Supporting Information

A Cooperative Pathway for Water Activation Process Using a Bimetallic Pt^0-Cu^I System

S. Jamali,*[a] S. Abedanzadeh,[a] N. K. Khaledi,[a] H. Samouei,[b] Z. Hendi,[a] S. Zacchini,[c] R. Kia,[a] H. R. Shahsavari[d]

Chemistry Department, Sharif University of Technology, P.O. Box 11155-3516, Tehran, Iran; Department of Chemistry, Texas A&M University, PO Box 30012, College Station, TX 77842-3012; Dipartimento di Chimica Industriale "Toso Montanari", Università di Bologna, Viale Risorgimento 4-40136 Bologna, Italy, Institute for Advanced Studies in Basic Sciences, Zanjan, Iran

2-NMR spectra

2.1- ^{1}H NMR spectrum of **1**

2.2- 2D-(^{1}H-^{13}C) HMBC NMR spectrum of **1**

2.3- ^{31}P NMR spectrum of **1**

2.4- Monitoring of the reaction **1** with pyridine using ^{1}H NMR spectroscopy

2.5- Monitoring of the reaction **1** with different concentration of pyridine using ^{1}H NMR spectroscopy

2.4- ^{31}P NMR spectrum of **4**

2.5- ^{1}H NMR spectrum of **4**

2.6- ^{13}C NMR spectrum of **4**

2.7- DEPT-135 spectrum of **4**

2.7- 2D-(^{1}H-^{13}C) HMBC NMR spectrum of **4**

3-Crystallography data

3.2- Crystallography data for **1**

3.3- Crystallography data for **4**

.

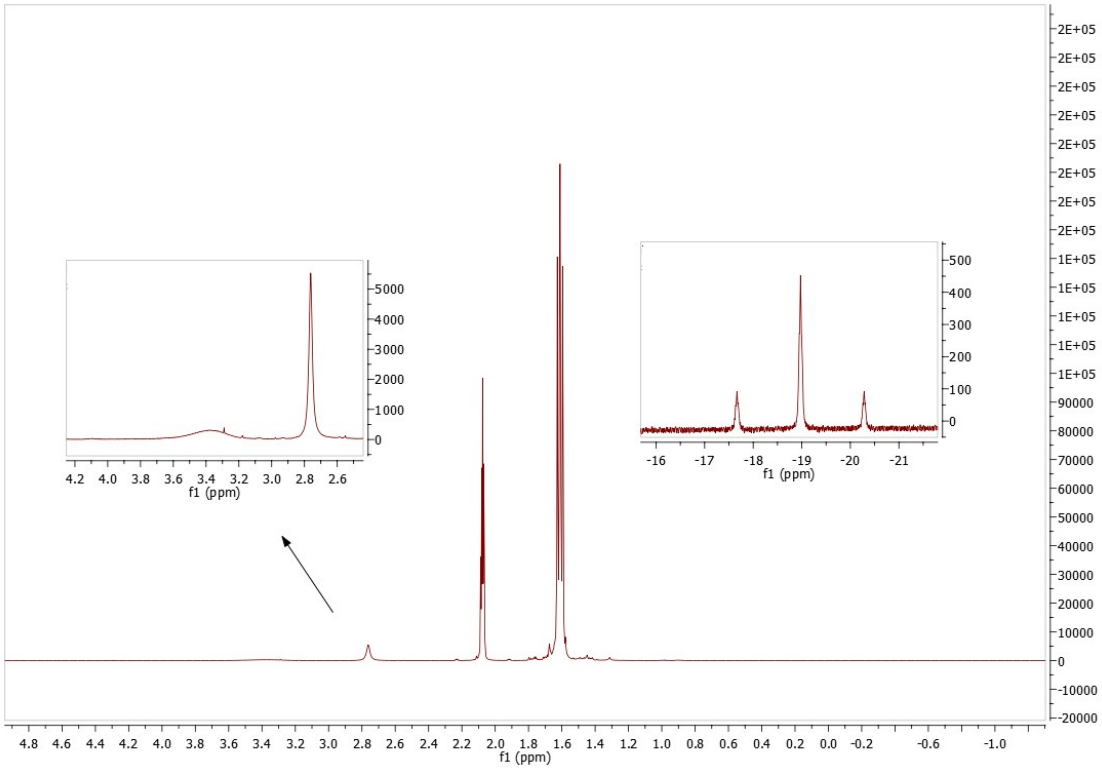


Figure S1. ^{1}H NMR spectrum of **1** in acetone-d_6 (Armar chemical Company). The insets show expansion of the hydride, water and acetonitrile regions

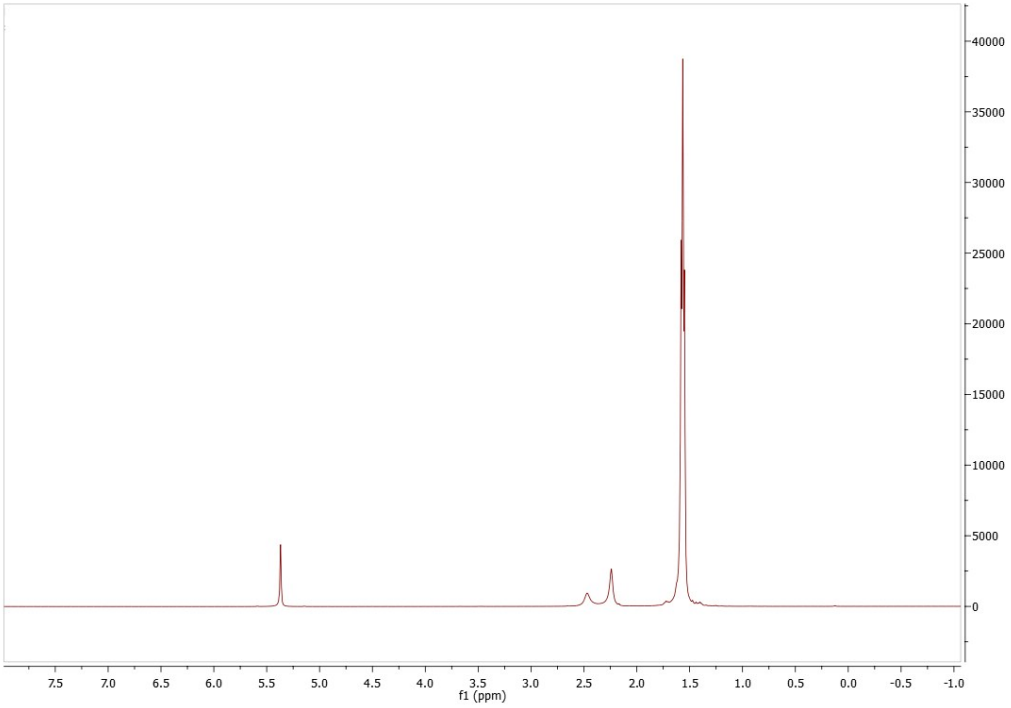


Figure S2. ^{1}H NMR spectrum of **1** in CD_2Cl_2 (Armar Chemical Company)

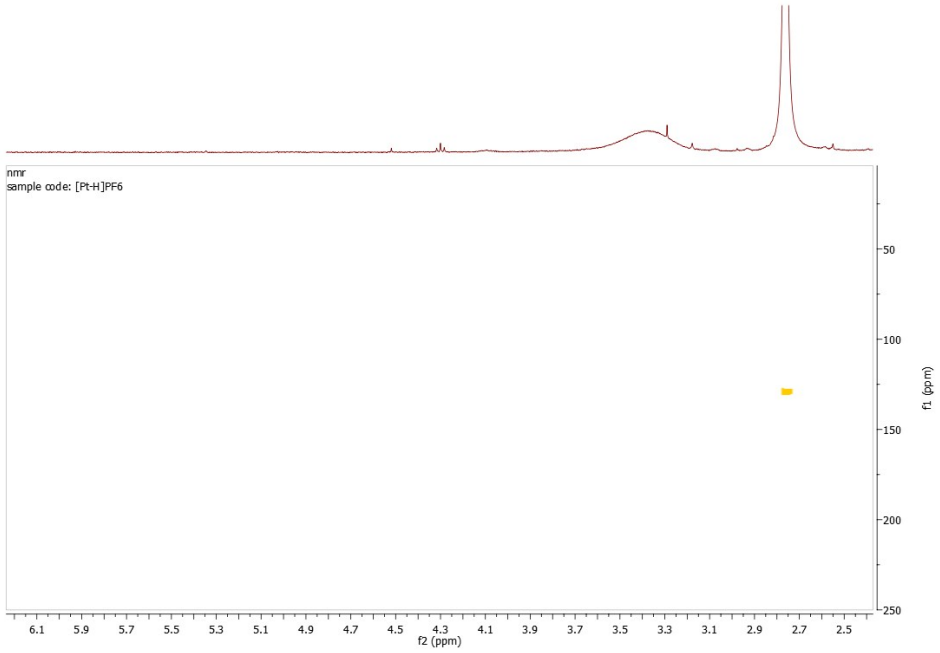


Figure S3. Expantion of the (^{1}H, ^{13}C)-HMBC NMR spectrum of **1** in acetone d_6 (Armar Chemical Company)

