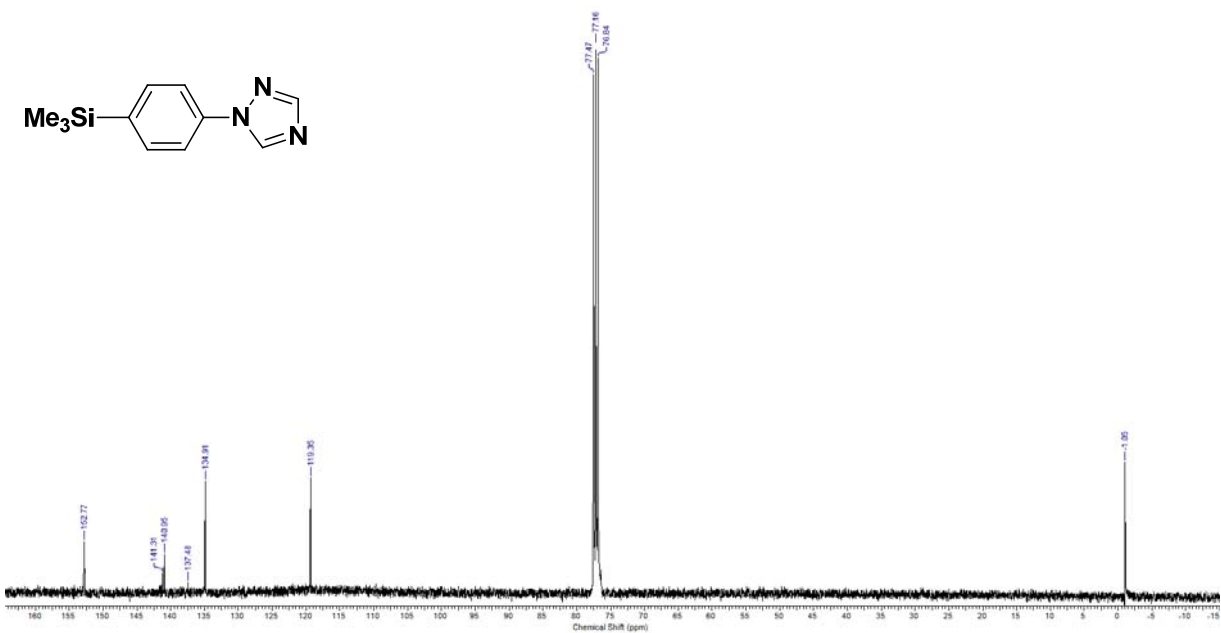
iv) ^{13}C NMR spectra of **2** in CDCl_3



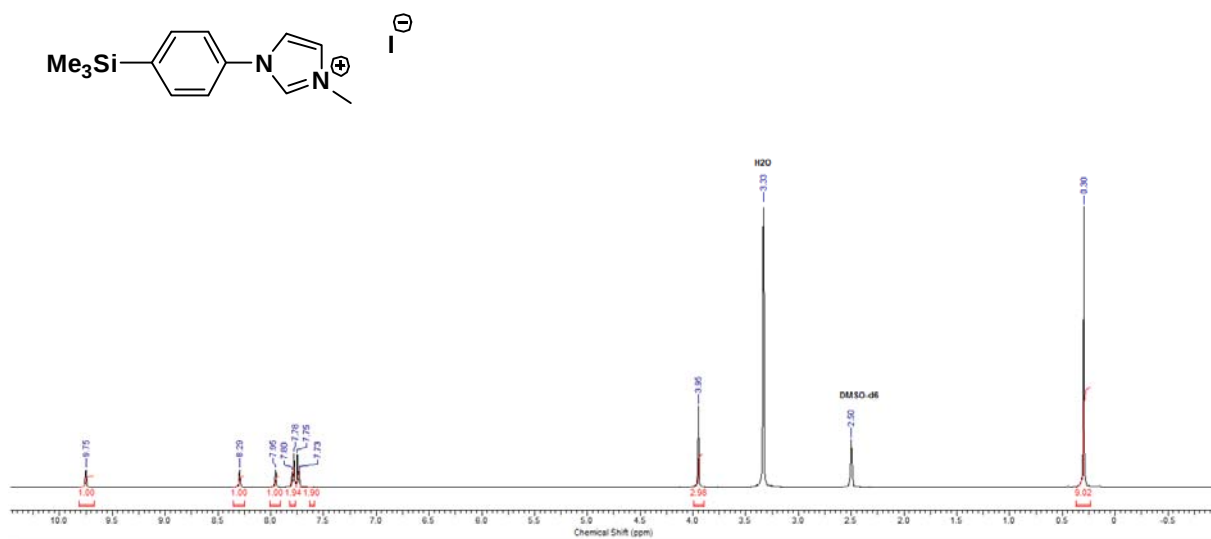
v) ^1H NMR spectra of **6** in CDCl_3



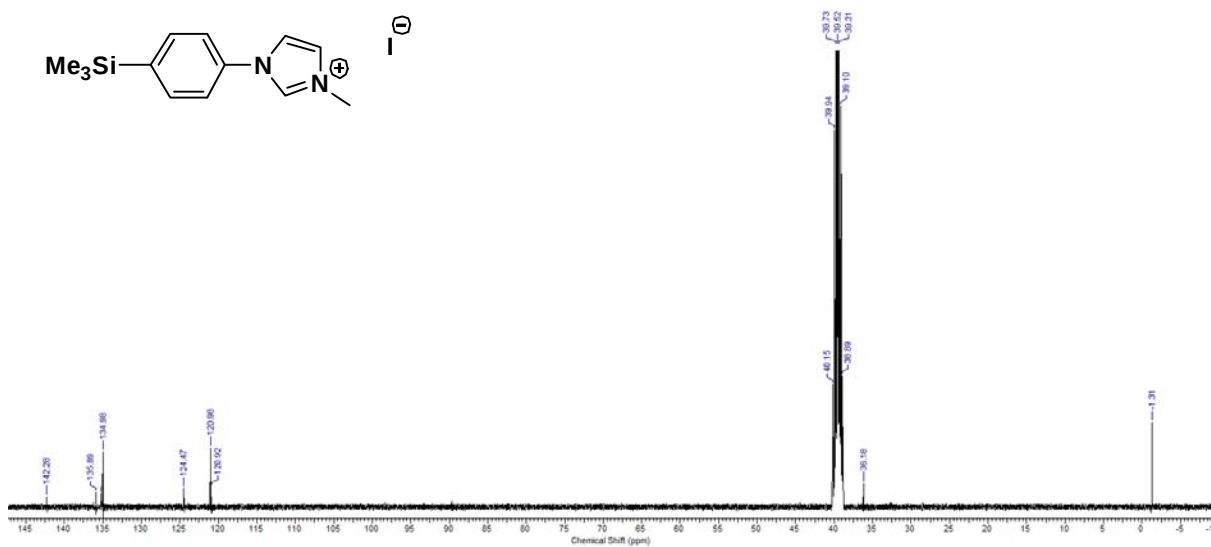
vi) ^{13}C NMR spectra of **6** in CDCl_3



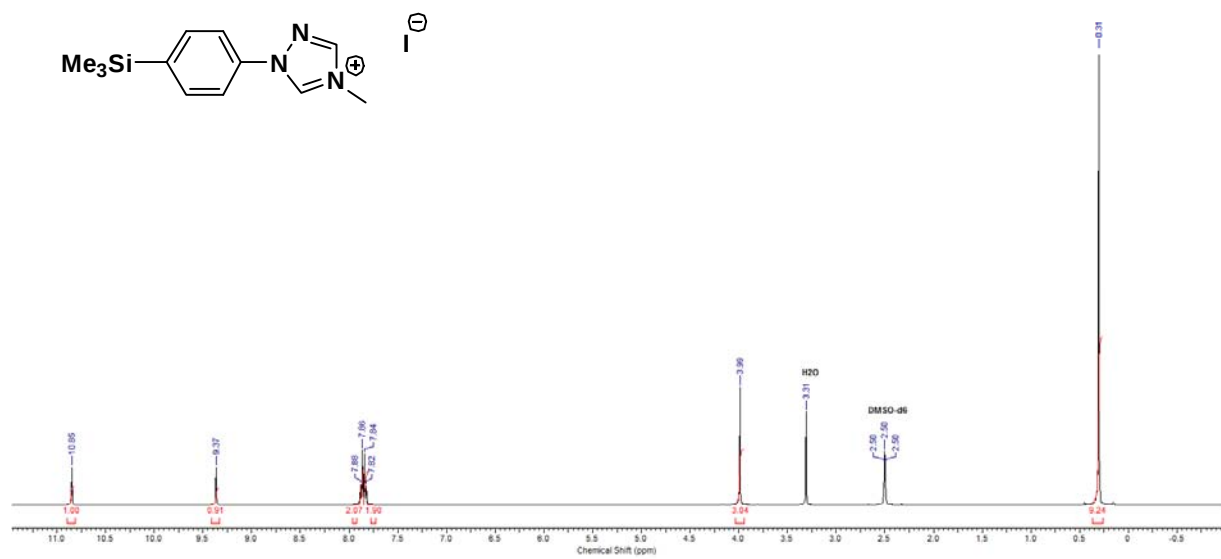
vii) ^1H NMR spectra of **7** in $\text{DMSO-}d_6$



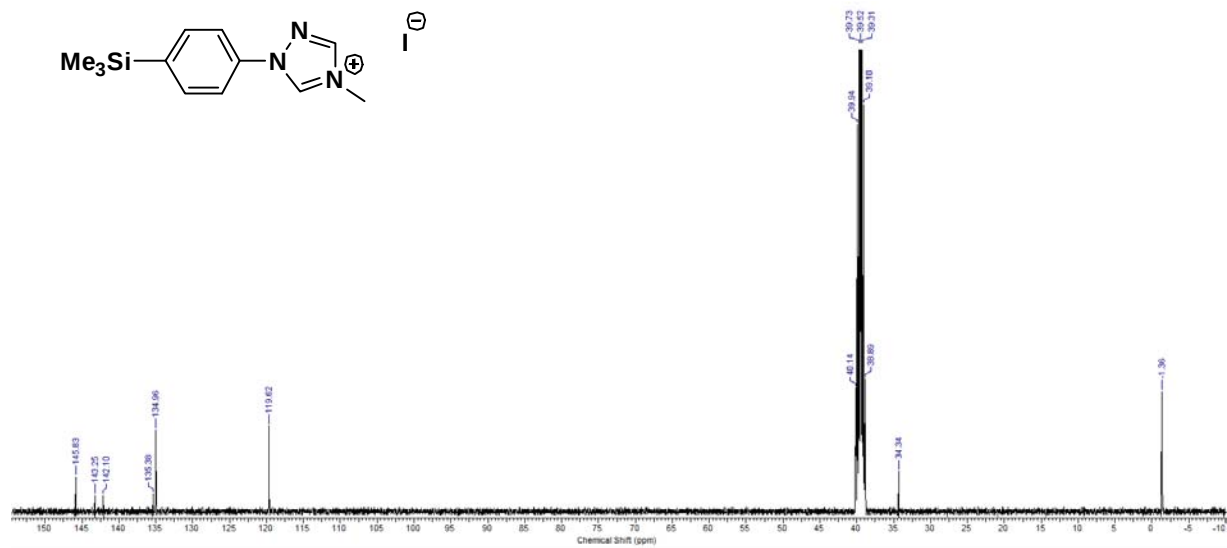
viii) ^{13}C NMR spectra of **7** in $\text{DMSO-}d_6$



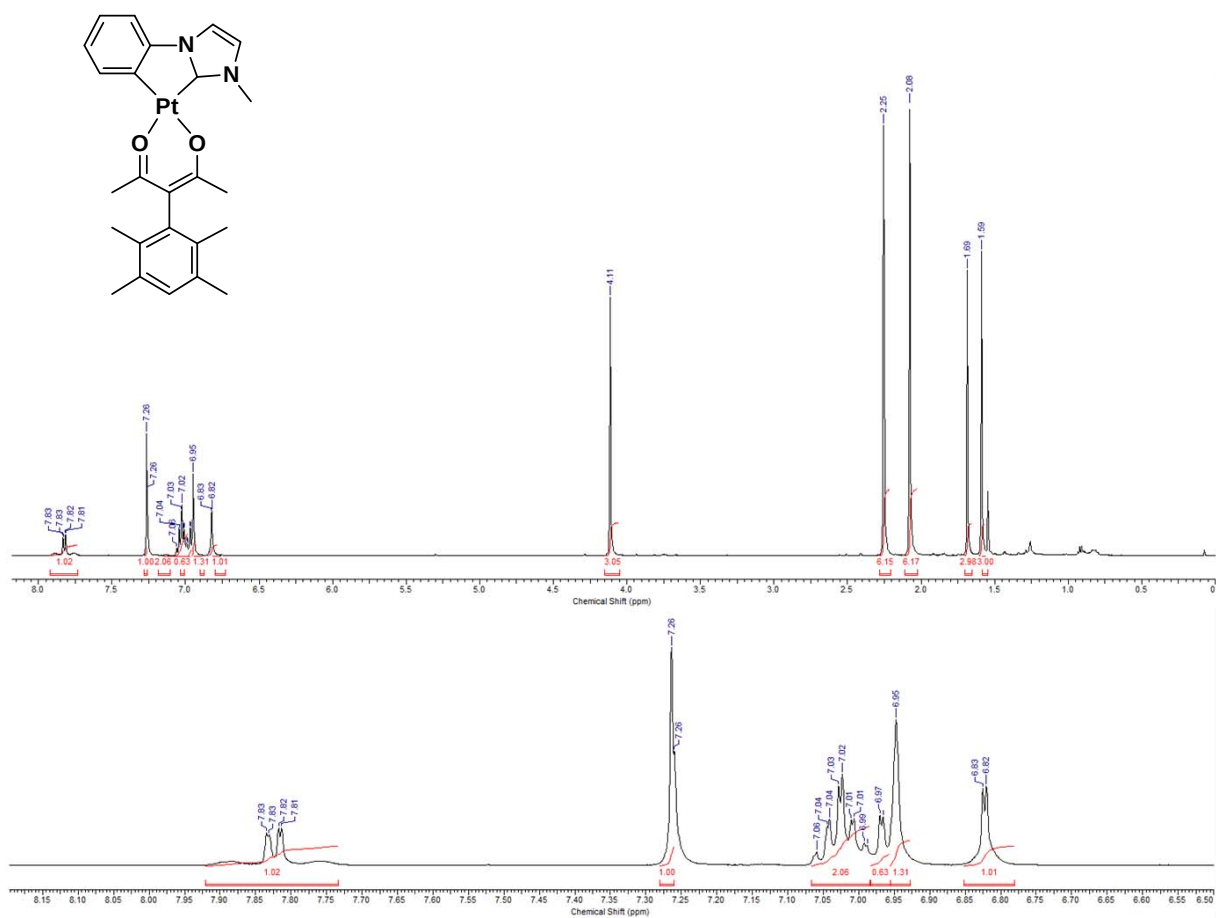
ix) ^1H NMR spectra of **8** in $\text{DMSO}-d_6$



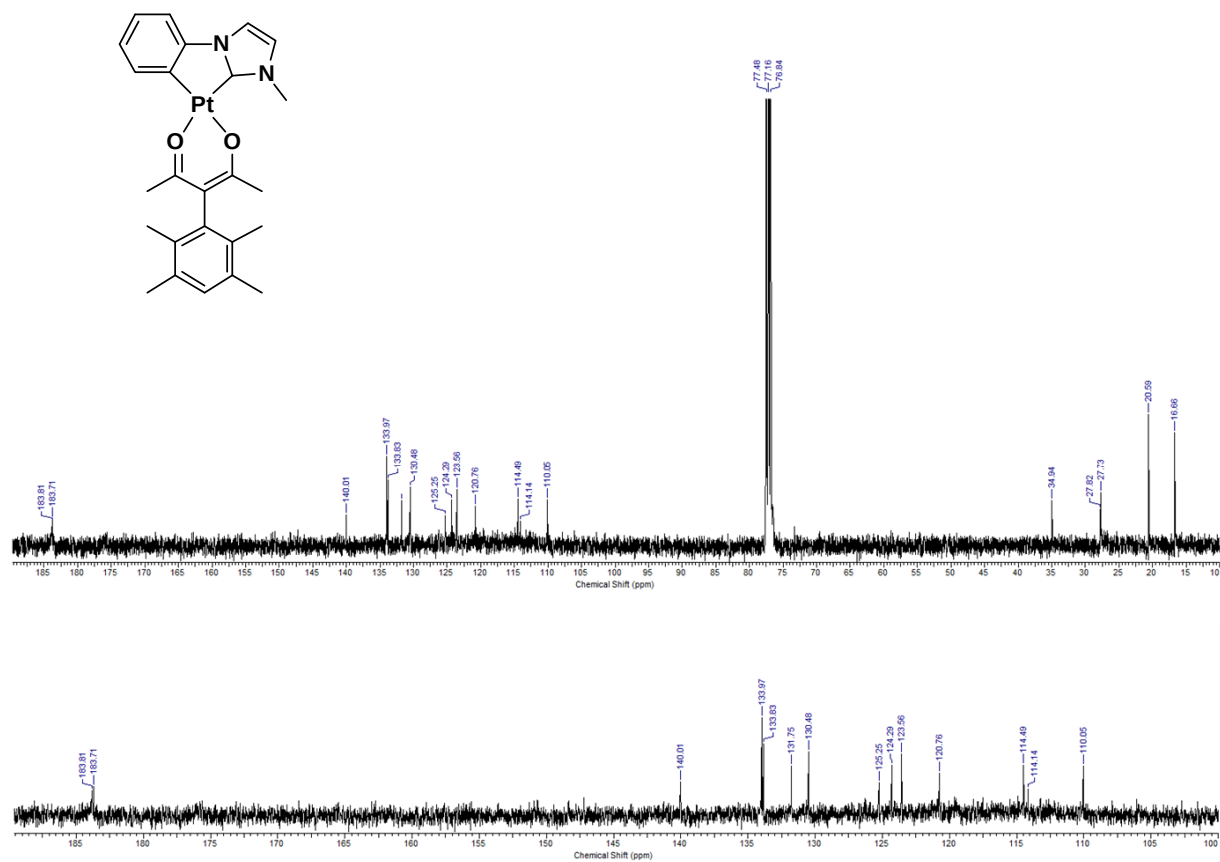
x) ^{13}C NMR spectra of **8** in $\text{DMSO}-d_6$