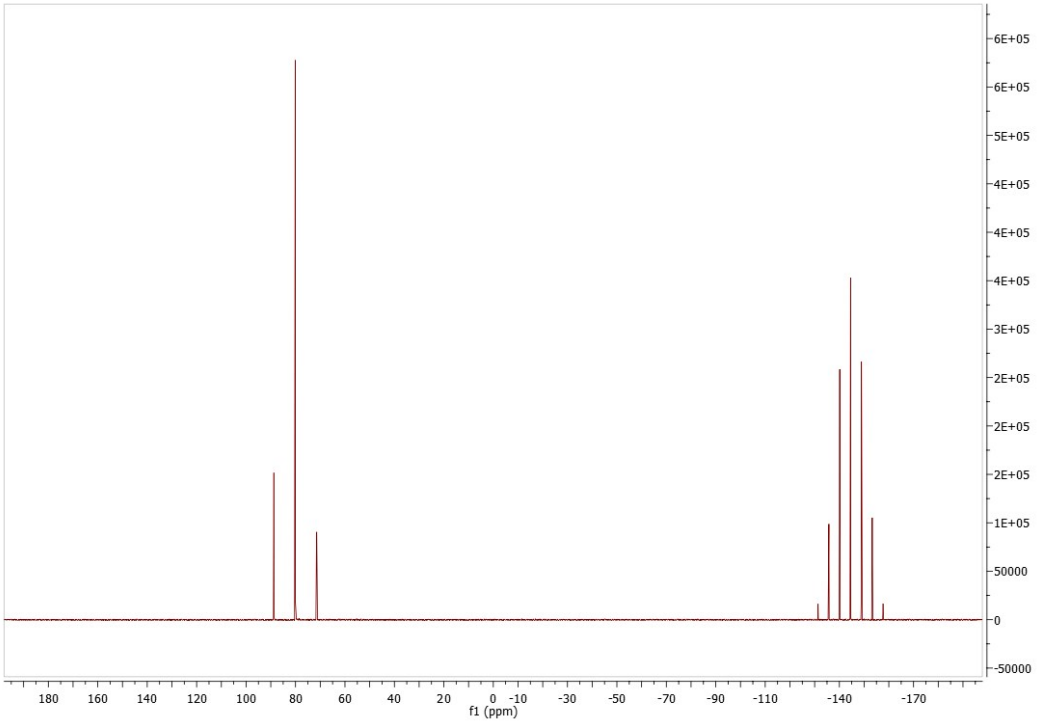


Figure S4. ^{31}P{^{1}H} NMR spectrum of **1** in acetone-d_6 (Armar Chemical Company).

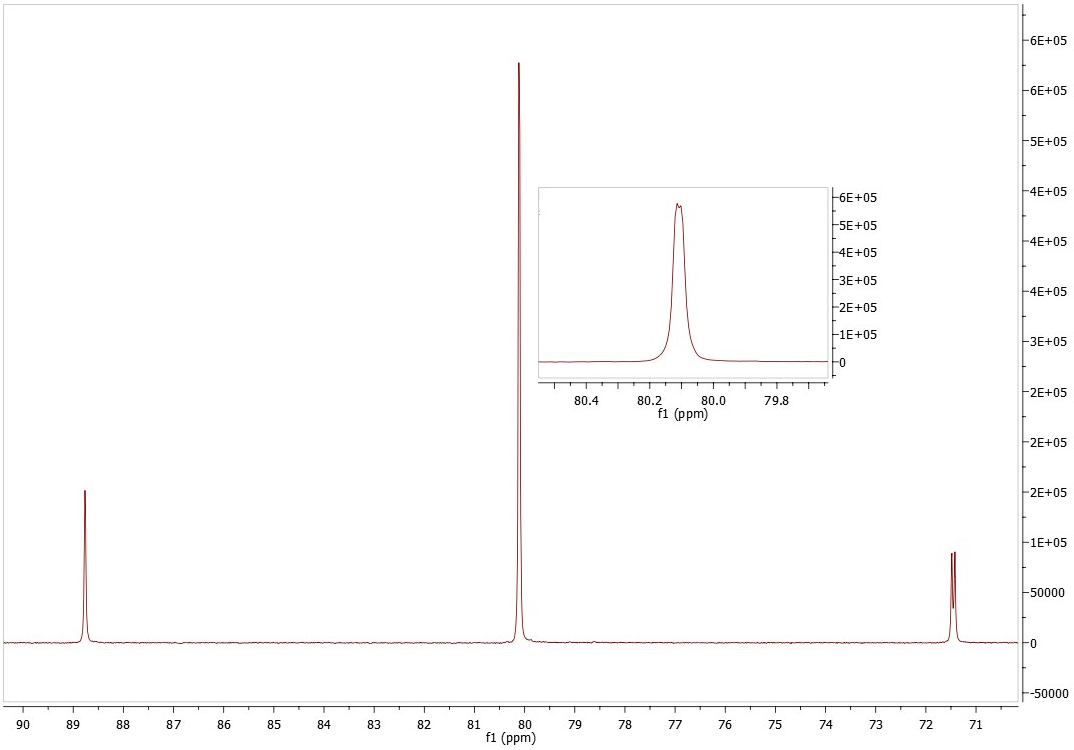


Figure S5. Expantion of the ^{31}P NMR spectrum of **1** in acetone d_6 (Armar Chemical Company)

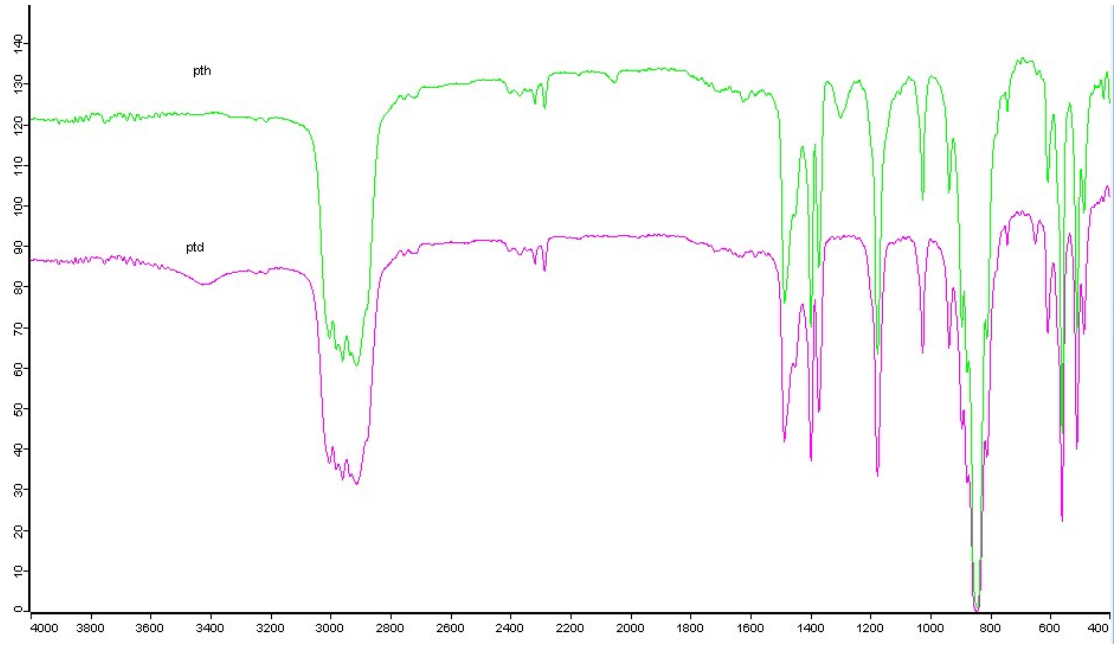


Figure S6.The IR spectrum of **1** (green) and the IR spectrum of **1**-d_1 (pink)

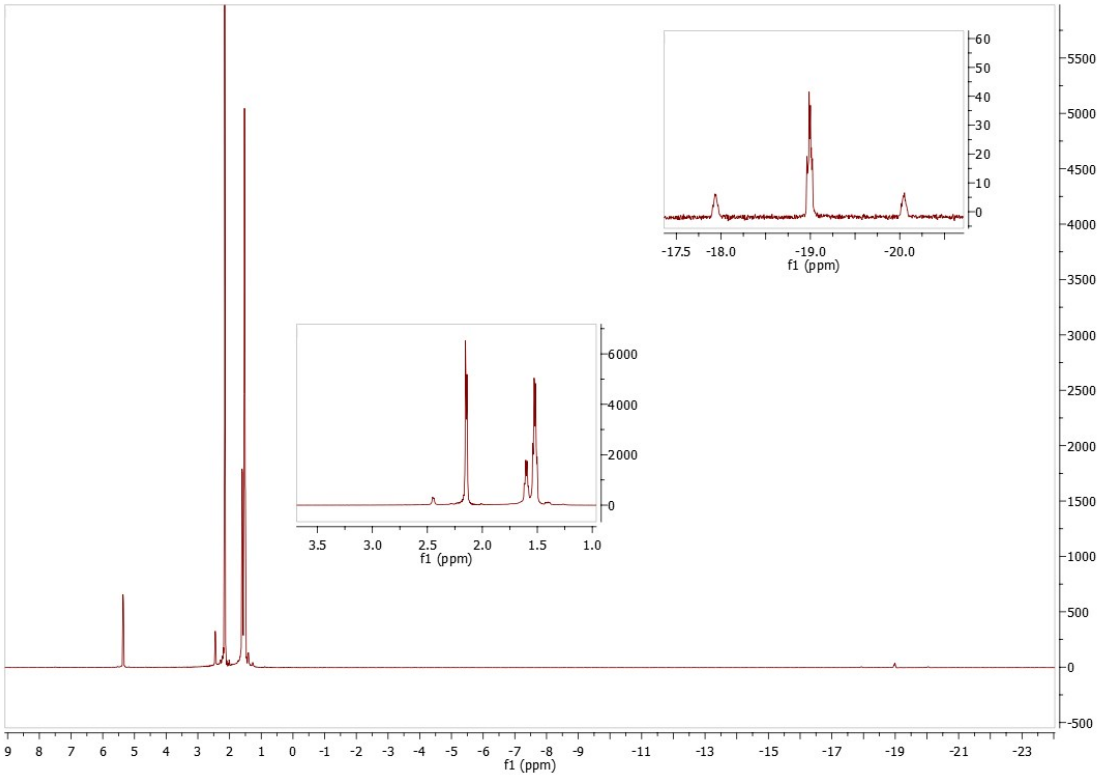


Figure S7. ^{1}H NMR spectrum of the reaction platinum(0) complex with the Cu(I) complex $[Cu(CH_3CN)_4]PF_6$ at -10 ˚C in CD_2Cl_2 (containing 0.5 water)

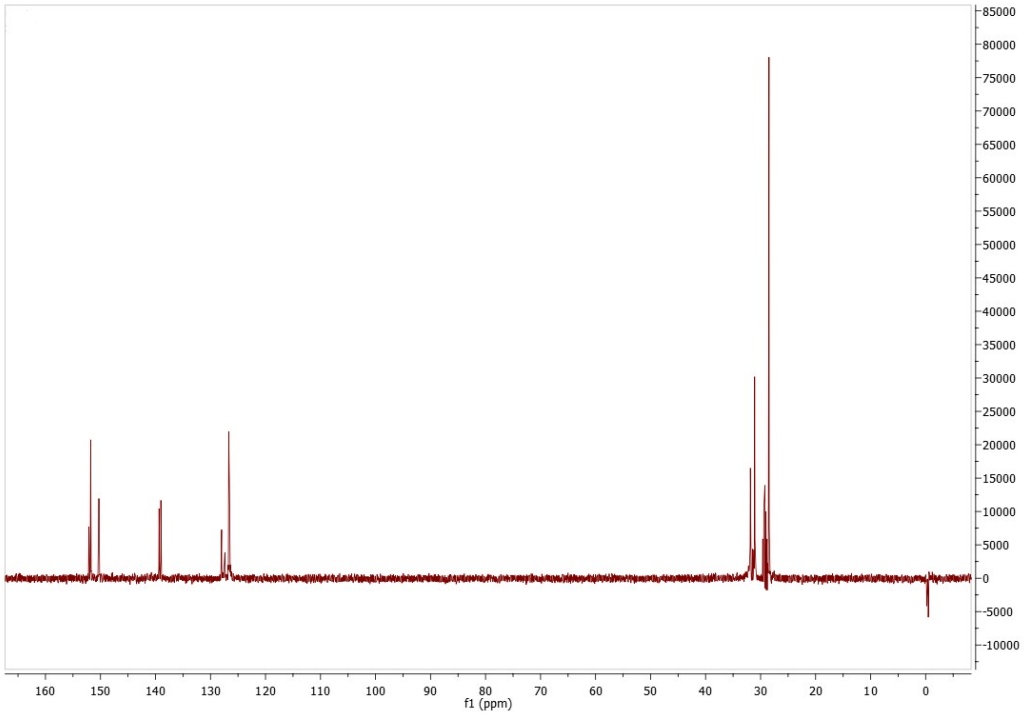


Figure S8. DEPT 135 NMR spectrum of **4** in acetone-d_6

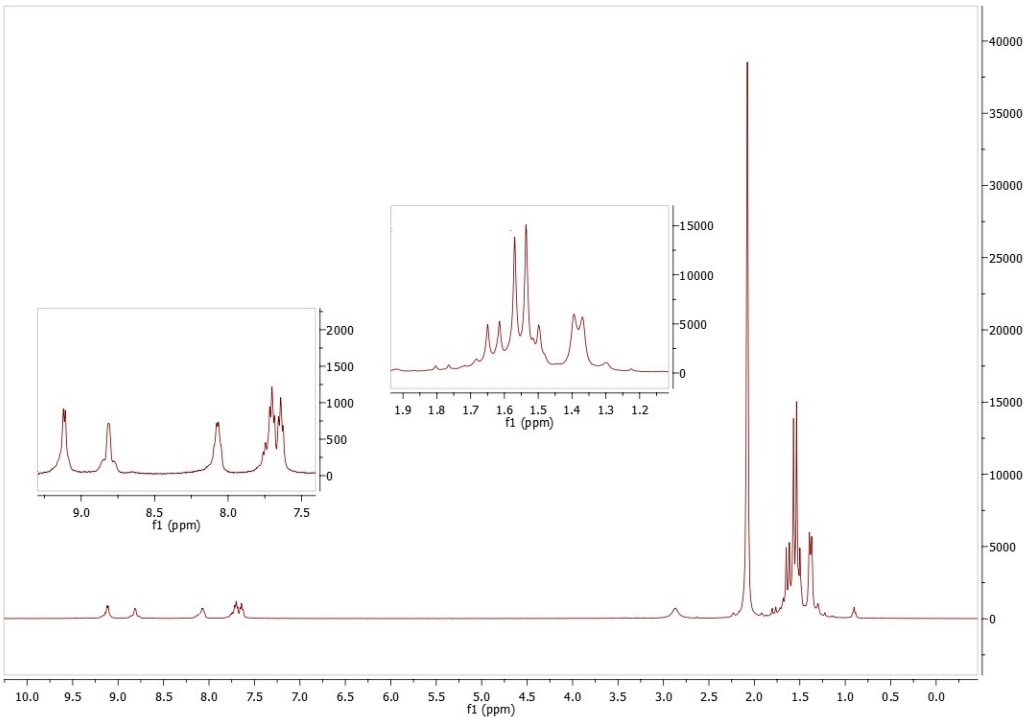


Figure S9. ^{1}H NMR spectrum of **4** in acetone d_6

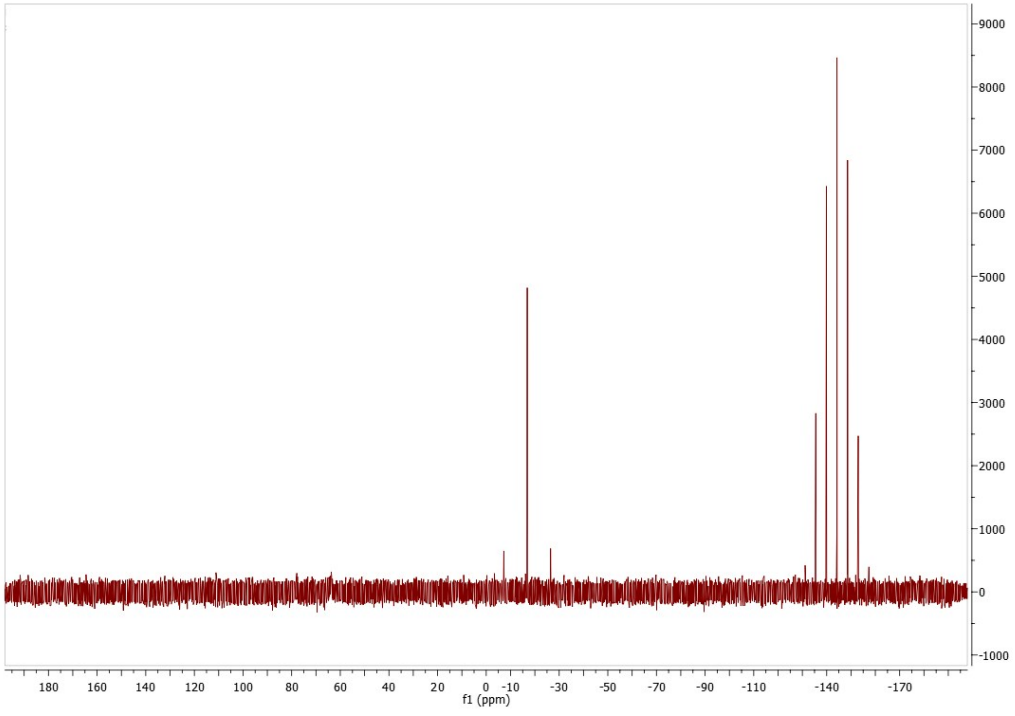


Figure S10. $^{31}P\{^{1}H\}$ NMR spectrum of **4** in acetone-d_6

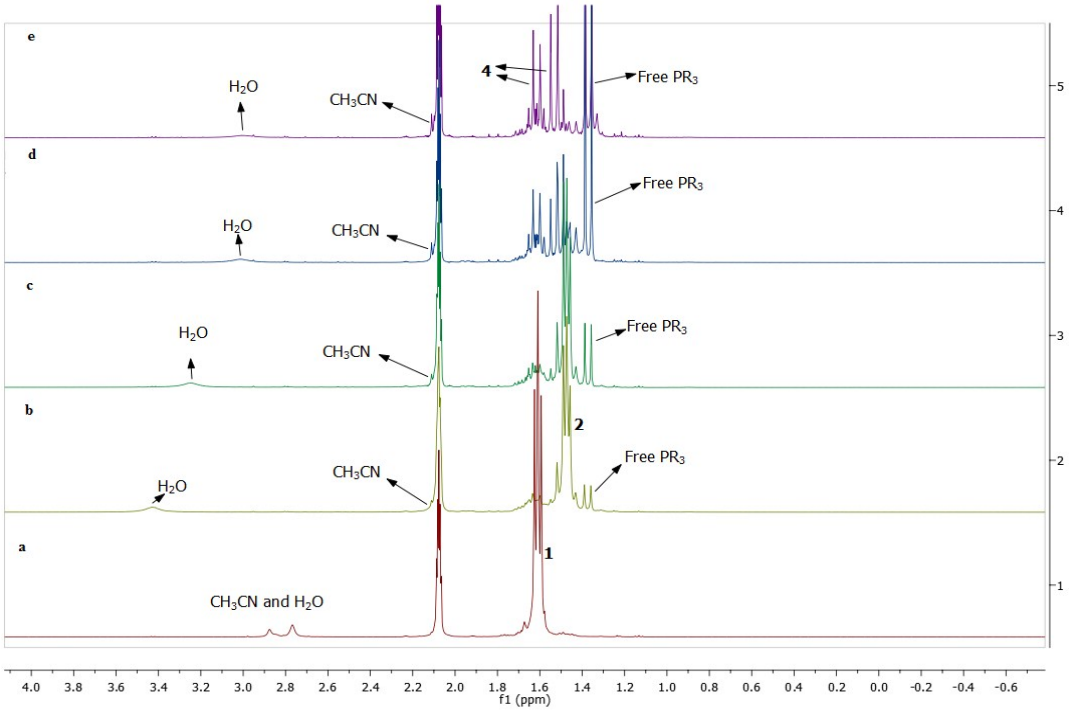


Figure S11. Monitoring of the reaction **1** with pyridine (ten-fold excess) using ^{1}H NMR spectroscopy. PR_3 =P^tBu_3