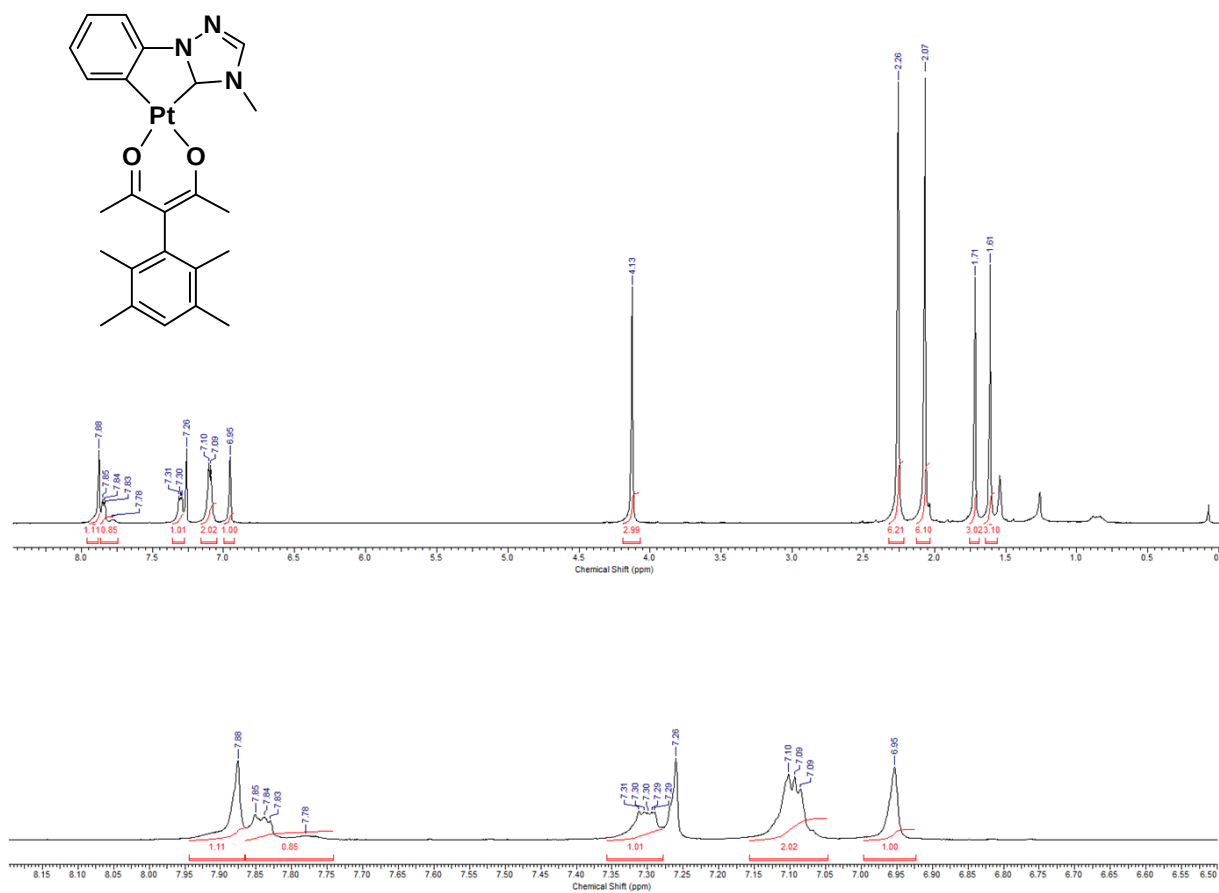
xi) ^1H NMR spectra of **Pt1** in CDCl_3



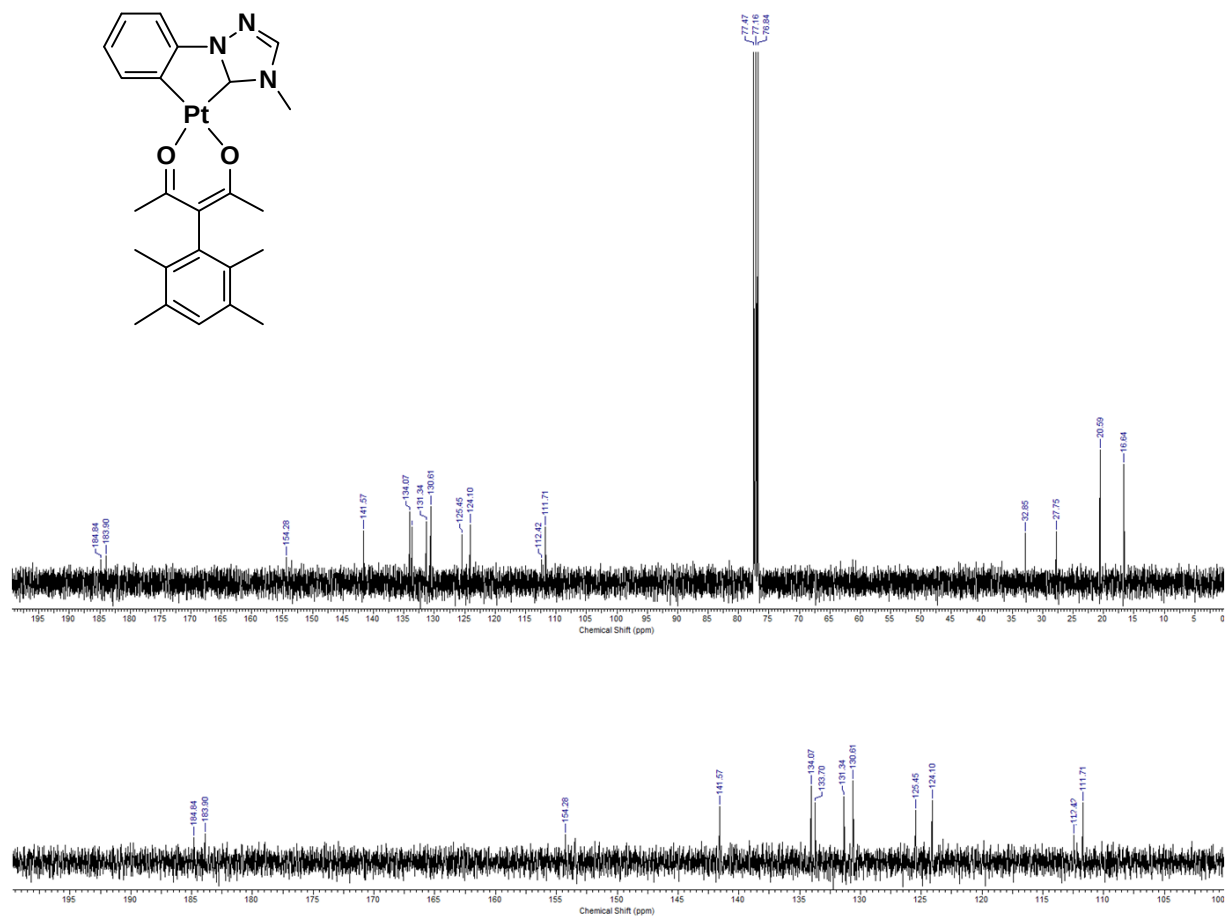
xii) ^{13}C NMR spectra of **Pt1** in CDCl_3



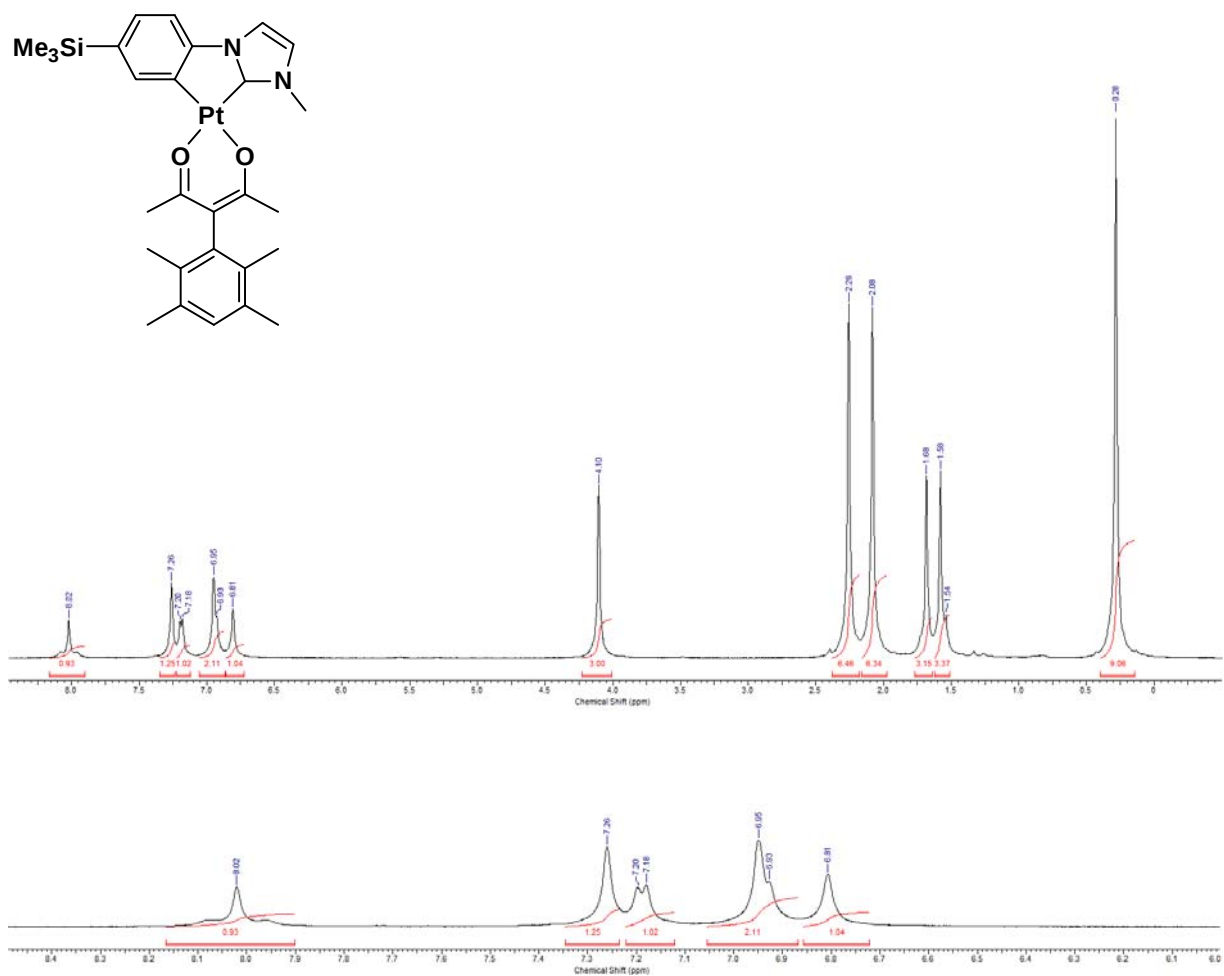
xiii) ^1H NMR spectra of **Pt2** in CDCl_3



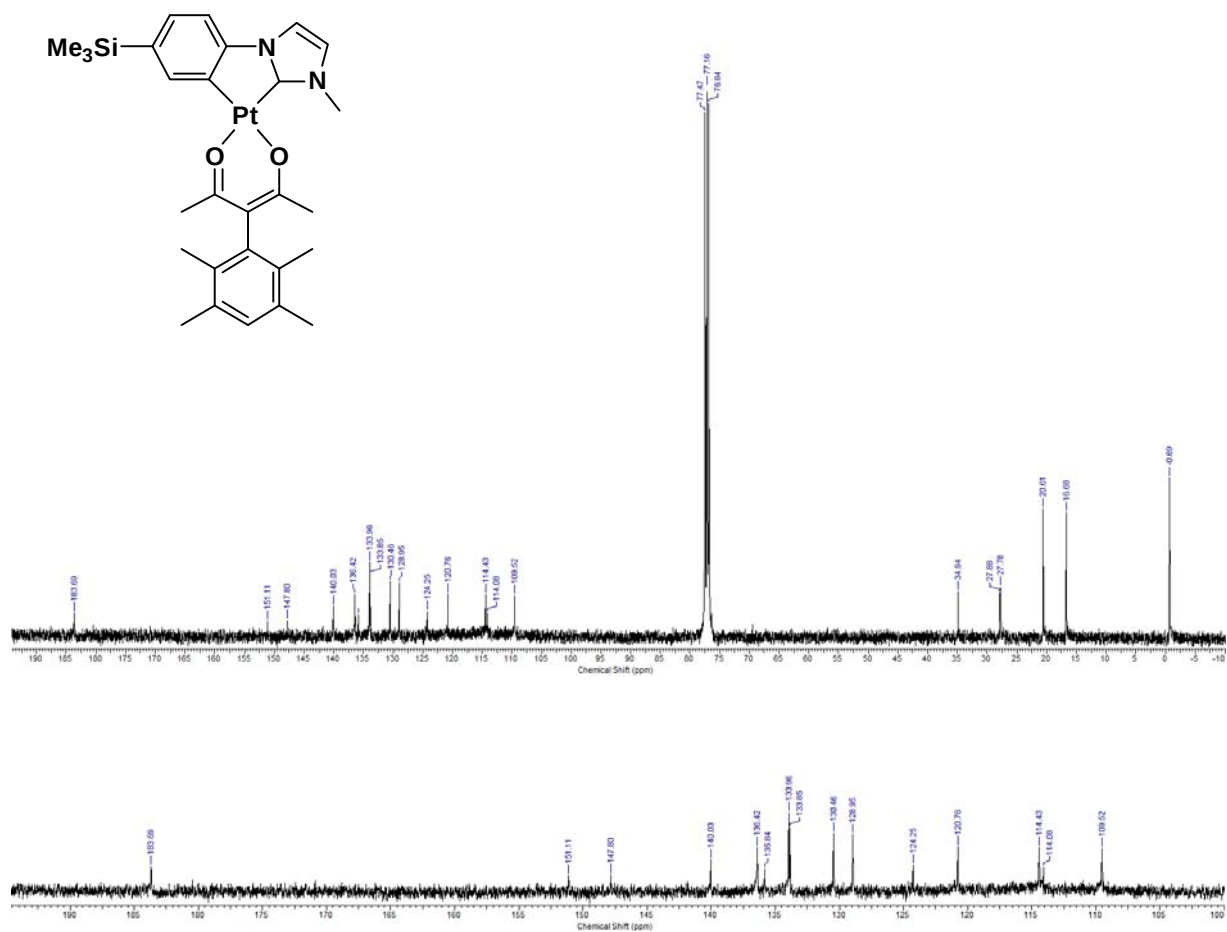
xiv) ^{13}C NMR spectra of **Pt2** in CDCl_3



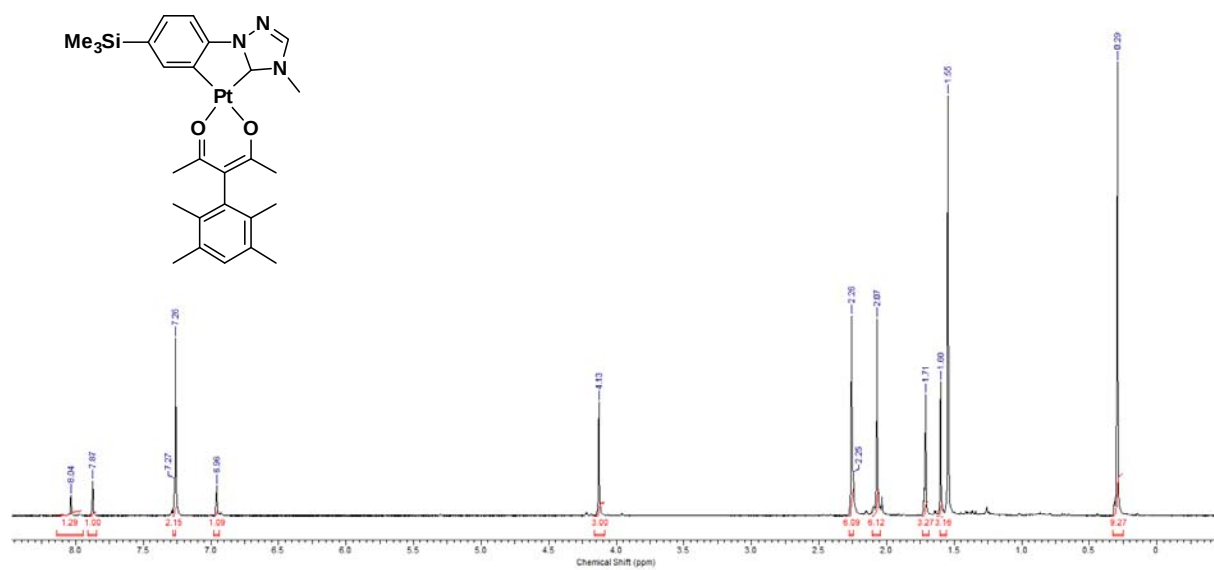
xv) ^1H NMR spectra of **Pt3** in CDCl_3



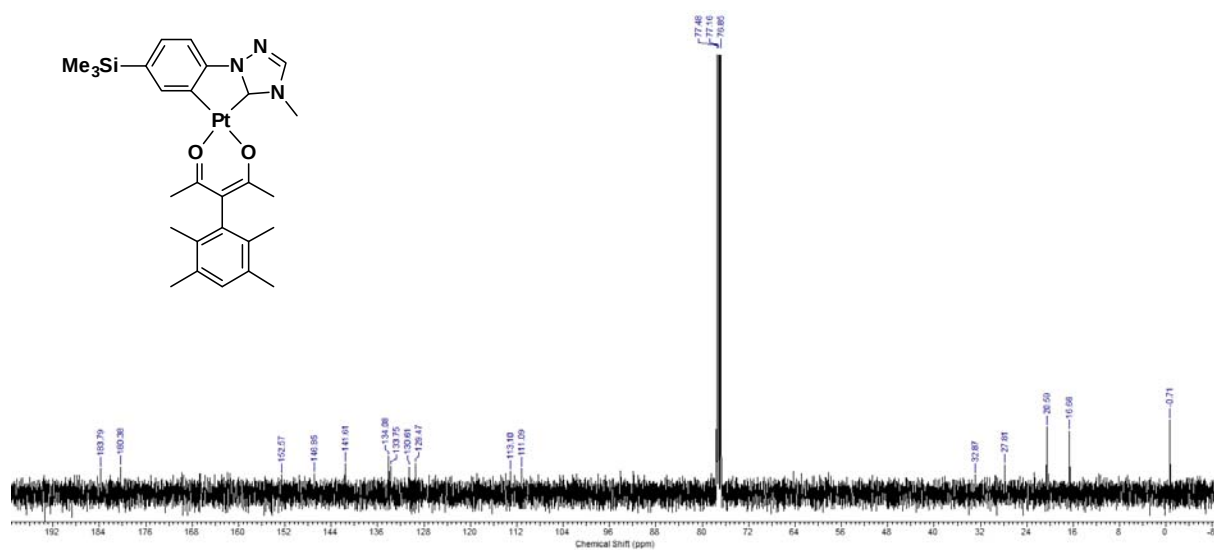
xvi) ^{13}C NMR spectra of **Pt3** in CDCl_3



xvii) ^1H NMR spectra of **Pt4** in CDCl_3



xviii) ^{13}C NMR spectra of **Pt4** in CDCl_3



II. Cyclic Voltammetry Data

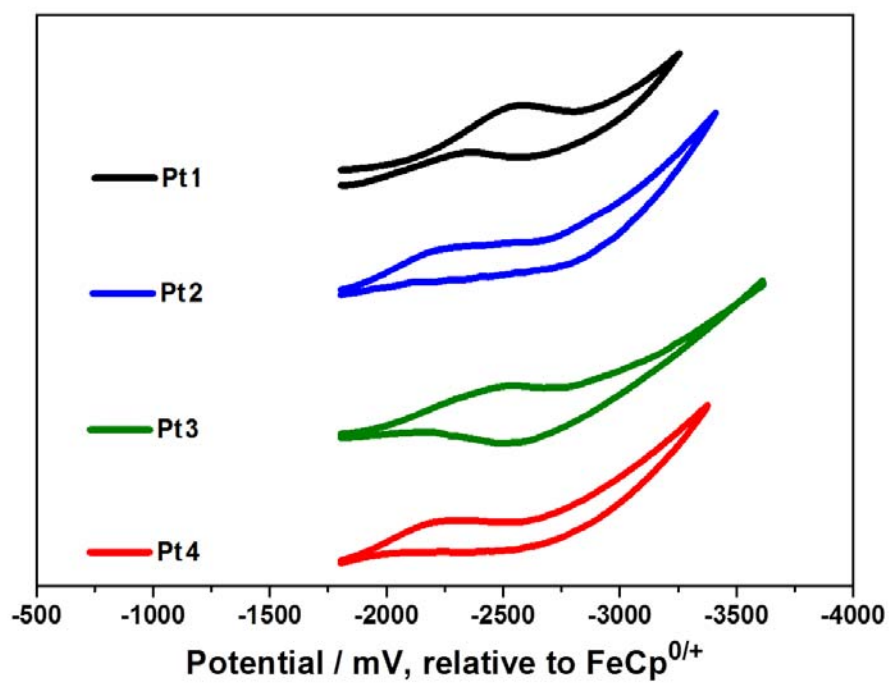


Fig S1. The reduction potential diagrams for complexes **Pt1**, **Pt2**, **Pt3**, and **Pt4** recorded in THF using $(n\text{-Bu})_4\text{NPF}_6$ as the electrolyte.

III. DFT Calculation Results of Pt(II) Complexes in Ground States

i) Comparison of the optimized structure for **Pt1**, **Pt2**, **Pt3**, and **Pt4**

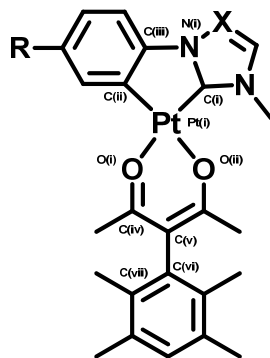
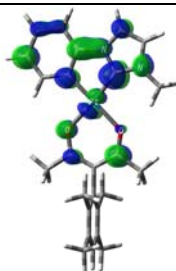
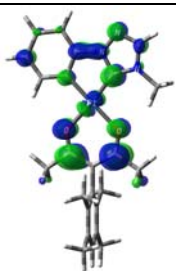
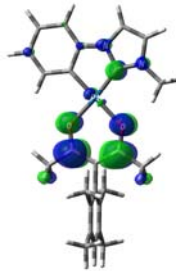
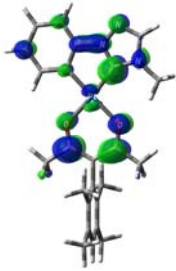
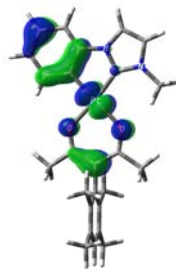
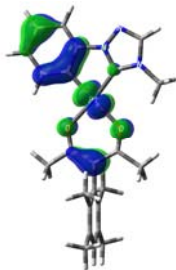
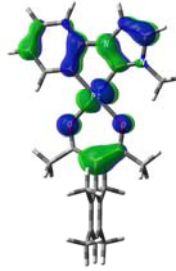
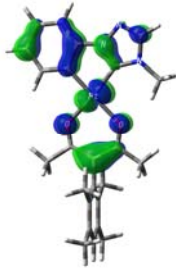
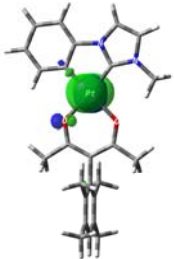
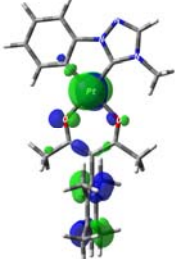
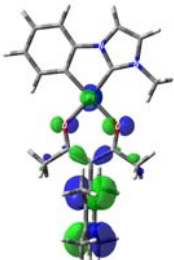
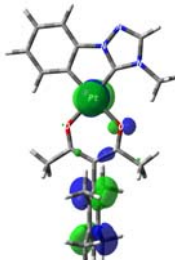
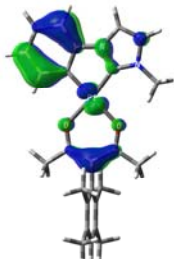
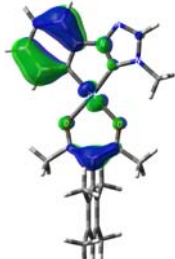


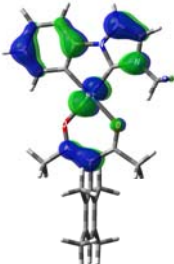
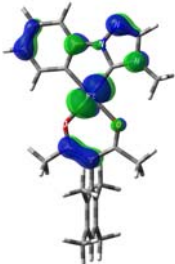
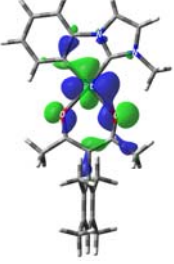
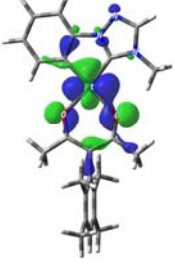
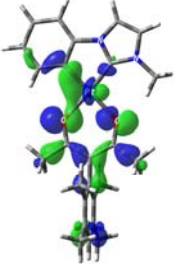
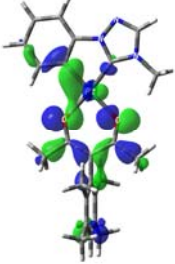
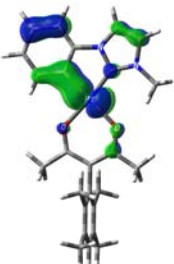
Table S1. Important bond lengths (Å), angle (°), and torsion angle (°) for the optimized structure.

	Pt1	Pt2	Pt3	Pt4
Pt(i)-C(i)	1.97093	1.96230	1.97082	1.96225
Pt(i)-C(ii)	2.00748	2.01583	2.00889	2.01735
Pt(i)-O(i)	2.08665	2.07778	2.08696	2.07765
Pt(i)-O(ii)	2.13994	2.13311	2.14369	2.13659
C(i)-Pt(i)-C(ii)	79.878	79.775	79.862	76.762
O(i)-Pt(i)-O(ii)	86.784	87.448	86.716	87.430
Pt(i)-C(i)-N(i)-C(iii)	0.000	0.001	-0.004	-0.005
N(i)-C(i)-Pt(i)-O(ii)	-179.999	-179.996	179.992	179.989
C(iv)-C(v)-C(vi)-C(vii)	89.901	89.902	-89.963	-89.970

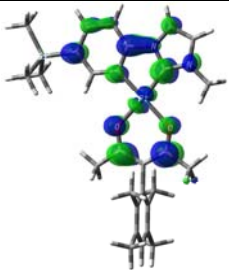
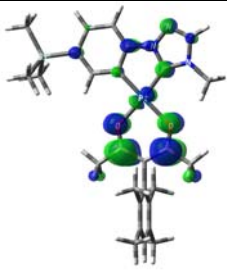
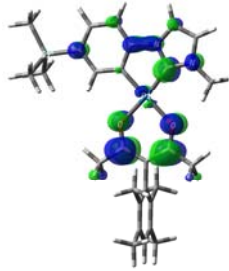
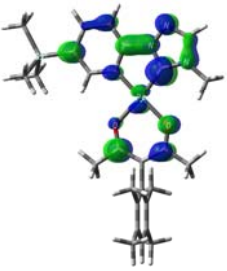
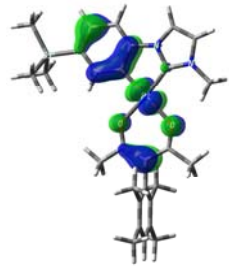
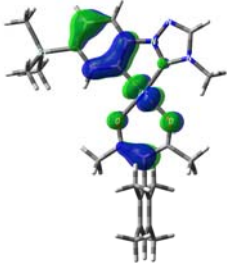
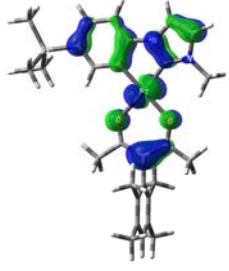
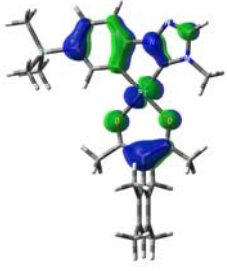
ii) Isodensity surface plots and energies for frontier orbitals of **Pt** complexes

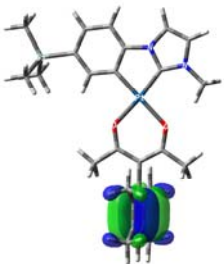
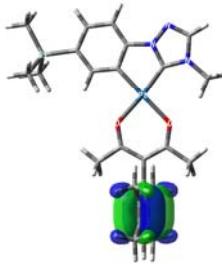
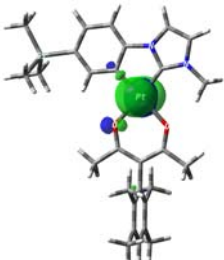
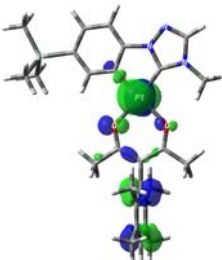
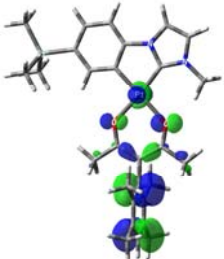
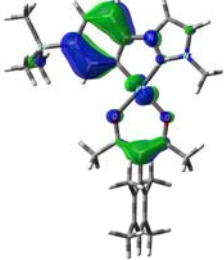
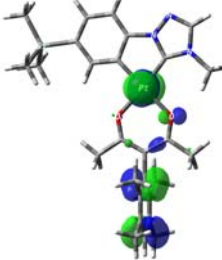
	Pt1	Pt2
LUMO+1	 -0.80 eV (Pt d orbital contribution: 4%)	 -0.97 eV (Pt d orbital contribution: 4%)
LUMO	 -0.95 eV (Pt d orbital contribution: 2%)	 -1.10 eV (Pt d orbital contribution: 2%)
HOMO	 -5.54 eV (Pt d orbital contribution: 28%)	 -5.65 eV (Pt d orbital contribution: 26%)
HOMO-1	 -5.66 eV (Pt d orbital contribution: 22%)	 -5.87 eV (Pt d orbital contribution: 17%)

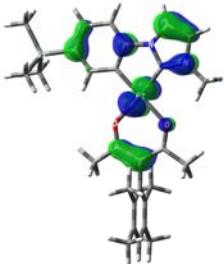
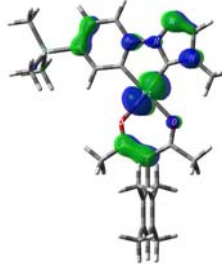
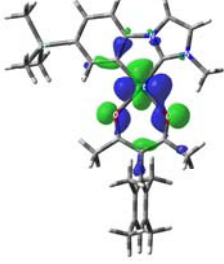
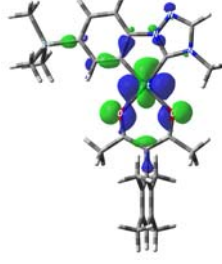
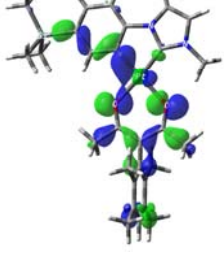
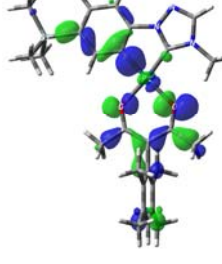
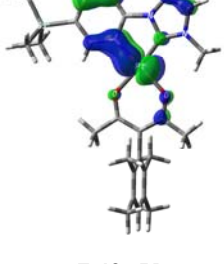
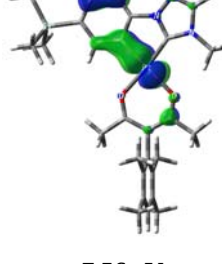
HOMO-2	 -5.97 eV	 -5.99 eV
HOMO-3	 -6.19 eV (Pt d orbital contribution: 68%)	 -6.24 eV (Pt d orbital contribution: 38%)
HOMO-4	 -6.23 eV (Pt d orbital contribution: 4%)	 -6.36 eV (Pt d orbital contribution: 33%)
HOMO-5	 -6.40 eV (Pt d orbital contribution: 9%)	 -6.50 eV (Pt d orbital contribution: 6%)

HOMO-6	 -6.57 eV (Pt d orbital contribution: 28%)	 -6.96 eV (Pt d orbital contribution: 50%)
HOMO-7	 -6.91 eV (Pt d orbital contribution: 55%)	 -7.03 eV (Pt d orbital contribution: 55%)
HOMO-8	 -7.11 eV (Pt d orbital contribution: 8%)	 -7.19 eV (Pt d orbital contribution: 6%)
HOMO-9	 -7.41 eV (Pt d orbital contribution: 48%)	 -7.58 eV (Pt d orbital contribution: 52%)

(isodensity contour = 0.04 au)

	Pt3	Pt4
LUMO+1	 -0.85 eV (Pt d orbital contribution: 4%)	 -0.98 eV (Pt d orbital contribution: 3%)
LUMO	 -0.96 eV (Pt d orbital contribution: 2%)	 -1.15 eV (Pt d orbital contribution: 3%)
HOMO	 -5.53 eV (Pt d orbital contribution: 28%)	 -5.65 eV (Pt d orbital contribution: 26%)
HOMO-1	 -5.65 eV (Pt d orbital contribution: 22%)	 -5.85 eV (Pt d orbital contribution: 16%)

HOMO-2	 -5.82 eV	 -5.99 eV
HOMO-3	 -6.19 eV (Pt d orbital contribution: 66%)	 -6.24 eV (Pt d orbital contribution: 38%)
HOMO-4	 -6.23 eV (Pt d orbital contribution: 5%)	 -6.36 eV (Pt d orbital contribution: 6%)
HOMO-5	 -6.35 eV (Pt d orbital contribution: 8%)	 -6.44 eV (Pt d orbital contribution: 32%)

HOMO-6	 -6.53 eV (Pt d orbital contribution: 30%)	 -6.93 eV (Pt d orbital contribution: 50%)
HOMO-7	 -6.89 eV (Pt d orbital contribution: 58%)	 -7.02 eV (Pt d orbital contribution: 58%)
HOMO-8	 -7.03 eV (Pt d orbital contribution: 5%)	 -7.11 eV (Pt d orbital contribution: 3%)
HOMO-9	 -7.40 eV (Pt d orbital contribution: 47%)	 -7.56 eV (Pt d orbital contribution: 51%)

(isodensity contour = 0.04 au)

IV. TD-DFT Calculation Results of Pt(II) Complexes

Table S2. TD-DFT calculated electronic transition configurations, excitation energy and oscillator strengths for the single and triplet transitions of **Pt1**.