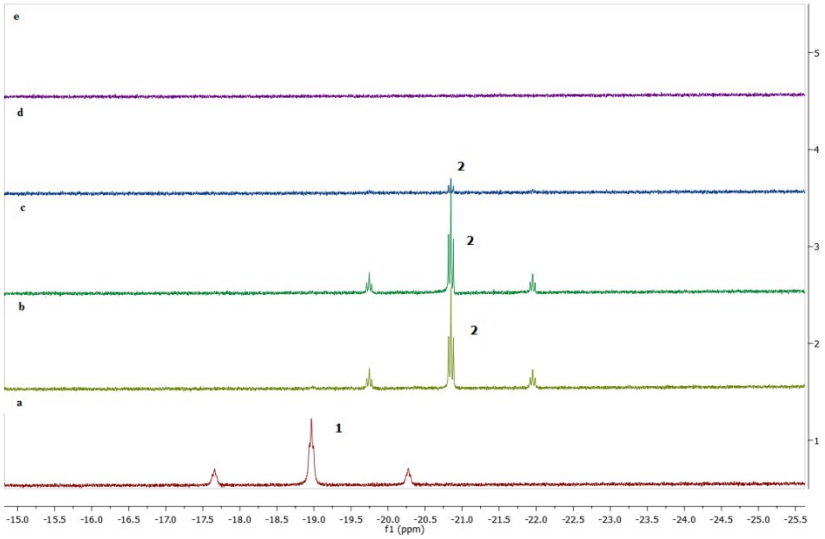
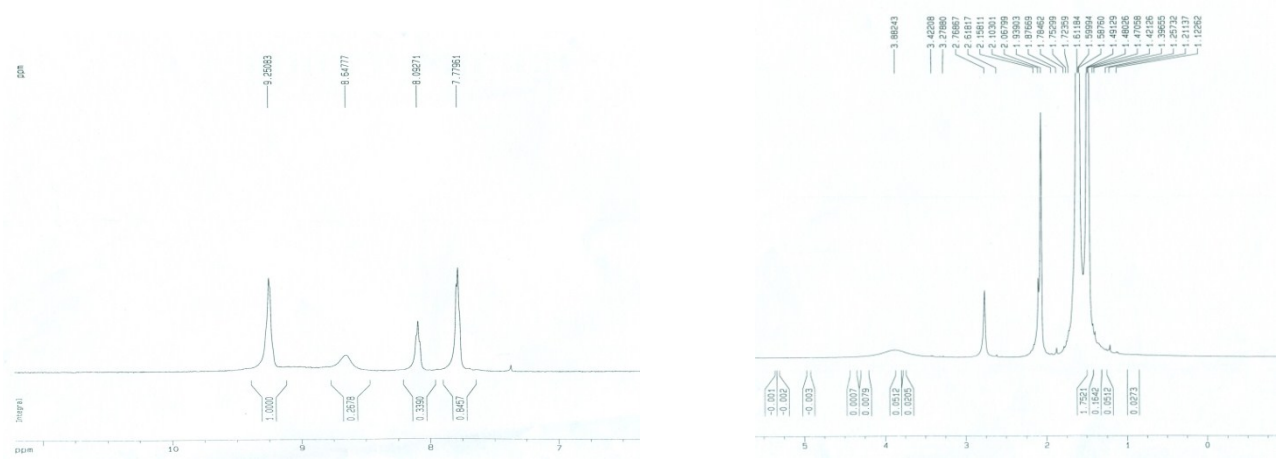


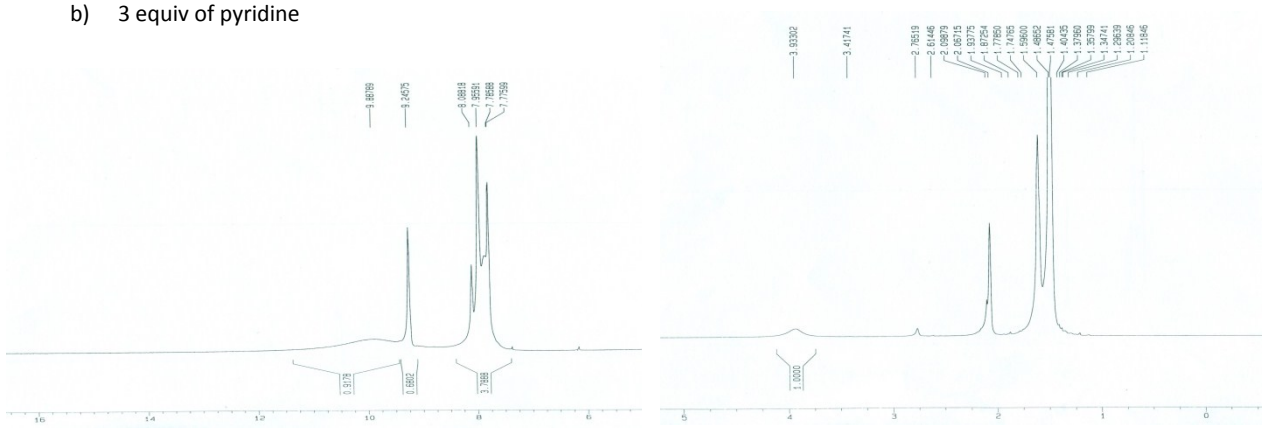
Figure S12. Monitoring of the reaction **1** with pyridine (ten-fold excess) using ^{1}H NMR spectroscopy (hydride region)

Figure S13. The following figures show monitoring the reaction with different concentration of pyridine using ^{1}H NMR spectroscopy in the acetone-d_6 in time frame 3 h.