Complex	Spin state	Transition configurations	Excitation energy (nm, eV)	Oscillator strength
Pt1	S ₁	HOMO-1 → LUMO (14%)	324.31 (3.82)	0.0032
		HOMO → LUMO (31%)		
		HOMO → LUMO+1 (42%)		
		HOMO-1 → LUMO+1 (9%)		
	S ₂	HOMO → LUMO (65%)	314.01 (3.95)	0.0127
		HOMO → LUMO+1 (21%)		
		HOMO-1 → LUMO (4%)		
		HOMO-1 → LUMO+1 (7%)		
	S ₃	HOMO-1 → LUMO (60%)	297.97 (4.16)	0.2788
		HOMO → LUMO+1 (29%)		
		HOMO-1 → LUMO+1 (7%)		
	S ₄	HOMO-3 → LUMO (97%)	291.67 (4.25)	0.0015
	S ₅	HOMO-1 → LUMO (18%)	290.35 (4.27)	0.0133
		HOMO-1 → LUMO+1 (72%)		
		HOMO-6 → LUMO (2%)		
		HOMO → LUMO+1 (4%)		
	S ₆	HOMO-4 → LUMO (29%)	281.41 (4.41)	0.0179
		HOMO-3 → LUMO+1 (62%)		
		HOMO-8 → LUMO (4%)		
	S ₇	HOMO-4 → LUMO (47%)	279.78 (4.43)	0.0028
		HOMO-4 → LUMO+1 (11%)		
		HOMO-3 → LUMO+1 (31%)		
		HOMO-8 → LUMO (6%)		
	S ₈	HOMO-2 → LUMO (92%)	274.92 (4.51)	0.0001
		HOMO-2 → LUMO+1 (8%)		
	S ₉	HOMO → LUMO+5 (80%)	268.64 (4.62)	0.0004
		HOMO-9 → LUMO+5 (3%)		
		HOMO → LUMO+4 (7%)		
	S ₁₀	HOMO-5 → LUMO+1 (25%)	264.20 (4.69)	0.0171
		HOMO → LUMO+2 (53%)		
		HOMO-5 → LUMO (6%)		
		HOMO-1 → LUMO+2 (9%)		
	T ₁	HOMO-1 → LUMO (34%)	422.77 (2.93)	0.0000
		HOMO → LUMO (42%)		
		HOMO-6 → LUMO (3%)		
		HOMO-5 → LUMO (7%)		
		HOMO-1 → LUMO+1 (6%)		
		HOMO → LUMO+1 (6%)		
	T ₂	HOMO-1 → LUMO-1 (23%)	388.70 (3.19)	0.0000
		HOMO → LUMO+1 (40%)		
		HOMO-5 → LUMO+2 (4%)		
		HOMO-1 → LUMO (7%)		
		HOMO → LUMO (9%)		
		HOMO → LUMO+6 (3%)		

Table S3. TD-DFT calculated electronic transition configurations, excitation energy and oscillator strengths for the single and triplet transitions of **Pt2**.

Complex	Spin state	Transition configurations	Excitation energy (nm, eV)	Oscillator strength
Pt2	S ₁	HOMO-1 → LUMO (12%)	334.02 (3.71)	0.0137
		HOMO → LUMO (61%)		
		HOMO → LUMO+1 (21%)		
	S ₂	HOMO → LUMO (34%)	313.36 (3.96)	0.0148
		HOMO → LUMO+1 (52%)		
		HOMO-1 → LUMO (7%)		
		HOMO-1 → LUMO+1 (4%)		
	S ₃	HOMO-1 → LUMO (65%)	299.75 (4.14)	0.2410
		HOMO → LUMO+1 (23%)		
		HOMO-1 → LUMO+1 (6%)		
	S ₄	HOMO-4 → LUMO (23%)	290.88 (4.26)	0.0075
		HOMO-3 → LUMO (72%)		
	S ₅	HOMO-1 → LUMO (10%)	285.28 (4.35)	0.0170
		HOMO-1 → LUMO+1 (81%)		
	S ₆	HOMO-4 → LUMO (19%)	284.18 (4.36)	0.0120
		HOMO-3 → LUMO+1 (68%)		
		HOMO-8 → LUMO (3%)		
		HOMO-4 → LUMO+1 (4%)		
	S ₇	HOMO-4 → LUMO (28%)	279.98 (4.43)	0.0005
		HOMO-4 → LUMO+1 (54%)		
		HOMO-8 → LUMO (3%)		
		HOMO-8 → LUMO+1 (3%)		
		HOMO-3 → LUMO (6%)		
	S ₈	HOMO-2 → LUMO (67%)	279.31 (4.44)	0.0002
		HOMO-2 → LUMO+1 (33%)		
	S ₉	HOMO-5 → LUMO (10%)	272.81 (4.54)	0.0186
		HOMO → LUMO+2 (74%)		
		HOMO-5 → LUMO+1 (8%)		
		HOMO-1 → LUMO+2 (4%)		
	S ₁₀	HOMO-5 → LUMO+4 (12%)	270.69 (4.58)	0.0002
		HOMO → LUMO+5 (75%)		
		HOMO-9 → LUMO+5 (3%)		
	T ₁	HOMO-1 → LUMO (21%)	421.71 (2.94)	0.0000
		HOMO-1 → LUMO+1 (22%)		
		HOMO → LUMO (26%)		
		HOMO → LUMO+1 (20%)		
		HOMO-5 → LUMO (4%)		
		HOMO-5 → LUMO+1 (4%)		
	T ₂	HOMO-1 → LUMO (20%)	399.66 (3.10)	0.0000
		HOMO-1 → LUMO+1 (10%)		
		HOMO → LUMO (28%)		
		HOMO → LUMO+1 (23%)		
		HOMO-5 → LUMO (2%)		
		HOMO-5 → LUMO+6 (3%)		
		HOMO → LUMO+6 (2%)		
		HOMO → LUMO+7 (2%)		

Table S4. TD-DFT calculated electronic transition configurations, excitation energy and oscillator strengths for the single and triplet transitions of **Pt3**.

Complex	Spin state	Transition configurations	Excitation energy (nm, eV)	Oscillator strength
Pt3	S ₁	HOMO-1 → LUMO (18%)	328.00 (3.78)	0.0078
		HOMO → LUMO (45%)		
		HOMO → LUMO+1 (28%)		
		HOMO-1 → LUMO+1 (5%)		
	S ₂	HOMO → LUMO (50%)	314.54 (3.94)	0.0088
		HOMO → LUMO+1 (32%)		
		HOMO-1 → LUMO (8%)		
		HOMO-1 → LUMO+1 (6%)		
	S ₃	HOMO-1 → LUMO (55%)	301.71 (4.11)	0.2704
		HOMO → LUMO+1 (34%)		
		HOMO-1 → LUMO+1 (7%)		
	S ₄	HOMO-3 → LUMO (94%)	292.69 (4.24)	0.0030
		HOMO-3 → LUMO+1 (3%)		
	S ₅	HOMO-1 → LUMO (16%)	291.58 (4.25)	0.0078
		HOMO-1 → LUMO+1 (77%)		
		HOMO-6 → LUMO (2%)		
	S ₆	HOMO-3 → LUMO+1 (86%)	284.44 (4.36)	0.0164
		HOMO-4 → LUMO (7%)		
		HOMO-3 → LUMO (3%)		
	S ₇	HOMO-4 → LUMO (55%)	280.43 (4.42)	0.0000
		HOMO-4 → LUMO+1 (25%)		
		HOMO-8 → LUMO (8%)		
		HOMO-8 → LUMO+1 (3%)		
	S ₈	HOMO-3 → LUMO+1 (6%)	275.21 (4.51)	0.0001
		HOMO-2 → LUMO (78%)		
	S ₉	HOMO-2 → LUMO+1 (22%)	269.15 (4.61)	0.0002
		HOMO → LUMO+5 (79%)		
		HOMO-9 → LUMO+5 (3%)		
	S ₁₀	HOMO → LUMO+4 (8%)	267.92 (4.63)	0.0106
		HOMO-5 → LUMO (16%)		
		HOMO-5 → LUMO+1 (22%)		
		HOMO-1 → LUMO+2 (10%)		
	T ₁	HOMO-1 → LUMO+2 (46%)	422.98 (2.93)	0.0000
		HOMO-1 → LUMO (25%)		
		HOMO-1 → LUMO+1 (13%)		
		HOMO → LUMO (34%)		
		HOMO → LUMO+1 (15%)		
		HOMO-6 → LUMO (3%)		
	T ₂	HOMO-5 → LUMO (5%)	395.03 (3.14)	0.0000
		HOMO-5 → LUMO+1 (3%)		
		HOMO-1 → LUMO (14%)		
		HOMO-1 → LUMO+1 (18%)		
		HOMO → LUMO (18%)		
		HOMO → LUMO+1 (30%)		
		HOMO-5 → LUMO+2 (3%)		
		HOMO → LUMO+6 (2%)		

Table S5. TD-DFT calculated electronic transition configurations, excitation energy and oscillator strengths for the single and triplet transitions of **Pt4**.

Complex	Spin state	Transition configurations	Excitation energy (nm, eV)	Oscillator strength
Pt4	S ₁	HOMO-1 → LUMO (13%) HOMO → LUMO (73%) HOMO → LUMO+1 (9%)	337.70 (3.67)	0.0184
	S ₂	HOMO-1 → LUMO (15%) HOMO → LUMO (20%) HOMO → LUMO+1 (59%) HOMO-1 → LUMO+1 (3%)	314.03 (3.95)	0.0132
	S ₃	HOMO-1 → LUMO (64%) HOMO → LUMO+1 (28%) HOMO → LUMO (3%)	303.99 (4.08)	0.2363
	S ₄	HOMO-5 → LUMO (27%) HOMO-3 → LUMO (59%)	293.40 (4.23)	0.0102
	S ₅	HOMO-1 → LUMO+1 (89%) HOMO-1 → LUMO (4%)	286.24 (4.33)	0.0195
	S ₆	HOMO-5 → LUMO (11%) HOMO-3 → LUMO+1 (3%) HOMO-5 → LUMO+1 (2%)	285.72 (4.34)	0.0075
	S ₇	HOMO-5 → LUMO (20%) HOMO-5 → LUMO+1 (64%) HOMO-8 → LUMO (3%) HOMO-8 → LUMO+1 (5%) HOMO-3 → LUMO (5%)	280.40 (4.42)	0.0000
	S ₈	HOMO-2 → LUMO (51%) HOMO-2 → LUMO+1 (49%)	279.67 (4.43)	0.0002
	S ₉	HOMO-4 → LUMO (23%) HOMO → LUMO+2 (60%) HOMO-4 → LUMO+1 (6%) HOMO-1 → LUMO+2 (5%)	275.19 (4.51)	0.0118
	S ₁₀	HOMO → LUMO+4 (13%) HOMO → LUMO+5 (72%) HOMO-9 → LUMO+5 (3%) HOMO-7 → LUMO (4%)	271.25 (4.57)	0.0001
	T ₁	HOMO-1 → LUMO (12%) HOMO-1 → LUMO+1 (30%) HOMO → LUMO (17%) HOMO → LUMO+1 (29%) HOMO-4 → LUMO (2%) HOMO-4 → LUMO+1 (7%)	421.97 (2.94)	0.0000
	T ₂	HOMO-1 → LUMO (27%) HOMO → LUMO (37%) HOMO → LUMO+1 (14%) HOMO-4 → LUMO (3%) HOMO-4 → LUMO+6 (3%) HOMO-1 → LUMO+1 (5%) HOMO → LUMO+7 (2%)	405.64 (3.06)	0.0000

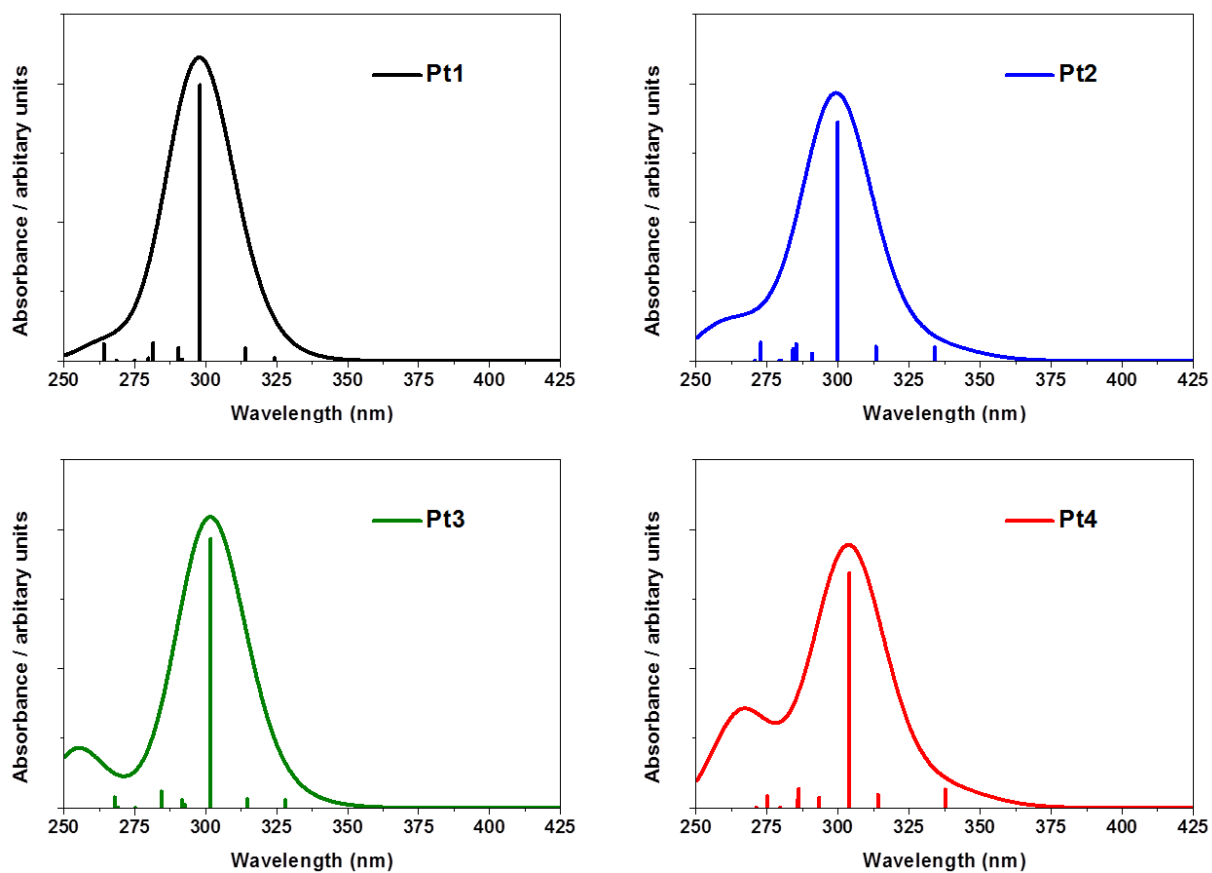


Fig S2. The calculated UV-Vis spectra of the Pt complexes.