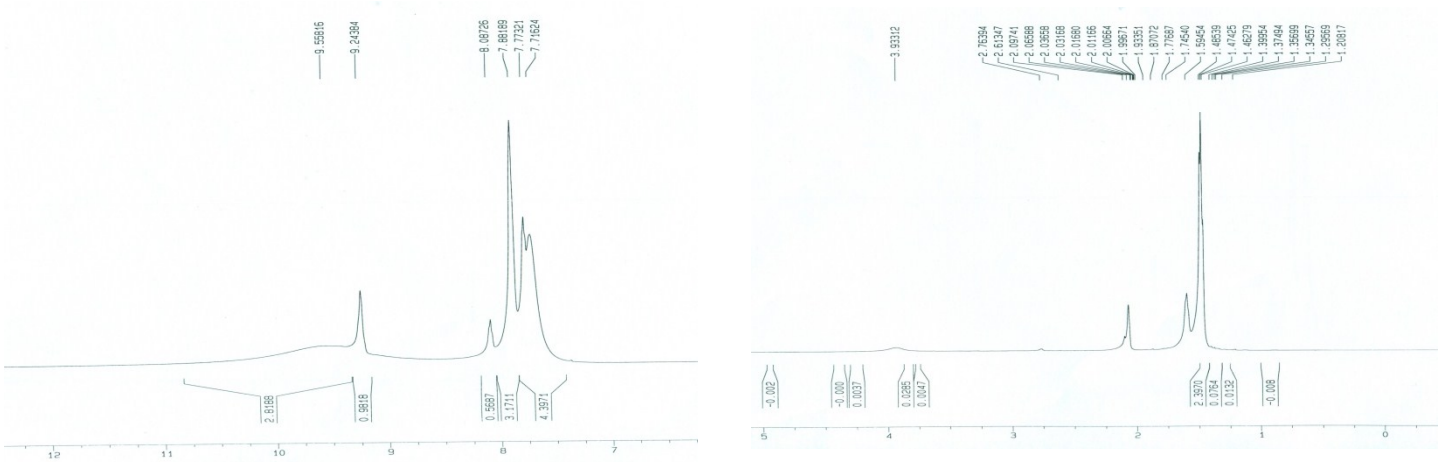
a) 2 equiv pyridine



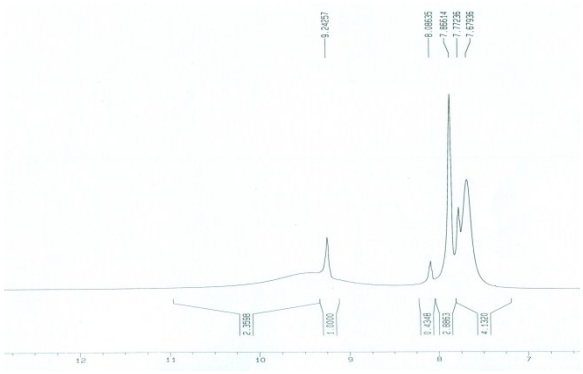
b) 3 equiv of pyridine

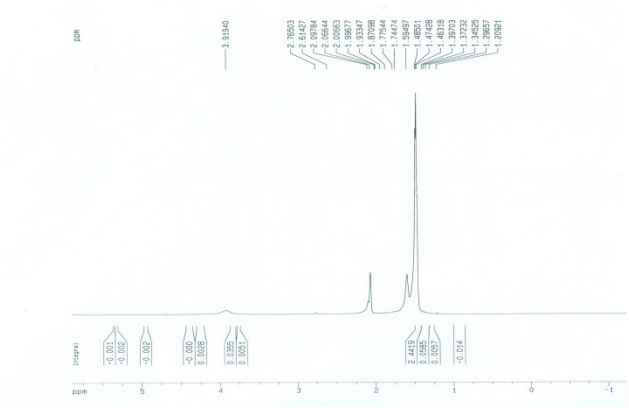


c) 4 equiv of pyridin

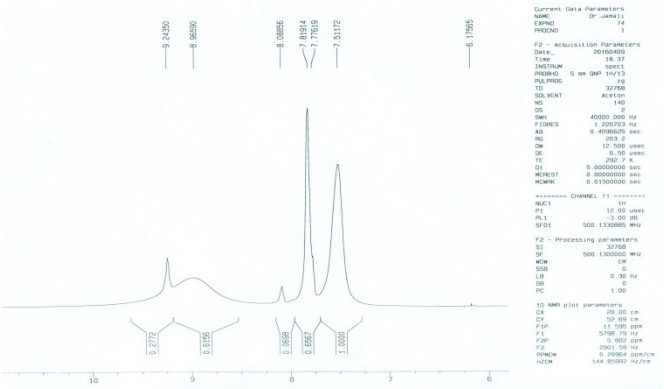


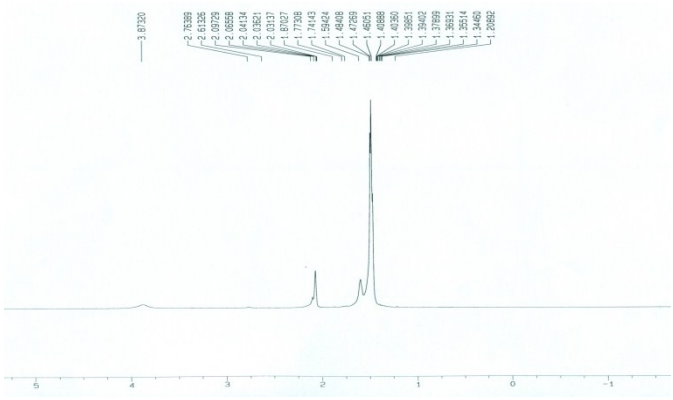
d) 5 equiv of pyridine



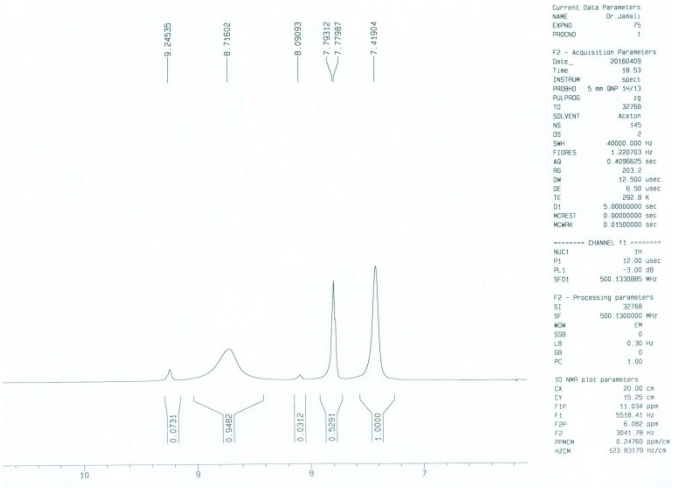


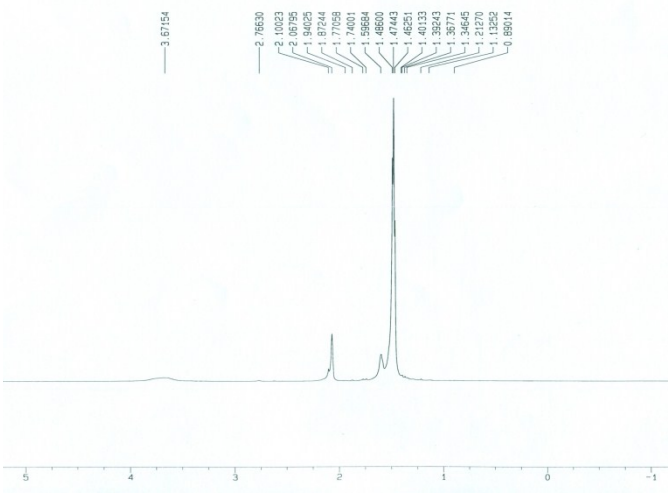
e) 6 equiv of pyridine





f) 10 equiv of pyridine





g) 20 equiv of pyridine

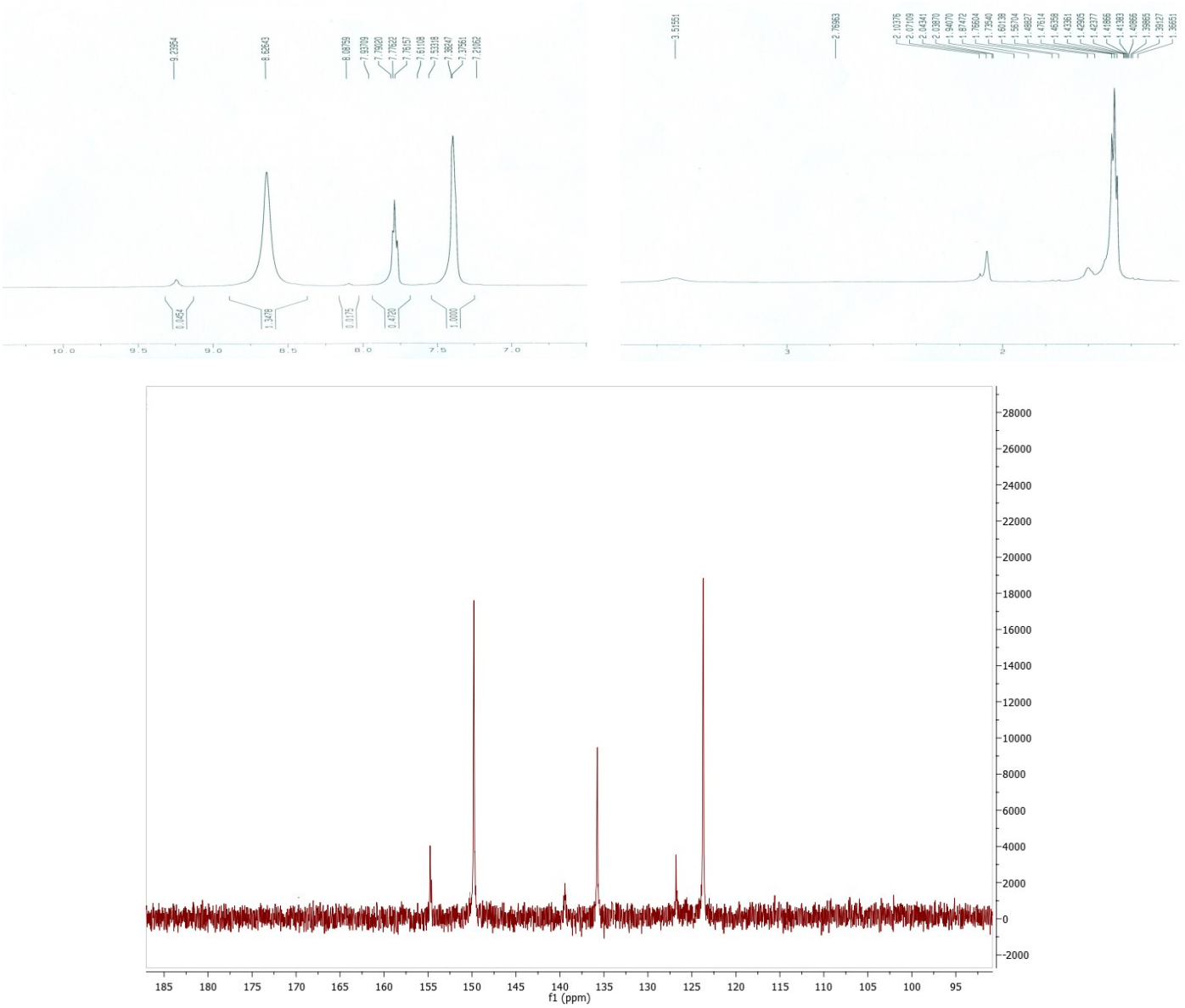


Figure S14. Pyridine region of the $^{13}C\{^{1}H\}$ NMR spectrum of the reaction between **1** and 2 equiv of pyridine that its ^{1}H NMR has shown in Figure S13 part (a)

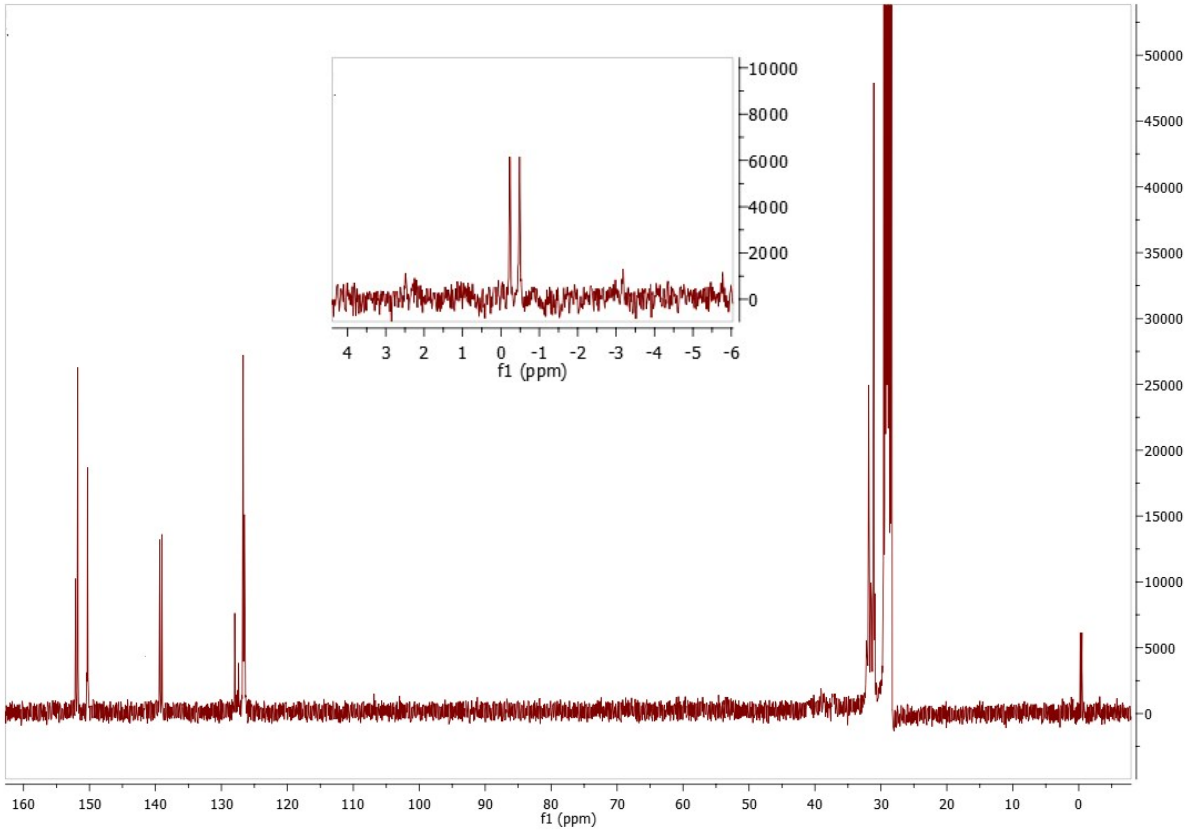


Figure S15. ^{13}C NMR spectrum of **4** in acetone-d_6

Table S1. Crystal data and structure refinement for **1**.

Identification code	1	
Empirical formula	$C_{26}H_{58}F_6NP_3Pt$	
Formula weight	786.73	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/n$	
Unit cell dimensions	a = 8.956(4) Å	α= 90°
	b = 12.531(5) Å	β= 91.695(5)°
	c = 29.404(13) Å	γ= 90°
Volume	3298(2) Å^3	
Z	4	
Density (calculated)	1.584 Mg/m^3	
Absorption coefficient	6.662 mm^{-1}	
F(000)	1592	
Theta range for data collection	1.767 to 27.818°	
Index ranges	-11<=h<=11, -16<=k<=16, -1<=l<=38	
Reflections collected	7774	
Independent reflections	7774 [R(int) = 0.063]	
Completeness to theta = 26.000°	99.9 %	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	7774 / 0 / 354	
Goodness-of-fit on F^2	1.086	
Final R indices [I > 2 σ (I)]	R1 = 0.0617, wR2 = 0.1436	
R indices (all data)	R1 = 0.0711, wR2 = 0.1475	
Largest diff. peak and hole	2.831 and -4.203 e.Å^{-3}	

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

Pt(1)-N(1)	2.099(9)
Pt(1)-P(1)	2.331(2)
Pt(1)-P(2)	2.343(2)
Pt(1)-H	1.2721
P(2)-C(15)	1.877(11)
P(2)-C(23)	1.891(10)
P(2)-C(19)	1.911(12)
P(1)-C(11)	1.888(11)
P(1)-C(3)	1.917(10)
P(1)-C(7)	1.920(12)
P(3)-F(5)	1.560(11)
P(3)-F(1)	1.562(10)
P(3)-F(6)	1.568(10)
P(3)-F(2)	1.571(8)
P(3)-F(3)	1.575(9)
P(3)-F(4)	1.589(8)
C(3)-C(5)	1.536(15)
C(3)-C(4)	1.541(14)
C(3)-C(6)	1.551(15)
N(1)-C(1)	1.123(14)
C(24)-C(23)	1.543(15)
C(24)-H(24A)	0.9600
C(24)-H(24B)	0.9600
C(24)-H(24C)	0.9600
C(17)-C(15)	1.549(16)
C(17)-H(17A)	0.9600
C(17)-H(17B)	0.9600
C(17)-H(17C)	0.9600
C(13)-C(11)	1.556(17)
C(13)-H(13A)	0.9600
C(13)-H(13B)	0.9600
C(13)-H(13C)	0.9600
C(15)-C(18)	1.523(15)
C(15)-C(16)	1.539(15)

C(2)-C(1)	1.446(15)
C(2)-H(2A)	0.9600
C(2)-H(2B)	0.9600
C(2)-H(2C)	0.9600
C(11)-C(14)	1.533(17)
C(11)-C(12)	1.543(15)
C(7)-C(9)	1.527(19)
C(7)-C(10)	1.535(18)
C(7)-C(8)	1.565(18)
C(25)-C(23)	1.545(14)
C(25)-H(25A)	0.9600
C(25)-H(25B)	0.9600
C(25)-H(25C)	0.9600
C(4)-H(4A)	0.9600
C(4)-H(4B)	0.9600
C(4)-H(4C)	0.9600
C(6)-H(6A)	0.9600
C(6)-H(6B)	0.9600
C(6)-H(6C)	0.9600
C(19)-C(21)	1.529(16)
C(19)-C(22)	1.530(16)
C(19)-C(20)	1.557(16)
C(18)-H(18A)	0.9600
C(18)-H(18B)	0.9600
C(18)-H(18C)	0.9600
C(23)-C(26)	1.540(15)
C(26)-H(26A)	0.9600
C(26)-H(26B)	0.9600
C(26)-H(26C)	0.9600
C(16)-H(16A)	0.9600
C(16)-H(16B)	0.9600
C(16)-H(16C)	0.9600
C(5)-H(5A)	0.9600
C(5)-H(5B)	0.9600
C(5)-H(5C)	0.9600
C(21)-H(21A)	0.9600

C(21)-H(21B)	0.9600
C(21)-H(21C)	0.9600
C(14)-H(14A)	0.9600
C(14)-H(14B)	0.9600
C(14)-H(14C)	0.9600
C(10)-H(10A)	0.9600
C(10)-H(10B)	0.9600
C(10)-H(10C)	0.9600
C(20)-H(20A)	0.9600
C(20)-H(20B)	0.9600
C(20)-H(20C)	0.9600
C(12)-H(12A)	0.9600
C(12)-H(12B)	0.9600
C(12)-H(12C)	0.9600
C(9)-H(9A)	0.9600
C(9)-H(9B)	0.9600
C(9)-H(9C)	0.9600
C(8)-H(8A)	0.9600
C(8)-H(8B)	0.9600
C(8)-H(8C)	0.9600
C(22)-H(22A)	0.9600
C(22)-H(22B)	0.9600
C(22)-H(22C)	0.9600

N(1)-Pt(1)-P(1)	97.6(2)
N(1)-Pt(1)-P(2)	99.0(2)
P(1)-Pt(1)-P(2)	163.38(9)
N(1)-Pt(1)-H	144.6
P(1)-Pt(1)-H	77.4
P(2)-Pt(1)-H	89.4
C(15)-P(2)-C(23)	109.8(5)
C(15)-P(2)-C(19)	109.6(5)
C(23)-P(2)-C(19)	107.4(5)
C(15)-P(2)-Pt(1)	105.3(3)
C(23)-P(2)-Pt(1)	113.6(3)
C(19)-P(2)-Pt(1)	111.2(3)

C(11)-P(1)-C(3)	109.9(5)
C(11)-P(1)-C(7)	108.8(6)
C(3)-P(1)-C(7)	106.8(5)
C(11)-P(1)-Pt(1)	109.1(4)
C(3)-P(1)-Pt(1)	112.3(3)
C(7)-P(1)-Pt(1)	110.0(4)
F(5)-P(3)-F(1)	93.6(9)
F(5)-P(3)-F(6)	89.6(8)
F(1)-P(3)-F(6)	176.7(8)
F(5)-P(3)-F(2)	88.2(6)
F(1)-P(3)-F(2)	87.6(6)
F(6)-P(3)-F(2)	91.8(6)
F(5)-P(3)-F(3)	176.7(8)
F(1)-P(3)-F(3)	89.4(8)
F(6)-P(3)-F(3)	87.3(6)
F(2)-P(3)-F(3)	90.7(5)
F(5)-P(3)-F(4)	92.1(6)
F(1)-P(3)-F(4)	91.0(6)
F(6)-P(3)-F(4)	89.5(6)
F(2)-P(3)-F(4)	178.6(6)
F(3)-P(3)-F(4)	89.0(5)
C(5)-C(3)-C(4)	107.7(9)
C(5)-C(3)-C(6)	107.1(10)
C(4)-C(3)-C(6)	108.7(9)
C(5)-C(3)-P(1)	110.9(7)
C(4)-C(3)-P(1)	114.8(8)
C(6)-C(3)-P(1)	107.3(7)
C(1)-N(1)-Pt(1)	178.0(11)
C(23)-C(24)-H(24A)	109.5
C(23)-C(24)-H(24B)	109.5
H(24A)-C(24)-H(24B)	109.5
C(23)-C(24)-H(24C)	109.5
H(24A)-C(24)-H(24C)	109.5
H(24B)-C(24)-H(24C)	109.5
C(15)-C(17)-H(17A)	109.5
C(15)-C(17)-H(17B)	109.5

H(17A)-C(17)-H(17B)	109.5
C(15)-C(17)-H(17C)	109.5
H(17A)-C(17)-H(17C)	109.5
H(17B)-C(17)-H(17C)	109.5
C(11)-C(13)-H(13A)	109.5
C(11)-C(13)-H(13B)	109.5
H(13A)-C(13)-H(13B)	109.5
C(11)-C(13)-H(13C)	109.5
H(13A)-C(13)-H(13C)	109.5
H(13B)-C(13)-H(13C)	109.5
C(18)-C(15)-C(16)	105.2(9)
C(18)-C(15)-C(17)	106.3(9)
C(16)-C(15)-C(17)	106.9(10)
C(18)-C(15)-P(2)	112.5(8)
C(16)-C(15)-P(2)	109.3(7)
C(17)-C(15)-P(2)	115.9(7)
C(1)-C(2)-H(2A)	109.5
C(1)-C(2)-H(2B)	109.5
H(2A)-C(2)-H(2B)	109.5
C(1)-C(2)-H(2C)	109.5
H(2A)-C(2)-H(2C)	109.5
H(2B)-C(2)-H(2C)	109.5
C(14)-C(11)-C(12)	108.6(10)
C(14)-C(11)-C(13)	104.5(10)
C(12)-C(11)-C(13)	108.8(10)
C(14)-C(11)-P(1)	109.3(8)
C(12)-C(11)-P(1)	116.1(8)
C(13)-C(11)-P(1)	108.9(8)
C(9)-C(7)-C(10)	105.6(11)
C(9)-C(7)-C(8)	110.7(12)
C(10)-C(7)-C(8)	105.2(11)
C(9)-C(7)-P(1)	109.7(9)
C(10)-C(7)-P(1)	113.0(9)
C(8)-C(7)-P(1)	112.4(9)
C(23)-C(25)-H(25A)	109.5
C(23)-C(25)-H(25B)	109.5