V. OLED Data

i) Pt1 & 26mCPy

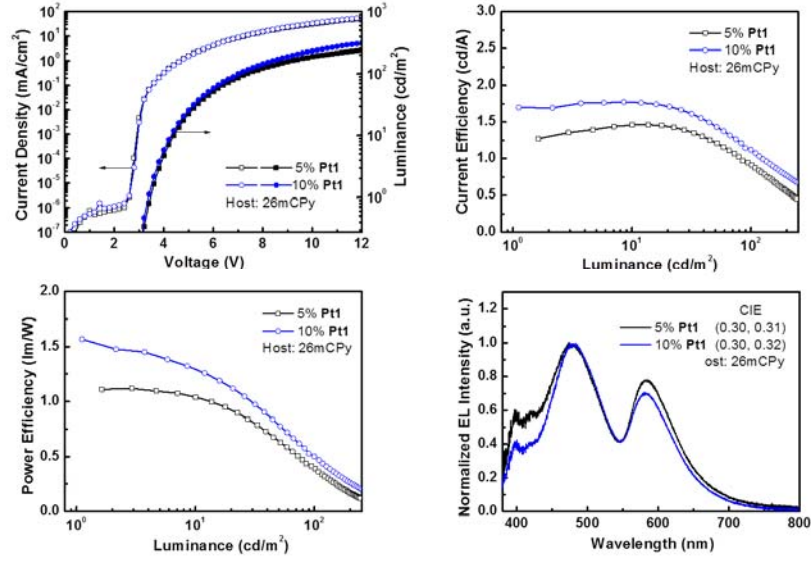


Fig S3. Luminance efficiency 26mCpy host devices for **Pt1**.

ii) Pt1 & POPCPA

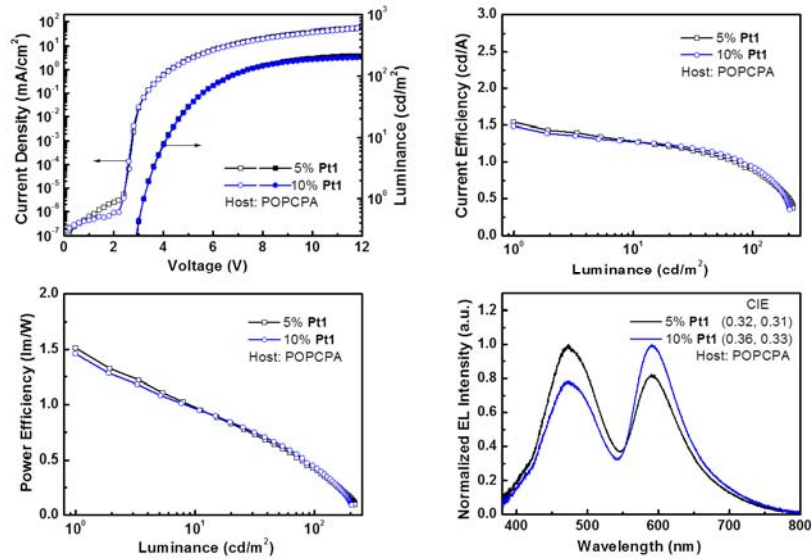


Fig S4. Luminance efficiency POPCPA host devices for **Pt1**.

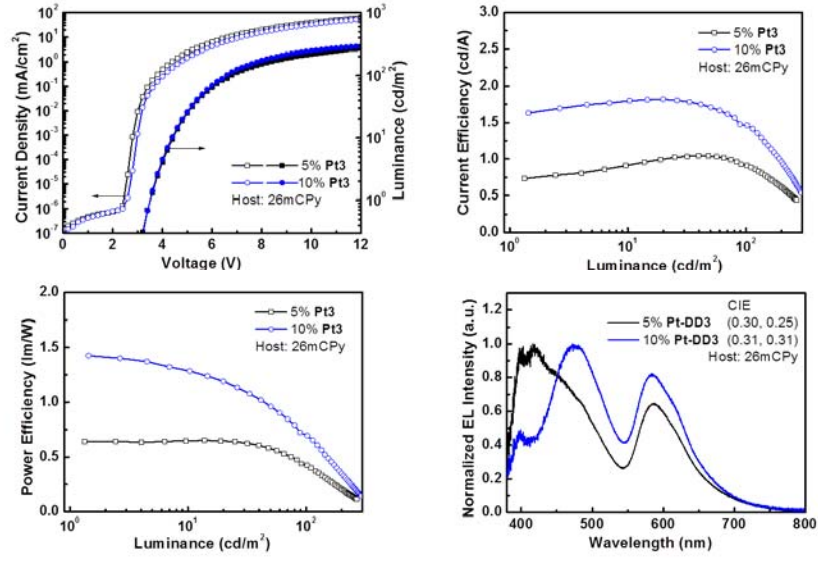
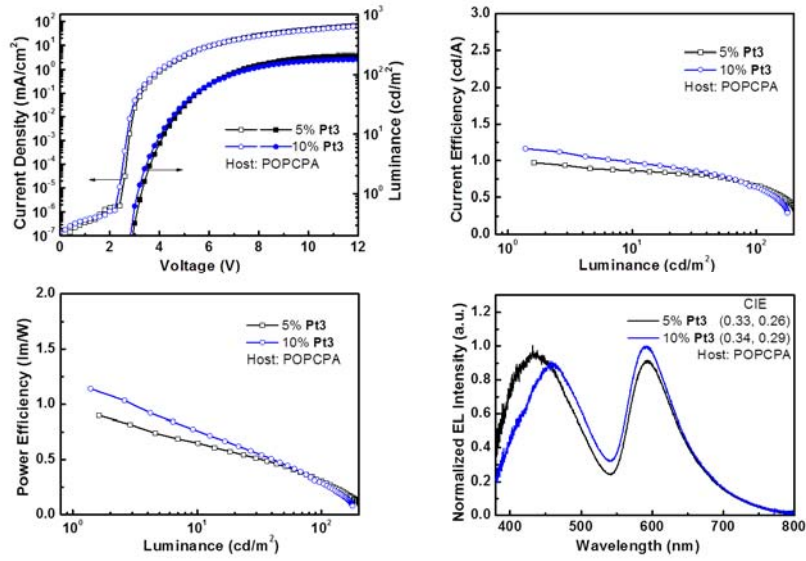
iii) **Pt3** & 26mCPyFig S5. Luminance efficiency 26mCpy host devices for **Pt3**.iv) **Pt3** & POPCPAFig S6. Luminance efficiency POPCPA host devices for **Pt3**.

Table S6. OLEDs characteristics for **Pt1** and **Pt3**.

Device	Host	EL			CIE (x,y)
		$\lambda_{\max}$ [nm] ^a	V_{on} [V] ^a	L [cd/m ² , V] ^b	
5% Pt1	POPCPA	473, 590	3.2	218, 12	(0.32, 0.31)
	26mCpy	400, 473, 590	3.6	242, 12	(0.30, 0.31)
10% Pt1	POPCPA	473, 590	3.2	203, 12	(0.36, 0.33)
	26mCpy	400, 475, 590	3.4	314, 12	(0.30, 0.32)
5% Pt3	POPCPA	431, 590	3.4	206, 12	(0.33, 0.26)
	26mCpy	400, 416, 585	3.6	269, 12	(0.34, 0.29)
10% Pt3	POPCPA	457, 592	3.2	178, 12	(0.30, 0.25)
	26mCpy	400, 472, 585	3.6	295, 12	(0.31, 0.31)

^a Value taken at I = 20 mA. ^b The applied voltage (V_{on}) is defined as brightness of 1 cd/m². ^c The luminance (L) is the maximum value.

VI. Phosphorescent Spectra of in the Solid State

i) **Pt1** (Neat and 50% POPCPA)

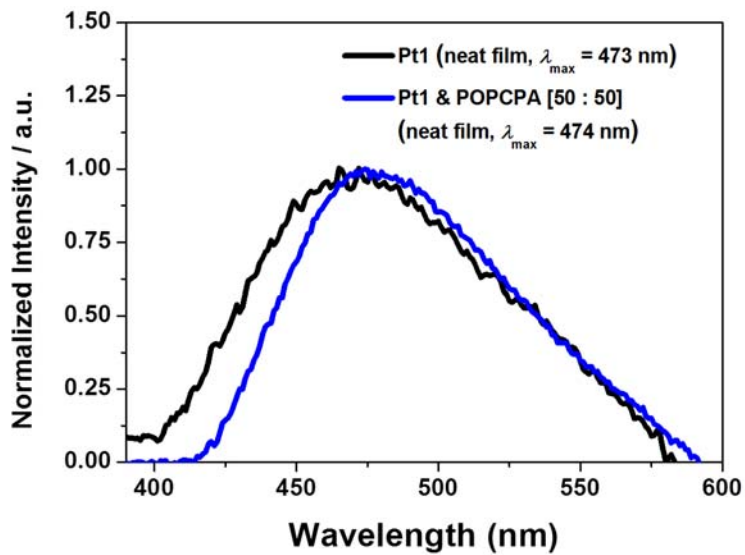


Fig S7. Emission spectra of **Pt1** (neat and 50% POPCPA).

ii) **Pt3** (Neat and 50% POPCPA)

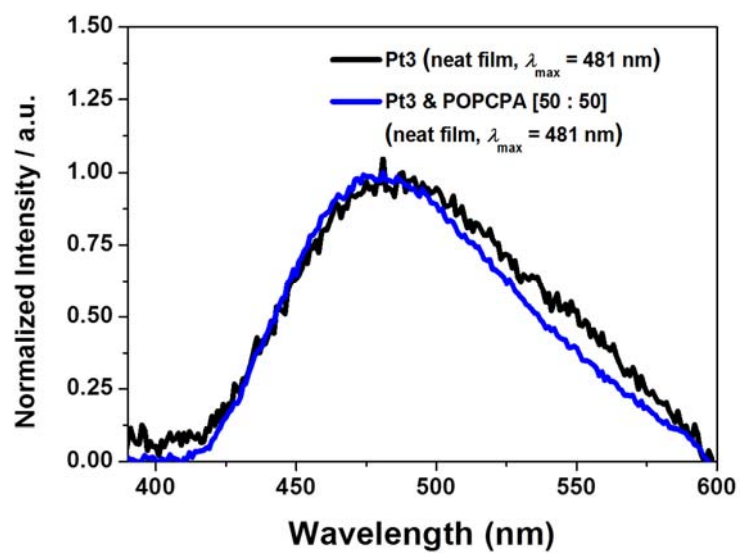


Fig S8. Emission spectra of **Pt3** (neat and 50% POPCPA).

VII. X-Ray Crystal Data

Single crystals of **Pt1** and **Pt3** were mounted on glass fibers and were collected on a Bruker Apex II single-crystal X-ray diffractometer with graphite-monochromated Mo K α radiation, operating at 50 kV and 30 mA and at 180 K. Data were processed on a PC with the aid of the Bruker SHELXTL software package (version 6.10)¹ and corrected for absorption effects. **Pt1** and **Pt3** belong to the triclinic crystal space group P-1 and the monoclinic space group P2₁/n, respectively. A methanol solvent molecule was located in the crystal lattice of **Pt1** and refined successfully. For **Pt3**, there are three independent molecules in the asymmetric unit. All non-hydrogen atoms were refined anisotropically. Complete crystal structure data can be found in the Supporting Information. The crystal data of **Pt1** and **Pt3** have been deposited at the Cambridge Crystallographic Data Center (CCDC No. 1013934 and 1013976, respectively).

i) **Pt1**

Table 1. Crystal data and structure refinement for Pt1.

Identification code	ko9	
Empirical formula	C ₂₆ H ₃₂ N ₂ O ₃ Pt	
Formula weight	615.63	
Temperature	180(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 8.5714(11) Å	$\alpha = 77.8100(10)^\circ$.
	b = 10.4125(13) Å	$\beta = 78.4930(10)^\circ$.
	c = 14.2062(18) Å	$\gamma = 82.4880(10)^\circ$.
Volume	1209.2(3) Å ³	
Z	2	
Density (calculated)	1.691 Mg/m ³	
Absorption coefficient	5.831 mm ⁻¹	
F(000)	608	
Crystal size	0.20 x 0.20 x 0.05 mm ³	
Theta range for data collection	1.49 to 26.50°.	
Index ranges	-10 ≤ h ≤ 10, -13 ≤ k ≤ 13, -17 ≤ l ≤ 17	
Reflections collected	12953	
Independent reflections	4962 [R(int) = 0.0206]	
Completeness to theta = 26.50°	99.1 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7592 and 0.3884	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	4962 / 0 / 300	
Goodness-of-fit on F ²	1.106	
Final R indices [I > 2sigma(I)]	R1 = 0.0185, wR2 = 0.0400	
R indices (all data)	R1 = 0.0211, wR2 = 0.0410	
Largest diff. peak and hole	0.705 and -0.390 e.Å ⁻³	

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for Pt1. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Pt(1)	7926(1)	845(1)	1530(1)	22(1)
O(1)	7928(2)	994(2)	2936(1)	29(1)
O(2)	9347(2)	2410(2)	1063(1)	26(1)
O(3)	5158(3)	3125(2)	834(2)	50(1)
N(1)	7049(3)	-584(2)	251(2)	24(1)
N(2)	8291(3)	999(2)	-701(2)	24(1)
C(1)	7812(3)	486(3)	252(2)	23(1)
C(2)	7839(3)	248(3)	-1282(2)	30(1)
C(3)	7057(3)	-734(3)	-696(2)	27(1)
C(4)	9123(4)	2189(3)	-1072(2)	32(1)
C(5)	6575(3)	-665(3)	1943(2)	25(1)
C(6)	5850(3)	-1204(3)	2885(2)	29(1)
C(7)	4933(3)	-2267(3)	3047(2)	31(1)
C(8)	4742(3)	-2828(3)	2282(2)	32(1)
C(9)	5460(3)	-2323(3)	1325(2)	28(1)
C(10)	6338(3)	-1256(3)	1189(2)	24(1)
C(11)	8463(4)	1602(3)	4323(2)	39(1)
C(12)	8707(3)	1765(3)	3226(2)	26(1)
C(13)	9713(3)	2702(3)	2635(2)	23(1)
C(14)	9969(3)	2960(3)	1600(2)	24(1)
C(15)	11063(4)	3992(3)	1034(2)	32(1)
C(16)	10552(3)	3494(3)	3127(2)	25(1)
C(17)	12019(3)	2974(3)	3409(2)	27(1)
C(18)	12805(3)	3749(3)	3834(2)	31(1)
C(19)	12126(4)	4987(3)	3957(2)	34(1)
C(20)	10671(4)	5525(3)	3679(2)	30(1)
C(21)	9858(3)	4760(3)	3271(2)	26(1)
C(22)	12765(4)	1624(3)	3261(2)	39(1)
C(23)	14381(4)	3219(4)	4177(3)	51(1)
C(24)	10016(4)	6901(3)	3833(2)	42(1)
C(25)	8248(4)	5295(3)	3001(2)	38(1)
C(26)	5467(4)	4212(3)	1200(3)	45(1)

Table 3. Bond lengths [$\text{\AA}$] and angles [$^\circ$] for Pt1.

Pt(1)-C(1)	1.953(3)	C(12)-C(13)	1.409(4)
Pt(1)-C(5)	1.993(3)	C(13)-C(14)	1.414(4)
Pt(1)-O(1)	2.0360(18)	C(13)-C(16)	1.512(3)
Pt(1)-O(2)	2.0779(18)	C(14)-C(15)	1.510(4)
O(1)-C(12)	1.284(3)	C(15)-H(15A)	0.9800
O(2)-C(14)	1.274(3)	C(15)-H(15B)	0.9800
O(3)-C(26)	1.416(4)	C(15)-H(15C)	0.9800
O(3)-H(3)	0.8400	C(16)-C(17)	1.402(4)
N(2)-C(1)	1.364(3)	C(16)-C(21)	1.412(4)
N(2)-C(3)	1.386(3)	C(17)-C(18)	1.408(4)
N(2)-C(10)	1.424(3)	C(17)-C(22)	1.505(4)
N(1)-C(1)	1.348(3)	C(18)-C(19)	1.374(4)
N(1)-C(2)	1.387(3)	C(18)-C(23)	1.523(4)
N(1)-C(4)	1.458(3)	C(19)-C(20)	1.395(4)
C(2)-C(3)	1.336(4)	C(19)-H(19A)	0.9500
C(2)-H(2A)	0.9500	C(20)-C(21)	1.399(4)
C(3)-H(3A)	0.9500	C(20)-C(24)	1.512(4)
C(4)-H(4A)	0.9800	C(21)-C(25)	1.511(4)
C(4)-H(4B)	0.9800	C(22)-H(22A)	0.9800
C(4)-H(4C)	0.9800	C(22)-H(22B)	0.9800
C(5)-C(6)	1.391(4)	C(22)-H(22C)	0.9800
C(5)-C(10)	1.402(4)	C(23)-H(23A)	0.9800
C(6)-C(7)	1.394(4)	C(23)-H(23B)	0.9800
C(6)-H(6A)	0.9500	C(23)-H(23C)	0.9800
C(7)-C(8)	1.384(4)	C(24)-H(24A)	0.9800
C(7)-H(7A)	0.9500	C(24)-H(24B)	0.9800
C(8)-C(9)	1.397(4)	C(24)-H(24C)	0.9800
C(8)-H(8A)	0.9500	C(25)-H(25A)	0.9800
C(9)-C(10)	1.381(4)	C(25)-H(25B)	0.9800
C(9)-H(9A)	0.9500	C(25)-H(25C)	0.9800
C(11)-C(12)	1.507(4)	C(26)-H(26A)	0.9800
C(11)-H(11A)	0.9800	C(26)-H(26B)	0.9800
C(11)-H(11B)	0.9800	C(26)-H(26C)	0.9800
C(11)-H(11C)	0.9800		