H(25A)-C(25)-H(25B)	109.5
C(23)-C(25)-H(25C)	109.5
H(25A)-C(25)-H(25C)	109.5
H(25B)-C(25)-H(25C)	109.5
N(1)-C(1)-C(2)	177.6(13)
C(3)-C(4)-H(4A)	109.5
C(3)-C(4)-H(4B)	109.5
H(4A)-C(4)-H(4B)	109.5
C(3)-C(4)-H(4C)	109.5
H(4A)-C(4)-H(4C)	109.5
H(4B)-C(4)-H(4C)	109.5
C(3)-C(6)-H(6A)	109.5
C(3)-C(6)-H(6B)	109.5
H(6A)-C(6)-H(6B)	109.5
C(3)-C(6)-H(6C)	109.5
H(6A)-C(6)-H(6C)	109.5
H(6B)-C(6)-H(6C)	109.5
C(21)-C(19)-C(22)	108.8(10)
C(21)-C(19)-C(20)	107.1(10)
C(22)-C(19)-C(20)	105.7(10)
C(21)-C(19)-P(2)	114.4(8)
C(22)-C(19)-P(2)	109.7(8)
C(20)-C(19)-P(2)	110.8(8)
C(15)-C(18)-H(18A)	109.5
C(15)-C(18)-H(18B)	109.5
H(18A)-C(18)-H(18B)	109.5
C(15)-C(18)-H(18C)	109.5
H(18A)-C(18)-H(18C)	109.5
H(18B)-C(18)-H(18C)	109.5
C(26)-C(23)-C(24)	108.0(9)
C(26)-C(23)-C(25)	106.3(9)
C(24)-C(23)-C(25)	106.6(9)
C(26)-C(23)-P(2)	109.2(7)
C(24)-C(23)-P(2)	109.5(7)
C(25)-C(23)-P(2)	116.9(8)
C(23)-C(26)-H(26A)	109.5

C(23)-C(26)-H(26B)	109.5
H(26A)-C(26)-H(26B)	109.5
C(23)-C(26)-H(26C)	109.5
H(26A)-C(26)-H(26C)	109.5
H(26B)-C(26)-H(26C)	109.5
C(15)-C(16)-H(16A)	109.5
C(15)-C(16)-H(16B)	109.5
H(16A)-C(16)-H(16B)	109.5
C(15)-C(16)-H(16C)	109.5
H(16A)-C(16)-H(16C)	109.5
H(16B)-C(16)-H(16C)	109.5
C(3)-C(5)-H(5A)	109.5
C(3)-C(5)-H(5B)	109.5
H(5A)-C(5)-H(5B)	109.5
C(3)-C(5)-H(5C)	109.5
H(5A)-C(5)-H(5C)	109.5
H(5B)-C(5)-H(5C)	109.5
C(19)-C(21)-H(21A)	109.5
C(19)-C(21)-H(21B)	109.5
H(21A)-C(21)-H(21B)	109.5
C(19)-C(21)-H(21C)	109.5
H(21A)-C(21)-H(21C)	109.5
H(21B)-C(21)-H(21C)	109.5
C(11)-C(14)-H(14A)	109.5
C(11)-C(14)-H(14B)	109.5
H(14A)-C(14)-H(14B)	109.5
C(11)-C(14)-H(14C)	109.5
H(14A)-C(14)-H(14C)	109.5
H(14B)-C(14)-H(14C)	109.5
C(7)-C(10)-H(10A)	109.5
C(7)-C(10)-H(10B)	109.5
H(10A)-C(10)-H(10B)	109.5
C(7)-C(10)-H(10C)	109.5
H(10A)-C(10)-H(10C)	109.5
H(10B)-C(10)-H(10C)	109.5
C(19)-C(20)-H(20A)	109.5

C(19)-C(20)-H(20B)	109.5
H(20A)-C(20)-H(20B)	109.5
C(19)-C(20)-H(20C)	109.5
H(20A)-C(20)-H(20C)	109.5
H(20B)-C(20)-H(20C)	109.5
C(11)-C(12)-H(12A)	109.5
C(11)-C(12)-H(12B)	109.5
H(12A)-C(12)-H(12B)	109.5
C(11)-C(12)-H(12C)	109.5
H(12A)-C(12)-H(12C)	109.5
H(12B)-C(12)-H(12C)	109.5
C(7)-C(9)-H(9A)	109.5
C(7)-C(9)-H(9B)	109.5
H(9A)-C(9)-H(9B)	109.5
C(7)-C(9)-H(9C)	109.5
H(9A)-C(9)-H(9C)	109.5
H(9B)-C(9)-H(9C)	109.5
C(7)-C(8)-H(8A)	109.5
C(7)-C(8)-H(8B)	109.5
H(8A)-C(8)-H(8B)	109.5
C(7)-C(8)-H(8C)	109.5
H(8A)-C(8)-H(8C)	109.5
H(8B)-C(8)-H(8C)	109.5
C(19)-C(22)-H(22A)	109.5
C(19)-C(22)-H(22B)	109.5
H(22A)-C(22)-H(22B)	109.5
C(19)-C(22)-H(22C)	109.5
H(22A)-C(22)-H(22C)	109.5
H(22B)-C(22)-H(22C)	109.5

Symmetry transformations used to generate equivalent atoms:

Table S3. Torsion angles [°] for **1**.

C(23)-P(2)-C(15)-C(18)	-163.8(8)
C(19)-P(2)-C(15)-C(18)	-46.1(9)
Pt(1)-P(2)-C(15)-C(18)	73.5(8)
C(23)-P(2)-C(15)-C(16)	79.7(8)
C(19)-P(2)-C(15)-C(16)	-162.6(8)
Pt(1)-P(2)-C(15)-C(16)	-42.9(8)
C(23)-P(2)-C(15)-C(17)	-41.1(10)
C(19)-P(2)-C(15)-C(17)	76.6(9)
Pt(1)-P(2)-C(15)-C(17)	-163.8(8)
C(3)-P(1)-C(11)-C(14)	76.3(9)
C(7)-P(1)-C(11)-C(14)	-167.2(8)
Pt(1)-P(1)-C(11)-C(14)	-47.2(9)
C(3)-P(1)-C(11)-C(12)	-46.9(11)
C(7)-P(1)-C(11)-C(12)	69.6(11)
Pt(1)-P(1)-C(11)-C(12)	-170.4(9)
C(3)-P(1)-C(11)-C(13)	-170.1(8)
C(7)-P(1)-C(11)-C(13)	-53.5(9)
Pt(1)-P(1)-C(11)-C(13)	66.4(8)
C(15)-P(2)-C(23)-C(26)	-50.2(8)
C(19)-P(2)-C(23)-C(26)	-169.2(7)
Pt(1)-P(2)-C(23)-C(26)	67.4(8)
C(15)-P(2)-C(23)-C(24)	-168.2(7)
C(19)-P(2)-C(23)-C(24)	72.7(8)
Pt(1)-P(2)-C(23)-C(24)	-50.6(8)
C(15)-P(2)-C(23)-C(25)	70.5(9)
C(19)-P(2)-C(23)-C(25)	-48.5(10)
Pt(1)-P(2)-C(23)-C(25)	-171.9(7)

Symmetry transformations used to generate equivalent atoms:

Table S4 - Hydrogen Bonds (Angstrom, Deg)

C2 -- H2A .. F2	0.9600	2.4500	3.405(17)	178.00	2_555
C2 -- H2C .. F6	0.9600	2.2500	3.116(19)	150.00	.
C5 -- H5A .. N1	0.9600	2.5600	3.418(19)	149.00	.
C14 -- H14C .. N1	0.9600	2.6200	3.339(19)	132.00	.
C24 -- H24C .. N1	0.9600	2.5400	3.163(17)	123.00	.
C26 -- H26A .. N1	0.9600	2.5400	3.320(18)	139.00	.

2555 = 1/2-x,1/2+y,1/2-z

Table S5. Crystal data and structure refinement for complex **4**.

Identification code	pp21n	
Empirical formula	C22 H36 F6 N2 P2 Pt	
Formula weight	699.56	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	*P*2(1)/*n*	
Unit cell dimensions	*a* = 11.4313(6) Å	α= 90°.
	b = 13.8224(8) Å	β= 106.597(3)°.
	c = 17.2917(10) Å	γ= 90°.
Volume	2618.4(3) Å^3	
Z	4	
Density (calculated)	1.775 Mg/m^3	
Absorption coefficient	5.537 mm^{-1}	
F(000)	1376	
Crystal size	0.18 x 0.16 x 0.12 mm^3	
Theta range for data collection	1.91 to 25.50°	
Index ranges	-13<=h<=13, -16<=k<=16, -20<=l<=20	
Reflections collected	35958	
Independent reflections	4785 [R(int) = 0.0610]	
Completeness to theta = 25.50°	98.1 %	
Absorption correction	Empirical	
Max. and min. transmission	0.5563 and 0.4356	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4785 / 0 / 307	
Goodness-of-fit on F^2	1.126	
Final R indices [I > 2σ (I)]	R1 = 0.0412, wR2 = 0.1198	
R indices (all data)	R1 = 0.0438, wR2 = 0.1219	
Largest diff. peak and hole	3.664 and -3.029 e.Å^{-3}	