C(1)-Pt(1)-C(5)	79.99(11)	C(5)-C(6)-C(7)	120.6(3)
C(1)-Pt(1)-O(1)	172.68(9)	C(5)-C(6)-H(6A)	119.7
C(5)-Pt(1)-O(1)	92.87(9)	C(7)-C(6)-H(6A)	119.7
C(1)-Pt(1)-O(2)	98.55(9)	C(8)-C(7)-C(6)	121.1(3)
C(5)-Pt(1)-O(2)	178.51(9)	C(8)-C(7)-H(7A)	119.4
O(1)-Pt(1)-O(2)	88.59(7)	C(6)-C(7)-H(7A)	119.4
C(12)-O(1)-Pt(1)	127.17(18)	C(7)-C(8)-C(9)	120.1(3)
C(14)-O(2)-Pt(1)	126.59(18)	C(7)-C(8)-H(8A)	119.9
C(26)-O(3)-H(3)	109.5	C(9)-C(8)-H(8A)	119.9
C(1)-N(2)-C(3)	110.9(2)	C(10)-C(9)-C(8)	117.2(3)
C(1)-N(2)-C(10)	115.6(2)	C(10)-C(9)-H(9A)	121.4
C(3)-N(2)-C(10)	133.3(2)	C(8)-C(9)-H(9A)	121.4
C(1)-N(1)-C(2)	110.0(2)	C(9)-C(10)-C(5)	124.6(3)
C(1)-N(1)-C(4)	125.3(2)	C(9)-C(10)-N(2)	123.5(2)
C(2)-N(1)-C(4)	124.7(2)	C(5)-C(10)-N(2)	111.8(2)
N(1)-C(1)-N(2)	104.9(2)	C(12)-C(11)-H(11A)	109.5
N(1)-C(1)-Pt(1)	138.5(2)	C(12)-C(11)-H(11B)	109.5
N(1)-C(1)-Pt(1)	116.6(2)	H(11A)-C(11)-H(11B)	109.5
C(3)-C(2)-N(1)	108.2(2)	C(12)-C(11)-H(11C)	109.5
C(3)-C(2)-H(2A)	125.9	H(11A)-C(11)-H(11C)	109.5
N(1)-C(2)-H(2A)	125.9	H(11B)-C(11)-H(11C)	109.5
C(2)-C(3)-N(2)	106.0(2)	O(1)-C(12)-C(13)	127.1(3)
C(2)-C(3)-H(3A)	127.0	O(1)-C(12)-C(11)	113.4(2)
N(2)-C(3)-H(3A)	127.0	C(13)-C(12)-C(11)	119.5(2)
N(1)-C(4)-H(4A)	109.5	C(12)-C(13)-C(14)	123.6(2)
N(1)-C(4)-H(4B)	109.5	C(12)-C(13)-C(16)	118.6(2)
H(4A)-C(4)-H(4B)	109.5	C(14)-C(13)-C(16)	117.8(2)
N(2)-C(4)-H(4C)	109.5	O(2)-C(14)-C(13)	126.6(2)
H(4A)-C(4)-H(4C)	109.5	O(2)-C(14)-C(15)	113.9(2)
H(4B)-C(4)-H(4C)	109.5	C(13)-C(14)-C(15)	119.5(2)
C(6)-C(5)-C(10)	116.3(2)	C(14)-C(15)-H(15A)	109.5
C(6)-C(5)-Pt(1)	128.0(2)	C(14)-C(15)-H(15B)	109.5
C(10)-C(5)-Pt(1)	115.7(2)	H(15A)-C(15)-H(15B)	109.5

C(14)-C(15)-H(15C)	109.5	H(22B)-C(22)-H(22C)	109.5
H(15A)-C(15)-H(15C)	109.5	C(18)-C(23)-H(23A)	109.5
H(15B)-C(15)-H(15C)	109.5	C(18)-C(23)-H(23B)	109.5
C(17)-C(16)-C(21)	121.4(2)	H(23A)-C(23)-H(23B)	109.5
C(17)-C(16)-C(13)	119.5(2)	C(18)-C(23)-H(23C)	109.5
C(21)-C(16)-C(13)	119.1(2)	H(23A)-C(23)-H(23C)	109.5
C(16)-C(17)-C(18)	118.5(3)	H(23B)-C(23)-H(23C)	109.5
C(16)-C(17)-C(22)	121.7(3)	C(20)-C(24)-H(24A)	109.5
C(18)-C(17)-C(22)	119.8(3)	C(20)-C(24)-H(24B)	109.5
C(19)-C(18)-C(17)	119.5(3)	H(24A)-C(24)-H(24B)	109.5
C(19)-C(18)-C(23)	119.8(3)	C(20)-C(24)-H(24C)	109.5
C(17)-C(18)-C(23)	120.6(3)	H(24A)-C(24)-H(24C)	109.5
C(18)-C(19)-C(20)	122.9(3)	H(24B)-C(24)-H(24C)	109.5
C(18)-C(19)-H(19A)	118.5	C(21)-C(25)-H(25A)	109.5
C(20)-C(19)-H(19A)	118.5	C(21)-C(25)-H(25B)	109.5
C(19)-C(20)-C(21)	118.4(3)	H(25A)-C(25)-H(25B)	109.5
C(19)-C(20)-C(24)	119.5(3)	C(21)-C(25)-H(25C)	109.5
C(21)-C(20)-C(24)	122.2(3)	H(25A)-C(25)-H(25C)	109.5
C(20)-C(21)-C(16)	119.3(3)	H(25B)-C(25)-H(25C)	109.5
C(20)-C(21)-C(25)	119.5(3)	O(3)-C(26)-H(26A)	109.5
C(16)-C(21)-C(25)	121.2(2)	O(3)-C(26)-H(26B)	109.5
C(17)-C(22)-H(22A)	109.5	H(26A)-C(26)-H(26B)	109.5
C(17)-C(22)-H(22B)	109.5	O(3)-C(26)-H(26C)	109.5
H(22A)-C(22)-H(22B)	109.5	H(26A)-C(26)-H(26C)	109.5
C(17)-C(22)-H(22C)	109.5	H(26B)-C(26)-H(26C)	109.5
H(22A)-C(22)-H(22C)	109.5		

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for Pt1. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12}]$

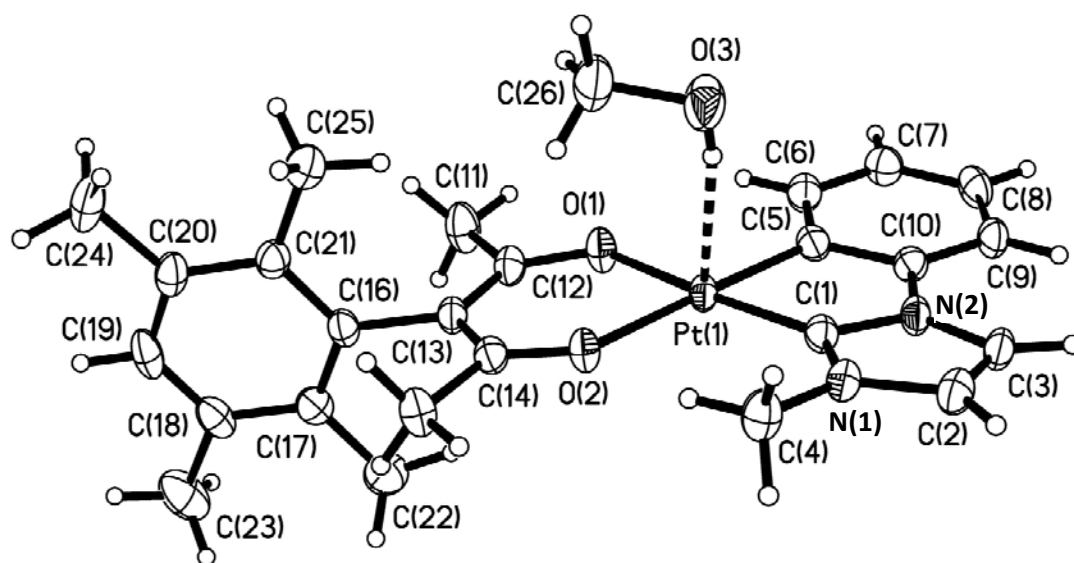
	U ¹¹	U ²²	U ³³	U ²³	U ¹³	U ¹²
Pt(1)	25(1)	19(1)	25(1)	-7(1)	-8(1)	-4(1)

O(1)	38(1)	30(1)	24(1)	-6(1)	-7(1)	-14(1)
O(2)	31(1)	26(1)	26(1)	-7(1)	-9(1)	-9(1)
O(3)	52(2)	32(1)	78(2)	-24(1)	-39(1)	11(1)
N(1)	29(1)	22(1)	24(1)	-7(1)	-8(1)	-2(1)
N(2)	27(1)	21(1)	29(1)	-9(1)	-9(1)	-4(1)
C(1)	24(1)	20(1)	28(2)	-7(1)	-9(1)	0(1)
C(2)	36(2)	29(2)	27(2)	-10(1)	-10(1)	-1(1)
C(3)	31(2)	25(2)	31(2)	-14(1)	-12(1)	0(1)
C(4)	43(2)	28(2)	28(2)	-5(1)	-6(1)	-10(1)
C(5)	24(1)	22(1)	31(2)	-5(1)	-9(1)	-2(1)
C(6)	31(2)	27(2)	31(2)	-8(1)	-8(1)	-3(1)
C(7)	33(2)	30(2)	30(2)	-4(1)	-4(1)	-7(1)
C(8)	32(2)	24(2)	42(2)	-4(1)	-11(1)	-11(1)
C(9)	31(2)	22(2)	34(2)	-9(1)	-8(1)	-6(1)
C(10)	24(1)	20(1)	29(2)	-6(1)	-7(1)	0(1)
C(11)	50(2)	45(2)	27(2)	-8(1)	-8(1)	-21(2)
C(12)	31(2)	24(2)	26(2)	-7(1)	-11(1)	-3(1)
C(13)	24(1)	20(1)	28(2)	-8(1)	-9(1)	-2(1)
C(14)	23(1)	19(1)	33(2)	-6(1)	-11(1)	0(1)
C(15)	36(2)	30(2)	32(2)	-4(1)	-10(1)	-11(1)
C(16)	26(1)	29(2)	22(1)	-7(1)	-4(1)	-9(1)
C(17)	28(2)	34(2)	20(1)	-5(1)	-4(1)	-6(1)
C(18)	29(2)	46(2)	21(1)	-3(1)	-5(1)	-14(1)
C(19)	43(2)	44(2)	20(1)	-6(1)	-3(1)	-27(2)
C(20)	40(2)	30(2)	21(1)	-9(1)	5(1)	-16(1)
C(21)	29(2)	27(2)	23(1)	-7(1)	-1(1)	-7(1)
C(22)	36(2)	44(2)	40(2)	-11(2)	-16(2)	5(2)
C(23)	39(2)	76(3)	42(2)	-6(2)	-19(2)	-15(2)
C(24)	66(2)	32(2)	29(2)	-13(1)	4(2)	-21(2)
C(25)	36(2)	31(2)	51(2)	-14(2)	-10(2)	-2(1)
C(26)	51(2)	35(2)	58(2)	-20(2)	-17(2)	-7(2)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^{-3}$) for Pt1.

	x	y	z	U(eq)
H(3)	5852	2493	951	60
H(2A)	8048	405	-1977	35
H(3A)	6600	-1399	-889	32
H(4A)	9307	2544	-522	49
H(4B)	8470	2848	-1466	49
H(4C)	10152	1973	-1479	49
H(6A)	5980	-844	3423	35
H(7A)	4431	-2613	3694	37
H(8A)	4121	-3557	2407	38
H(9A)	5348	-2697	790	33
H(11A)	7667	972	4624	58
H(11B)	8085	2456	4514	58
H(11C)	9478	1272	4546	58
H(15A)	11223	3973	335	47
H(15B)	12096	3809	1255	47
H(15C)	10579	4866	1145	47
H(19A)	12672	5498	4245	41
H(22A)	12024	1185	3019	59
H(22B)	12997	1100	3885	59
H(22C)	13761	1708	2783	59
H(23A)	14799	3914	4399	76
H(23B)	15153	2937	3634	76
H(23C)	14204	2465	4718	76
H(24A)	9476	7349	3290	62
H(24B)	10896	7399	3858	62
H(24C)	9252	6845	4450	62
H(25A)	7778	4604	2806	57
H(25B)	8381	6048	2455	57
H(25C)	7539	5581	3566	57

H(26A)	4756	4987	981	89(15)
H(26B)	6582	4400	957	100(16)
H(26C)	5276	4001	1917	115(19)



ii) **Pt-3**

Table 1. Crystal data and structure refinement for Pt3.

Identification code	ko9a	
Empirical formula	C ₈₄ H ₁₀₈ N ₆ O ₆ Pt ₃ Si ₃	
Formula weight	1967.30	
Temperature	180(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/n	
Unit cell dimensions	a = 24.1524(8) Å	$\alpha = 90^\circ$.
	b = 13.0815(4) Å	$\beta = 101.612(2)^\circ$.
	c = 27.3864(9) Å	$\gamma = 90^\circ$.
Volume	8475.6(5) Å ³	
Z	4	
Density (calculated)	1.542 Mg/m ³	
Absorption coefficient	5.034 mm ⁻¹	
F(000)	3912	
Crystal size	0.26 x 0.26 x 0.21 mm ³	
Theta range for data collection	1.03 to 26.73°	
Index ranges	-26 ≤ h ≤ 30, -16 ≤ k ≤ 16, -34 ≤ l ≤ 34	
Reflections collected	74804	
Independent reflections	17996 [R(int) = 0.0490]	
Completeness to theta = 26.73°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.4207 and 0.3533	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	17996 / 0 / 949	
Goodness-of-fit on F ²	1.136	
Final R indices [I > 2σ(I)]	R1 = 0.0645, wR2 = 0.1563	
R indices (all data)	R1 = 0.0837, wR2 = 0.1648	
Largest diff. peak and hole	6.135 and -1.753 e.Å ⁻³	

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for Pt3. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	$U(\text{eq})$
Pt(1)	7827(1)	4574(1)	3558(1)	27(1)
Pt(2)	9370(1)	1167(1)	2091(1)	27(1)
Pt(3)	8724(1)	6129(1)	9378(1)	30(1)
Si(1)	7729(1)	6965(3)	7274(1)	36(1)
Si(2)	8323(1)	3583(2)	5689(1)	35(1)
Si(3)	10315(1)	1780(2)	4225(1)	36(1)
O(1)	7893(3)	5771(6)	9202(2)	33(2)
O(2)	8716(3)	5674(6)	10103(3)	41(2)
O(3)	8637(3)	4888(6)	3903(2)	33(2)
O(4)	8029(3)	5098(6)	2900(2)	37(2)
O(5)	10155(3)	575(5)	2294(2)	30(2)
O(6)	9366(3)	647(6)	1369(3)	36(2)
N(1)	9974(4)	6591(9)	9823(4)	52(3)
N(2)	9685(4)	6861(7)	9038(3)	37(2)
N(3)	6667(4)	4132(7)	2877(3)	35(2)
N(4)	6780(3)	3696(7)	3647(3)	33(2)
N(5)	8206(4)	2002(7)	1596(3)	40(2)
N(6)	8482(4)	2277(7)	2381(3)	37(2)
C(1)	9511(4)	6517(9)	9451(4)	35(2)
C(2)	10423(5)	6979(12)	9633(5)	63(4)
C(3)	10253(5)	7158(10)	9150(5)	50(3)
C(4)	10003(6)	6286(14)	10337(5)	75(5)
C(5)	9261(4)	6914(7)	8596(4)	30(2)
C(6)	8746(4)	6548(7)	8697(3)	26(2)
C(7)	8293(4)	6594(8)	8270(3)	29(2)
C(8)	8352(4)	6955(8)	7795(4)	32(2)
C(9)	8882(5)	7294(8)	7751(4)	37(2)
C(10)	9343(4)	7252(8)	8149(4)	36(2)

C(11)	6986(4)	5160(9)	9228(4)	38(2)
C(12)	7590(4)	5348(8)	9485(4)	30(2)
C(13)	7758(5)	5090(8)	9988(4)	34(2)
C(14)	8313(5)	5270(9)	10269(4)	44(3)
C(15)	8453(6)	4967(13)	10815(4)	64(4)
C(16)	7336(5)	4535(8)	10236(4)	34(2)
C(17)	7261(5)	3489(8)	10162(4)	35(2)
C(18)	6871(5)	2947(7)	10375(4)	33(2)
C(19)	6569(5)	3517(7)	10661(4)	33(2)
C(20)	6633(5)	4570(8)	10733(4)	38(3)
C(21)	7022(5)	5073(7)	10529(4)	36(2)
C(22)	7088(6)	6218(9)	10604(5)	55(4)
C(23)	6271(6)	5122(10)	11037(5)	60(4)
C(24)	6761(6)	1838(8)	10301(4)	46(3)
C(25)	7600(5)	2906(9)	9843(4)	45(3)
C(26)	7088(5)	7377(10)	7502(4)	42(3)
C(27)	7590(6)	5645(12)	7031(6)	70(4)
C(28)	7860(6)	7851(16)	6775(5)	90(6)
C(29)	7047(4)	4154(8)	3319(4)	28(2)
C(30)	6170(5)	3670(9)	2945(4)	44(3)
C(31)	6243(4)	3382(9)	3427(4)	42(3)
C(32)	6746(5)	4585(10)	2414(4)	46(3)
C(33)	7101(5)	3633(8)	4147(4)	34(2)
C(34)	7619(4)	3998(7)	4207(4)	25(2)
C(35)	7977(4)	4027(7)	4645(4)	29(2)
C(36)	7807(4)	3614(7)	5080(4)	30(2)
C(37)	7261(4)	3207(8)	5007(4)	32(2)
C(38)	6894(4)	3220(8)	4541(4)	33(2)
C(39)	9601(5)	5307(10)	4060(4)	43(3)
C(40)	9035(4)	5229(8)	3705(4)	30(2)
C(41)	8997(4)	5542(8)	3199(4)	32(2)
C(42)	8502(5)	5458(9)	2838(4)	37(2)
C(43)	8501(6)	5779(12)	2313(4)	60(4)

C(44)	9526(4)	5995(8)	3072(4)	31(2)
C(45)	9910(5)	5389(8)	2874(4)	36(2)
C(46)	10405(5)	5836(9)	2801(4)	37(2)
C(47)	10515(5)	6845(8)	2902(4)	36(2)
C(48)	10142(5)	7461(8)	3086(4)	37(3)
C(49)	9641(5)	7034(8)	3171(4)	34(2)
C(50)	9239(7)	7671(11)	3392(5)	62(4)
C(51)	10294(7)	8568(10)	3199(5)	67(4)
C(52)	10837(5)	5206(10)	2584(5)	53(3)
C(53)	9796(6)	4281(9)	2764(5)	51(3)
C(54)	8629(4)	1837(8)	1971(4)	33(2)
C(55)	7799(5)	2586(10)	1761(5)	55(4)
C(56)	7957(5)	2740(10)	2247(5)	49(3)
C(57)	8175(5)	1666(11)	1091(5)	52(3)
C(58)	8873(4)	2187(7)	2841(4)	30(2)
C(59)	9354(4)	1649(6)	2763(3)	21(2)
C(60)	9776(4)	1550(7)	3203(4)	28(2)
C(61)	9720(4)	1954(7)	3675(4)	32(2)
C(62)	9228(5)	2474(8)	3695(4)	36(3)
C(63)	8798(5)	2595(8)	3283(4)	36(2)
C(64)	8938(6)	2770(12)	5616(5)	64(4)
C(65)	7981(6)	3082(9)	6186(4)	47(3)
C(66)	8594(6)	4878(10)	5866(5)	58(4)
C(67)	11047(4)	-115(9)	2285(4)	37(2)
C(68)	10449(4)	122(8)	2021(4)	30(2)
C(69)	10261(4)	-188(8)	1525(4)	31(2)
C(70)	9732(5)	89(8)	1234(4)	36(2)
C(71)	9580(5)	-260(11)	694(4)	51(3)
C(72)	10663(5)	-827(8)	1295(4)	33(2)
C(73)	11013(5)	-347(8)	1005(4)	36(2)
C(74)	11395(4)	-924(7)	805(4)	32(2)
C(75)	11441(5)	-1960(8)	912(4)	37(2)
C(76)	11107(5)	-2442(8)	1197(4)	35(2)

C(77)	10705(4)	-1877(8)	1376(4)	33(2)
C(78)	10327(5)	-2392(9)	1675(4)	42(3)
C(79)	11200(5)	-3577(9)	1305(4)	43(3)
C(80)	11799(6)	-430(10)	519(5)	55(3)
C(81)	10980(6)	798(9)	911(5)	53(3)
C(82)	10969(5)	2222(11)	4031(5)	55(3)
C(83)	10409(6)	426(10)	4416(5)	53(3)
C(84)	10178(6)	2554(14)	4766(5)	74(5)

Table 3. Bond lengths [$\text{\AA}$] and angles [$^\circ$] for Pt3.

Pt(1)-C(29)	1.946(10)	Si(3)-C(61)	1.876(11)
Pt(1)-O(3)	2.036(7)	Si(3)-C(84)	1.878(13)
Pt(1)-O(4)	2.078(7)	O(1)-C(12)	1.293(11)
Pt(1)-C(34)	2.081(10)	O(2)-C(14)	1.269(13)
Pt(2)-C(59)	1.953(9)	O(3)-C(40)	1.274(11)
Pt(2)-C(54)	1.960(10)	O(4)-C(42)	1.277(12)
Pt(2)-O(5)	2.021(6)	O(5)-C(68)	1.275(11)
Pt(2)-O(6)	2.089(7)	O(6)-C(70)	1.258(12)
Pt(3)-C(1)	1.938(10)	N(1)-C(1)	1.357(13)
Pt(3)-C(6)	1.953(9)	N(1)-C(2)	1.390(16)
Pt(3)-O(1)	2.022(7)	N(1)-C(4)	1.450(16)
Pt(3)-O(2)	2.078(7)	N(2)-C(1)	1.361(14)
Si(1)-C(8)	1.854(11)	N(2)-C(3)	1.399(13)
Si(1)-C(27)	1.856(15)	N(2)-C(5)	1.420(13)
Si(1)-C(26)	1.861(11)	N(3)-C(29)	1.364(13)
Si(1)-C(28)	1.865(14)	N(3)-C(30)	1.390(15)
Si(2)-C(66)	1.845(12)	N(3)-C(32)	1.446(14)
Si(2)-C(65)	1.848(11)	N(4)-C(29)	1.345(13)
Si(2)-C(36)	1.870(11)	N(4)-C(31)	1.379(13)
Si(2)-C(64)	1.871(14)	N(4)-C(33)	1.434(14)
Si(3)-C(83)	1.847(13)	N(5)-C(54)	1.313(13)
Si(3)-C(82)	1.857(13)	N(5)-C(55)	1.391(14)

N(5)-C(57)	1.439(15)	C(39)-C(40)	1.514(15)
N(6)-C(54)	1.369(14)	C(40)-C(41)	1.431(13)
N(6)-C(56)	1.387(13)	C(41)-C(42)	1.394(15)
N(6)-C(58)	1.419(13)	C(41)-C(44)	1.510(13)
C(2)-C(3)	1.325(18)	C(42)-C(43)	1.499(15)
C(5)-C(10)	1.352(14)	C(44)-C(49)	1.403(14)
C(5)-C(6)	1.412(13)	C(44)-C(45)	1.410(14)
C(6)-C(7)	1.432(14)	C(45)-C(46)	1.380(15)
C(7)-C(8)	1.419(13)	C(45)-C(53)	1.494(15)
C(8)-C(9)	1.382(14)	C(46)-C(47)	1.363(15)
C(9)-C(10)	1.394(15)	C(46)-C(52)	1.541(15)
C(11)-C(12)	1.508(14)	C(47)-C(48)	1.377(15)
C(12)-C(13)	1.397(14)	C(48)-C(49)	1.394(15)
C(13)-C(14)	1.424(16)	C(48)-C(51)	1.510(16)
C(13)-C(16)	1.518(14)	C(49)-C(50)	1.497(15)
C(14)-C(15)	1.517(15)	C(55)-C(56)	1.325(18)
C(16)-C(17)	1.390(15)	C(58)-C(63)	1.369(14)
C(16)-C(21)	1.399(14)	C(58)-C(59)	1.410(12)
C(17)-C(18)	1.398(15)	C(59)-C(60)	1.421(13)
C(17)-C(25)	1.517(14)	C(60)-C(61)	1.426(14)
C(18)-C(19)	1.389(14)	C(61)-C(62)	1.381(14)
C(18)-C(24)	1.481(14)	C(62)-C(63)	1.378(16)
C(19)-C(20)	1.396(15)	C(67)-C(68)	1.511(14)
C(20)-C(21)	1.357(15)	C(68)-C(69)	1.403(14)
C(20)-C(23)	1.506(14)	C(69)-C(70)	1.409(14)
C(21)-C(22)	1.516(15)	C(69)-C(72)	1.510(14)
C(30)-C(31)	1.349(16)	C(70)-C(71)	1.522(14)
C(33)-C(34)	1.318(14)	C(72)-C(77)	1.393(15)
C(33)-C(38)	1.388(14)	C(72)-C(73)	1.417(15)
C(34)-C(35)	1.331(14)	C(73)-C(74)	1.387(14)
C(35)-C(36)	1.440(13)	C(73)-C(81)	1.518(15)
C(36)-C(37)	1.397(14)	C(74)-C(75)	1.386(14)
C(37)-C(38)	1.399(14)	C(74)-C(80)	1.514(15)

C(75)-C(76)	1.381(15)	C(65)-Si(2)-C(64)	111.1(6)
C(76)-C(77)	1.388(15)	C(36)-Si(2)-C(64)	108.6(5)
C(76)-C(79)	1.521(15)	C(83)-Si(3)-C(82)	108.4(6)
C(77)-C(78)	1.502(15)	C(83)-Si(3)-C(61)	112.0(5)
		C(82)-Si(3)-C(61)	106.9(5)
C(29)-Pt(1)-O(3)	171.3(3)	C(83)-Si(3)-C(84)	109.0(7)
C(29)-Pt(1)-O(4)	100.5(3)	C(82)-Si(3)-C(84)	110.7(7)
O(3)-Pt(1)-O(4)	87.9(3)	C(61)-Si(3)-C(84)	109.9(6)
C(29)-Pt(1)-C(34)	78.6(4)	C(12)-O(1)-Pt(3)	127.6(6)
O(3)-Pt(1)-C(34)	93.0(3)	C(14)-O(2)-Pt(3)	128.1(7)
O(4)-Pt(1)-C(34)	178.0(3)	C(40)-O(3)-Pt(1)	127.6(6)
C(59)-Pt(2)-C(54)	79.8(4)	C(42)-O(4)-Pt(1)	127.5(7)
C(59)-Pt(2)-O(5)	93.5(3)	C(68)-O(5)-Pt(2)	128.3(6)
C(54)-Pt(2)-O(5)	172.9(4)	C(70)-O(6)-Pt(2)	126.6(6)
C(59)-Pt(2)-O(6)	178.6(3)	C(1)-N(1)-C(2)	109.4(10)
C(54)-Pt(2)-O(6)	99.0(4)	C(1)-N(1)-C(4)	125.4(10)
O(5)-Pt(2)-O(6)	87.8(3)	C(2)-N(1)-C(4)	125.2(10)
C(1)-Pt(3)-C(6)	79.2(4)	C(1)-N(2)-C(3)	111.1(10)
C(1)-Pt(3)-O(1)	172.2(4)	C(1)-N(2)-C(5)	115.8(8)
C(6)-Pt(3)-O(1)	93.1(3)	C(3)-N(2)-C(5)	132.9(10)
C(1)-Pt(3)-O(2)	100.0(4)	C(29)-N(3)-C(30)	109.5(9)
C(6)-Pt(3)-O(2)	179.0(4)	C(29)-N(3)-C(32)	125.8(9)
O(1)-Pt(3)-O(2)	87.7(3)	C(30)-N(3)-C(32)	124.5(9)
C(8)-Si(1)-C(27)	109.2(6)	C(29)-N(4)-C(31)	112.1(9)
C(8)-Si(1)-C(26)	110.1(5)	C(29)-N(4)-C(33)	115.1(8)
C(27)-Si(1)-C(26)	106.7(6)	C(31)-N(4)-C(33)	132.8(9)
C(8)-Si(1)-C(28)	109.7(6)	C(54)-N(5)-C(55)	109.1(10)
C(27)-Si(1)-C(28)	111.1(8)	C(54)-N(5)-C(57)	125.7(10)
C(26)-Si(1)-C(28)	110.0(7)	C(55)-N(5)-C(57)	125.1(10)
C(66)-Si(2)-C(65)	108.6(6)	C(54)-N(6)-C(56)	110.0(10)
C(66)-Si(2)-C(36)	110.5(5)	C(54)-N(6)-C(58)	117.2(8)
C(65)-Si(2)-C(36)	110.4(5)	C(56)-N(6)-C(58)	132.8(10)
C(66)-Si(2)-C(64)	107.6(7)	N(1)-C(1)-N(2)	104.8(9)

N(1)-C(1)-Pt(3)	137.7(9)	C(17)-C(18)-C(24)	123.9(10)
N(2)-C(1)-Pt(3)	117.4(7)	C(18)-C(19)-C(20)	123.7(9)
C(3)-C(2)-N(1)	109.2(11)	C(21)-C(20)-C(19)	119.1(9)
C(2)-C(3)-N(2)	105.4(11)	C(21)-C(20)-C(23)	121.5(10)
C(10)-C(5)-C(6)	125.7(10)	C(19)-C(20)-C(23)	119.5(10)
C(10)-C(5)-N(2)	125.1(9)	C(20)-C(21)-C(16)	119.5(9)
C(6)-C(5)-N(2)	109.2(9)	C(20)-C(21)-C(22)	119.0(10)
C(5)-C(6)-C(7)	112.5(8)	C(16)-C(21)-C(22)	121.4(10)
C(5)-C(6)-Pt(3)	118.4(7)	N(4)-C(29)-N(3)	104.9(9)
C(7)-C(6)-Pt(3)	129.0(7)	N(4)-C(29)-Pt(1)	117.5(7)
C(8)-C(7)-C(6)	124.3(9)	N(3)-C(29)-Pt(1)	137.5(8)
C(9)-C(8)-C(7)	116.8(9)	C(31)-C(30)-N(3)	107.9(10)
C(9)-C(8)-Si(1)	123.6(8)	C(30)-C(31)-N(4)	105.6(10)
C(7)-C(8)-Si(1)	119.6(7)	C(34)-C(33)-C(38)	121.7(10)
C(8)-C(9)-C(10)	121.9(10)	C(34)-C(33)-N(4)	114.5(9)
C(5)-C(10)-C(9)	118.8(9)	C(38)-C(33)-N(4)	123.8(10)
O(1)-C(12)-C(13)	127.5(10)	C(33)-C(34)-C(35)	123.3(10)
O(1)-C(12)-C(11)	113.7(9)	C(33)-C(34)-Pt(1)	114.2(7)
C(13)-C(12)-C(11)	118.8(9)	C(35)-C(34)-Pt(1)	122.4(7)
C(12)-C(13)-C(14)	123.1(10)	C(34)-C(35)-C(36)	119.7(9)
C(12)-C(13)-C(16)	117.9(9)	C(37)-C(36)-C(35)	116.2(9)
C(14)-C(13)-C(16)	118.8(9)	C(37)-C(36)-Si(2)	124.0(8)
O(2)-C(14)-C(13)	125.6(10)	C(35)-C(36)-Si(2)	119.7(8)
O(2)-C(14)-C(15)	115.2(11)	C(36)-C(37)-C(38)	122.2(9)
C(13)-C(14)-C(15)	119.2(11)	C(33)-C(38)-C(37)	116.9(10)
C(17)-C(16)-C(21)	120.6(10)	O(3)-C(40)-C(41)	127.3(9)
C(17)-C(16)-C(13)	119.0(9)	O(3)-C(40)-C(39)	114.2(9)
C(21)-C(16)-C(13)	120.3(9)	C(41)-C(40)-C(39)	118.4(9)
C(16)-C(17)-C(18)	121.1(10)	C(42)-C(41)-C(40)	122.8(9)
C(16)-C(17)-C(25)	120.7(10)	C(42)-C(41)-C(44)	120.9(9)
C(18)-C(17)-C(25)	118.2(10)	C(40)-C(41)-C(44)	116.3(9)
C(19)-C(18)-C(17)	115.9(9)	O(4)-C(42)-C(41)	126.8(9)
C(19)-C(18)-C(24)	120.2(10)	O(4)-C(42)-C(43)	113.7(10)

C(41)-C(42)-C(43)	119.5(10)	C(62)-C(61)-Si(3)	123.7(8)
C(49)-C(44)-C(45)	119.9(9)	C(60)-C(61)-Si(3)	119.1(7)
C(49)-C(44)-C(41)	118.7(9)	C(63)-C(62)-C(61)	122.5(10)
C(45)-C(44)-C(41)	121.3(9)	C(58)-C(63)-C(62)	117.9(9)
C(46)-C(45)-C(44)	118.2(10)	O(5)-C(68)-C(69)	126.3(9)
C(46)-C(45)-C(53)	120.9(10)	O(5)-C(68)-C(67)	113.9(9)
C(44)-C(45)-C(53)	120.9(9)	C(69)-C(68)-C(67)	119.7(9)
C(47)-C(46)-C(45)	121.4(10)	C(68)-C(69)-C(70)	123.5(9)
C(47)-C(46)-C(52)	118.5(10)	C(68)-C(69)-C(72)	117.0(9)
C(45)-C(46)-C(52)	120.2(10)	C(70)-C(69)-C(72)	119.5(9)
C(46)-C(47)-C(48)	121.8(10)	O(6)-C(70)-C(69)	126.6(9)
C(47)-C(48)-C(49)	118.6(10)	O(6)-C(70)-C(71)	114.3(10)
C(47)-C(48)-C(51)	119.2(11)	C(69)-C(70)-C(71)	119.1(10)
C(49)-C(48)-C(51)	122.2(11)	C(77)-C(72)-C(73)	119.6(10)
C(48)-C(49)-C(44)	120.1(9)	C(77)-C(72)-C(69)	120.8(10)
C(48)-C(49)-C(50)	120.0(11)	C(73)-C(72)-C(69)	119.6(9)
C(44)-C(49)-C(50)	119.8(10)	C(74)-C(73)-C(72)	119.9(10)
N(5)-C(54)-N(6)	106.4(9)	C(74)-C(73)-C(81)	119.1(10)
N(5)-C(54)-Pt(2)	138.2(8)	C(72)-C(73)-C(81)	121.0(10)
N(6)-C(54)-Pt(2)	115.4(8)	C(75)-C(74)-C(73)	118.7(10)
C(56)-C(55)-N(5)	109.2(10)	C(75)-C(74)-C(80)	119.6(9)
C(55)-C(56)-N(6)	105.2(11)	C(73)-C(74)-C(80)	121.4(9)
C(63)-C(58)-C(59)	126.0(10)	C(76)-C(75)-C(74)	122.4(10)
C(63)-C(58)-N(6)	124.9(9)	C(75)-C(76)-C(77)	119.1(10)
C(59)-C(58)-N(6)	109.0(9)	C(75)-C(76)-C(79)	118.5(10)
C(58)-C(59)-C(60)	112.9(8)	C(77)-C(76)-C(79)	122.5(10)
C(58)-C(59)-Pt(2)	118.5(7)	C(76)-C(77)-C(72)	120.2(10)
C(60)-C(59)-Pt(2)	128.5(6)	C(76)-C(77)-C(78)	120.0(10)
C(59)-C(60)-C(61)	123.5(8)	C(72)-C(77)-C(78)	119.8(10)
C(62)-C(61)-C(60)	117.3(10)		

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for Pt3. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Pt(1)	28(1)	30(1)	25(1)	0(1)	9(1)	4(1)
Pt(2)	21(1)	29(1)	32(1)	7(1)	8(1)	5(1)
Pt(3)	24(1)	38(1)	28(1)	-1(1)	5(1)	-5(1)
Si(1)	33(2)	49(2)	28(1)	-3(1)	12(1)	-5(1)
Si(2)	43(2)	35(2)	28(1)	4(1)	10(1)	-6(1)
Si(3)	39(2)	38(2)	34(2)	-1(1)	12(1)	8(1)
O(1)	23(4)	48(4)	28(3)	-2(3)	5(3)	-8(3)
O(2)	18(3)	65(5)	38(4)	11(4)	2(3)	-14(4)
O(3)	29(4)	43(4)	27(3)	-3(3)	7(3)	-1(3)
O(4)	38(4)	48(5)	26(3)	1(3)	8(3)	-2(4)
O(5)	26(4)	37(4)	31(3)	2(3)	15(3)	12(3)
O(6)	30(4)	45(4)	31(4)	4(3)	1(3)	7(3)
N(1)	33(5)	69(7)	45(6)	6(5)	-8(4)	-12(5)
N(2)	27(5)	36(5)	47(5)	-5(4)	6(4)	-11(4)
N(3)	27(5)	39(5)	38(5)	-5(4)	1(4)	8(4)
N(4)	23(4)	36(5)	40(5)	4(4)	8(4)	6(4)
N(5)	24(5)	46(6)	47(5)	6(4)	2(4)	2(4)
N(6)	25(4)	35(5)	51(5)	7(4)	14(4)	5(4)
C(1)	25(5)	41(6)	36(6)	-3(5)	-3(4)	-2(5)
C(2)	23(6)	98(12)	63(9)	4(8)	-2(6)	-13(7)
C(3)	21(5)	57(8)	68(8)	3(7)	-2(5)	-11(5)
C(4)	53(9)	115(14)	46(8)	11(8)	-13(7)	-27(9)
C(5)	22(5)	24(5)	44(6)	-7(4)	10(4)	-3(4)
C(6)	28(5)	25(5)	30(5)	-6(4)	22(4)	-4(4)
C(7)	21(5)	37(6)	30(5)	-4(4)	10(4)	-3(4)
C(8)	28(5)	42(6)	28(5)	-6(4)	13(4)	0(5)
C(9)	39(6)	32(6)	47(6)	4(5)	21(5)	-7(5)
C(10)	25(5)	41(6)	46(6)	-2(5)	14(5)	-8(5)

C(11)	33(6)	41(6)	37(6)	5(5)	5(5)	-9(5)
C(12)	30(5)	35(5)	30(5)	-5(4)	18(4)	-4(4)
C(13)	46(6)	31(5)	26(5)	-4(4)	11(5)	1(5)
C(14)	53(7)	51(7)	27(5)	3(5)	5(5)	-2(6)
C(15)	54(8)	101(12)	31(6)	11(7)	-3(6)	-6(8)
C(16)	37(6)	36(6)	31(5)	4(5)	12(4)	0(5)
C(17)	46(7)	35(6)	20(5)	3(4)	1(4)	8(5)
C(18)	46(6)	21(5)	28(5)	6(4)	-4(4)	0(5)
C(19)	47(6)	26(5)	30(5)	0(4)	18(5)	-14(5)
C(20)	49(7)	36(6)	34(5)	2(5)	23(5)	7(5)
C(21)	59(7)	17(5)	37(6)	-2(4)	20(5)	-3(5)
C(22)	84(10)	30(6)	63(8)	-2(6)	43(8)	-10(6)
C(23)	90(11)	47(7)	58(8)	2(6)	51(8)	16(7)
C(24)	69(9)	28(6)	37(6)	6(5)	2(6)	-7(6)
C(25)	66(8)	33(6)	39(6)	-2(5)	16(6)	12(6)
C(26)	34(6)	59(8)	35(6)	4(5)	10(5)	4(6)
C(27)	44(8)	87(11)	76(10)	-36(9)	8(7)	13(8)
C(28)	54(9)	171(19)	44(8)	45(10)	7(7)	-28(11)
C(29)	27(5)	29(5)	30(5)	-3(4)	7(4)	13(4)
C(30)	33(6)	56(7)	42(6)	-6(6)	7(5)	5(6)
C(31)	21(5)	50(7)	56(7)	-20(6)	8(5)	-14(5)
C(32)	37(6)	62(8)	37(6)	3(6)	4(5)	18(6)
C(33)	42(6)	30(5)	38(6)	0(4)	23(5)	11(5)
C(34)	15(4)	16(4)	43(5)	-7(4)	3(4)	8(4)
C(35)	34(6)	21(5)	38(5)	-2(4)	22(5)	2(4)
C(36)	31(5)	27(5)	33(5)	-5(4)	10(4)	5(4)
C(37)	35(6)	29(5)	37(5)	1(4)	20(5)	2(4)
C(38)	24(5)	37(6)	41(6)	3(5)	13(4)	2(4)
C(39)	36(6)	55(7)	39(6)	10(5)	7(5)	-7(6)
C(40)	30(5)	34(6)	29(5)	-2(4)	10(4)	-4(4)
C(41)	31(5)	37(6)	33(5)	-7(4)	20(4)	-6(5)
C(42)	41(6)	40(6)	35(5)	-7(5)	18(5)	-10(5)
C(43)	62(9)	91(11)	32(6)	9(7)	17(6)	-6(8)

C(44)	36(6)	29(5)	32(5)	-2(4)	17(4)	-3(4)
C(45)	40(6)	32(6)	40(6)	0(5)	20(5)	-11(5)
C(46)	40(6)	41(6)	34(5)	8(5)	16(5)	0(5)
C(47)	37(6)	39(6)	30(5)	4(5)	5(4)	-6(5)
C(48)	51(7)	29(5)	30(5)	3(4)	5(5)	-13(5)
C(49)	45(6)	28(5)	31(5)	5(4)	14(5)	8(5)
C(50)	95(11)	54(8)	44(7)	-1(6)	31(7)	15(8)
C(51)	100(12)	41(7)	58(8)	-2(6)	14(8)	-27(8)
C(52)	48(7)	54(8)	67(8)	3(6)	36(7)	-2(6)
C(53)	61(8)	32(6)	73(9)	-19(6)	43(7)	-18(6)
C(54)	27(5)	26(5)	49(6)	9(5)	13(5)	3(4)
C(55)	20(6)	56(8)	82(10)	-4(7)	-6(6)	24(6)
C(56)	21(5)	47(7)	76(9)	2(6)	3(6)	10(5)
C(57)	36(7)	66(9)	50(7)	14(6)	2(5)	5(6)
C(58)	28(5)	19(5)	46(6)	7(4)	13(4)	0(4)
C(59)	18(4)	12(4)	39(5)	13(4)	19(4)	6(3)
C(60)	21(5)	26(5)	40(5)	8(4)	15(4)	6(4)
C(61)	33(6)	22(5)	44(6)	3(4)	19(5)	-4(4)
C(62)	46(6)	30(5)	41(6)	9(5)	31(5)	13(5)
C(63)	34(6)	24(5)	55(7)	-1(5)	23(5)	4(4)
C(64)	50(8)	87(11)	53(8)	20(8)	6(6)	16(8)
C(65)	66(8)	44(7)	33(6)	9(5)	16(6)	-3(6)
C(66)	76(10)	52(8)	43(7)	-9(6)	6(7)	-26(7)
C(67)	27(5)	54(7)	28(5)	-7(5)	2(4)	7(5)
C(68)	29(5)	33(5)	32(5)	2(4)	13(4)	3(4)
C(69)	22(5)	36(6)	32(5)	-3(4)	2(4)	4(4)
C(70)	44(6)	38(6)	27(5)	2(4)	12(5)	6(5)
C(71)	45(7)	77(9)	30(6)	-3(6)	7(5)	1(7)
C(72)	37(6)	30(5)	29(5)	-7(4)	-1(4)	-2(5)
C(73)	41(6)	35(6)	32(5)	-5(5)	10(5)	6(5)
C(74)	34(6)	14(5)	52(6)	-4(4)	18(5)	2(4)
C(75)	42(6)	35(6)	39(6)	-3(5)	18(5)	6(5)
C(76)	41(6)	39(6)	22(5)	-8(4)	0(4)	-6(5)

C(77)	33(6)	37(6)	25(5)	-2(4)	-2(4)	-1(5)
C(78)	49(7)	43(7)	36(6)	0(5)	14(5)	5(6)
C(79)	43(7)	44(7)	39(6)	-7(5)	1(5)	13(5)
C(80)	74(9)	41(7)	63(8)	1(6)	45(7)	1(7)
C(81)	62(9)	27(6)	77(9)	5(6)	31(7)	-1(6)
C(82)	49(8)	65(9)	53(7)	3(7)	14(6)	2(7)
C(83)	56(8)	51(8)	48(7)	10(6)	4(6)	4(6)
C(84)	72(10)	111(13)	35(7)	-23(8)	0(7)	4(9)

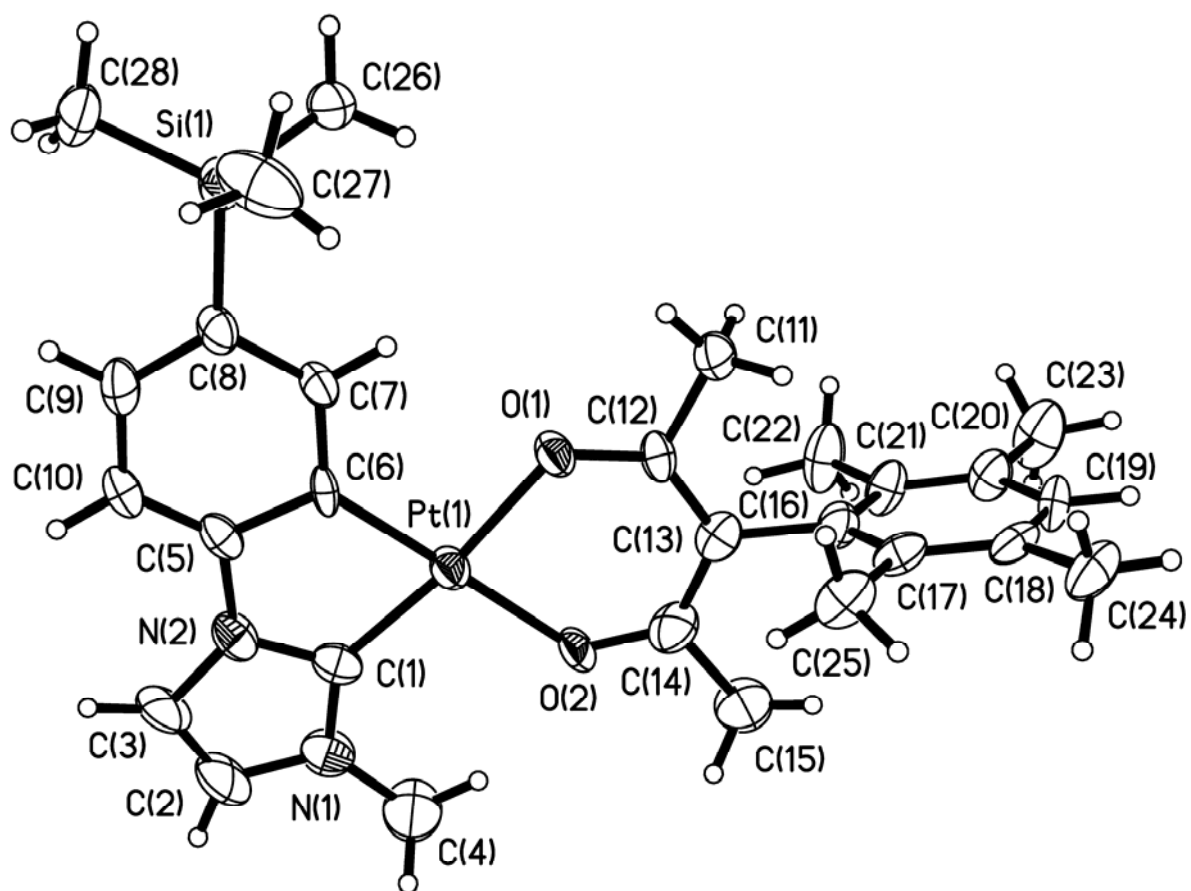
Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^{-3}$) for Pt3.

	x	y	z	U(eq)
H(2A)	10794	7098	9820	75
H(3A)	10470	7431	8928	60
H(4A)	9645	5966	10369	112
H(4B)	10071	6889	10553	112
H(4C)	10312	5796	10436	112
H(7A)	7930	6368	8308	35
H(9A)	8933	7563	7441	45
H(10A)	9707	7458	8108	43
H(11A)	6954	5202	8867	56
H(11B)	6741	5677	9335	56
H(11C)	6869	4479	9317	56
H(15A)	8852	4775	10907	96
H(15B)	8217	4385	10870	96
H(15C)	8379	5545	11020	96
H(19A)	6305	3171	10816	39
H(22A)	7164	6373	10961	82
H(22B)	6739	6561	10440	82
H(22C)	7403	6460	10459	82
H(23A)	6095	5717	10850	90

H(23B)	6507	5348	11352	90
H(23C)	5977	4659	11105	90
H(24A)	7115	1459	10408	69
H(24B)	6610	1702	9948	69
H(24C)	6486	1619	10499	69
H(25A)	7653	2199	9961	68
H(25B)	7969	3232	9865	68
H(25C)	7396	2909	9495	68
H(26A)	7159	8043	7667	64
H(26B)	7001	6873	7740	64
H(26C)	6768	7433	7220	64
H(27A)	7877	5454	6840	104
H(27B)	7215	5615	6813	104
H(27C)	7606	5171	7310	104
H(28A)	8066	7488	6554	136
H(28B)	8085	8434	6928	136
H(28C)	7498	8096	6582	136
H(30A)	5838	3573	2697	52
H(31A)	5979	3035	3582	51
H(32A)	7076	5040	2480	69
H(32B)	6409	4978	2265	69
H(32C)	6808	4044	2183	69
H(35A)	8342	4318	4671	34
H(37A)	7136	2911	5282	38
H(38A)	6521	2959	4497	40
H(39A)	9548	5224	4404	65
H(39B)	9769	5977	4024	65
H(39C)	9853	4769	3984	65
H(43A)	8153	6156	2179	91
H(43B)	8522	5171	2108	91
H(43C)	8829	6218	2307	91
H(47A)	10858	7129	2845	43
H(50A)	8857	7387	3295	93

H(50B)	9242	8374	3269	93
H(50C)	9355	7668	3756	93
H(51A)	10687	8686	3172	100
H(51B)	10249	8729	3539	100
H(51C)	10044	9007	2961	100
H(52A)	11171	5627	2576	79
H(52B)	10666	4989	2245	79
H(52C)	10949	4603	2793	79
H(53A)	10146	3891	2866	77
H(53B)	9652	4190	2406	77
H(53C)	9514	4036	2949	77
H(55A)	7460	2836	1557	66
H(56A)	7754	3093	2459	59
H(57A)	8496	1218	1076	77
H(57B)	8185	2261	876	77
H(57C)	7821	1290	977	77
H(60A)	10114	1196	3183	33
H(62A)	9183	2759	4003	43
H(63A)	8461	2950	3306	43
H(64A)	9134	3087	5374	96
H(64B)	8804	2090	5498	96
H(64C)	9200	2708	5939	96
H(65A)	7702	3578	6254	70
H(65B)	8268	2970	6489	70
H(65C)	7792	2434	6078	70
H(66A)	8277	5331	5890	87
H(66B)	8791	5140	5612	87
H(66C)	8856	4850	6189	87
H(67A)	11129	242	2606	55
H(67B)	11312	113	2079	55
H(67C)	11088	-854	2341	55
H(71A)	9175	-418	607	76
H(71B)	9798	-873	650	76

H(71C)	9667	285	476	76
H(75A)	11711	-2352	785	45
H(78A)	10555	-2814	1935	63
H(78B)	10053	-2826	1454	63
H(78C)	10124	-1873	1828	63
H(79A)	10835	-3929	1244	64
H(79B)	11389	-3670	1655	64
H(79C)	11438	-3862	1088	64
H(80A)	12101	-912	492	83
H(80B)	11963	185	696	83
H(80C)	11594	-242	185	83
H(81A)	11072	944	586	80
H(81B)	11250	1148	1173	80
H(81C)	10597	1039	915	80
H(82A)	11292	2140	4309	83
H(82B)	10929	2944	3935	83
H(82C)	11031	1814	3747	83
H(83A)	10718	369	4708	79
H(83B)	10501	23	4141	79
H(83C)	10059	168	4499	79
H(84A)	10514	2541	5035	111
H(84B)	9857	2263	4887	111
H(84C)	10093	3261	4660	111



VIII. References

1. *SHELXTL Version 6.14*, Bruker AXS, Madison, WI, 2000-2003.