Table S6 Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **4**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Pt(1)	3708(1)	2413(1)	1803(1)	14(1)
P(1)	3522(2)	2561(1)	489(1)	15(1)
P(2)	5527(2)	6319(1)	2963(1)	22(1)
F(5)	5675(6)	7246(4)	3537(3)	41(1)
F(6)	6529(4)	6755(4)	2574(3)	33(1)
F(2)	5421(6)	5394(4)	2405(4)	54(2)
F(4)	6597(6)	5808(4)	3638(3)	54(2)
F(1)	4497(5)	6873(5)	2302(3)	52(2)
F(3)	4550(6)	5879(4)	3360(4)	61(2)
N(2)	3652(6)	2689(4)	2982(4)	19(1)
N(1)	4557(5)	1038(4)	2162(3)	18(1)
C(9)	2876(6)	1576(5)	-260(4)	20(1)
C(10)	1974(7)	986(6)	65(4)	25(2)
C(11)	2226(7)	1976(6)	-1104(4)	25(2)
C(2)	2387(6)	3564(5)	467(4)	19(1)
C(5)	4986(6)	3052(5)	340(4)	18(1)
C(205)	3995(6)	3571(5)	3306(4)	20(1)
C(7)	5410(7)	3919(6)	904(4)	26(2)
C(4)	1077(6)	3191(6)	313(5)	24(2)
C(8)	6009(7)	2292(6)	600(5)	25(2)
C(203)	3369(7)	3202(6)	4477(4)	27(2)
C(105)	5800(7)	974(5)	2401(4)	20(1)
C(101)	3931(7)	212(5)	2137(4)	22(1)
C(1)	2906(6)	3715(5)	1397(4)	21(2)
C(104)	6400(7)	104(6)	2587(4)	25(2)
C(201)	3172(6)	2062(6)	3409(4)	22(2)
C(202)	3027(8)	2282(7)	4150(5)	31(2)
C(204)	3858(7)	3846(6)	4051(4)	24(2)
C(12)	3877(7)	859(6)	-328(5)	29(2)
C(3)	2359(7)	4456(6)	-55(5)	28(2)
C(102)	4470(8)	-679(6)	2326(4)	27(2)

C(103)	5730(8)	-736(6)	2547(5)	30(2)
C(6)	4842(7)	3357(6)	-540(4)	23(2)

Table S7. Bond lengths [Å] and angles [°] for **4**.

Pt(1)-C(1)	2.050(7)
Pt(1)-N(2)	2.093(7)
Pt(1)-N(1)	2.144(6)
Pt(1)-P(1)	2.230(2)
P(1)-C(9)	1.878(7)
P(1)-C(5)	1.892(7)
P(1)-C(2)	1.892(7)
P(2)-F(1)	1.584(5)
P(2)-F(2)	1.586(6)
P(2)-F(3)	1.589(6)
P(2)-F(4)	1.595(5)
P(2)-F(5)	1.599(5)
P(2)-F(6)	1.603(5)
N(2)-C(205)	1.352(9)
N(2)-C(201)	1.352(10)
N(1)-C(101)	1.342(9)
N(1)-C(105)	1.364(9)
C(9)-C(11)	1.540(9)
C(9)-C(10)	1.541(10)
C(9)-C(12)	1.544(10)
C(10)-H(10A)	0.9800
C(10)-H(10B)	0.9800
C(10)-H(10C)	0.9800
C(11)-H(11A)	0.9800
C(11)-H(11B)	0.9800
C(11)-H(11C)	0.9800
C(2)-C(3)	1.523(10)
C(2)-C(4)	1.534(10)
C(2)-C(1)	1.561(10)
C(5)-C(7)	1.534(10)
C(5)-C(8)	1.539(10)
C(5)-C(6)	1.542(9)
C(205)-C(204)	1.394(10)
C(205)-H(205)	0.9500

C(7)-H(7A)	0.9800
C(7)-H(7B)	0.9800
C(7)-H(7C)	0.9800
C(4)-H(4A)	0.9800
C(4)-H(4B)	0.9800
C(4)-H(4C)	0.9800
C(8)-H(8A)	0.9800
C(8)-H(8B)	0.9800
C(8)-H(8C)	0.9800
C(203)-C(204)	1.373(11)
C(203)-C(202)	1.401(12)
C(203)-H(203)	0.9500
C(105)-C(104)	1.375(10)
C(105)-H(105)	0.9500
C(101)-C(102)	1.374(11)
C(101)-H(101)	0.9500
C(1)-H(1A)	0.9900
C(1)-H(1B)	0.9900
C(104)-C(103)	1.382(12)
C(104)-H(104)	0.9500
C(201)-C(202)	1.372(12)
C(201)-H(201)	0.9500
C(202)-H(202)	0.9500
C(204)-H(204)	0.9500
C(12)-H(12A)	0.9800
C(12)-H(12B)	0.9800
C(12)-H(12C)	0.9800
C(3)-H(3A)	0.9800
C(3)-H(3B)	0.9800
C(3)-H(3C)	0.9800
C(102)-C(103)	1.383(12)
C(102)-H(102)	0.9500
C(103)-H(103)	0.9500
C(6)-H(6A)	0.9800
C(6)-H(6B)	0.9800
C(6)-H(6C)	0.9800

C(1)-Pt(1)-N(2)	92.2(3)
C(1)-Pt(1)-N(1)	176.8(2)
N(2)-Pt(1)-N(1)	91.0(2)
C(1)-Pt(1)-P(1)	70.6(2)
N(2)-Pt(1)-P(1)	162.79(18)
N(1)-Pt(1)-P(1)	106.23(16)
C(9)-P(1)-C(5)	110.8(3)
C(9)-P(1)-C(2)	112.7(3)
C(5)-P(1)-C(2)	111.3(3)
C(9)-P(1)-Pt(1)	122.7(2)
C(5)-P(1)-Pt(1)	110.0(2)
C(2)-P(1)-Pt(1)	87.3(2)
F(1)-P(2)-F(2)	92.2(4)
F(1)-P(2)-F(3)	91.5(4)
F(2)-P(2)-F(3)	90.7(3)
F(1)-P(2)-F(4)	177.3(4)
F(2)-P(2)-F(4)	89.8(4)
F(3)-P(2)-F(4)	90.1(4)
F(1)-P(2)-F(5)	89.2(3)
F(2)-P(2)-F(5)	178.3(4)
F(3)-P(2)-F(5)	90.1(3)
F(4)-P(2)-F(5)	88.7(3)
F(1)-P(2)-F(6)	89.3(3)
F(2)-P(2)-F(6)	89.3(3)
F(3)-P(2)-F(6)	179.1(4)
F(4)-P(2)-F(6)	89.0(3)
F(5)-P(2)-F(6)	89.8(3)
C(205)-N(2)-C(201)	117.8(7)
C(205)-N(2)-Pt(1)	118.8(5)
C(201)-N(2)-Pt(1)	123.0(5)
C(101)-N(1)-C(105)	117.0(6)
C(101)-N(1)-Pt(1)	123.5(5)
C(105)-N(1)-Pt(1)	119.5(5)
C(11)-C(9)-C(10)	110.1(6)
C(11)-C(9)-C(12)	109.0(6)

C(10)-C(9)-C(12)	106.0(6)
C(11)-C(9)-P(1)	112.5(5)
C(10)-C(9)-P(1)	107.7(5)
C(12)-C(9)-P(1)	111.4(5)
C(9)-C(10)-H(10A)	109.5
C(9)-C(10)-H(10B)	109.5
H(10A)-C(10)-H(10B)	109.5
C(9)-C(10)-H(10C)	109.5
H(10A)-C(10)-H(10C)	109.5
H(10B)-C(10)-H(10C)	109.5
C(9)-C(11)-H(11A)	109.5
C(9)-C(11)-H(11B)	109.5
H(11A)-C(11)-H(11B)	109.5
C(9)-C(11)-H(11C)	109.5
H(11A)-C(11)-H(11C)	109.5
H(11B)-C(11)-H(11C)	109.5
C(3)-C(2)-C(4)	108.3(6)
C(3)-C(2)-C(1)	116.1(6)
C(4)-C(2)-C(1)	106.8(6)
C(3)-C(2)-P(1)	120.3(5)
C(4)-C(2)-P(1)	112.8(5)
C(1)-C(2)-P(1)	91.2(4)
C(7)-C(5)-C(8)	105.8(6)
C(7)-C(5)-C(6)	109.8(6)
C(8)-C(5)-C(6)	109.4(6)
C(7)-C(5)-P(1)	108.9(5)
C(8)-C(5)-P(1)	110.1(5)
C(6)-C(5)-P(1)	112.6(5)
N(2)-C(205)-C(204)	122.1(7)
N(2)-C(205)-H(205)	118.9
C(204)-C(205)-H(205)	118.9
C(5)-C(7)-H(7A)	109.5
C(5)-C(7)-H(7B)	109.5
H(7A)-C(7)-H(7B)	109.5
C(5)-C(7)-H(7C)	109.5
H(7A)-C(7)-H(7C)	109.5

H(7B)-C(7)-H(7C)	109.5
C(2)-C(4)-H(4A)	109.5
C(2)-C(4)-H(4B)	109.5
H(4A)-C(4)-H(4B)	109.5
C(2)-C(4)-H(4C)	109.5
H(4A)-C(4)-H(4C)	109.5
H(4B)-C(4)-H(4C)	109.5
C(5)-C(8)-H(8A)	109.5
C(5)-C(8)-H(8B)	109.5
H(8A)-C(8)-H(8B)	109.5
C(5)-C(8)-H(8C)	109.5
H(8A)-C(8)-H(8C)	109.5
H(8B)-C(8)-H(8C)	109.5
C(204)-C(203)-C(202)	118.8(7)
C(204)-C(203)-H(203)	120.6
C(202)-C(203)-H(203)	120.6
N(1)-C(105)-C(104)	122.3(7)
N(1)-C(105)-H(105)	118.9
C(104)-C(105)-H(105)	118.9
N(1)-C(101)-C(102)	123.8(7)
N(1)-C(101)-H(101)	118.1
C(102)-C(101)-H(101)	118.1
C(2)-C(1)-Pt(1)	103.7(4)
C(2)-C(1)-H(1A)	111.0
Pt(1)-C(1)-H(1A)	111.0
C(2)-C(1)-H(1B)	111.0
Pt(1)-C(1)-H(1B)	111.0
H(1A)-C(1)-H(1B)	109.0
C(105)-C(104)-C(103)	119.4(7)
C(105)-C(104)-H(104)	120.3
C(103)-C(104)-H(104)	120.3
N(2)-C(201)-C(202)	123.0(8)
N(2)-C(201)-H(201)	118.5
C(202)-C(201)-H(201)	118.5
C(201)-C(202)-C(203)	118.9(8)
C(201)-C(202)-H(202)	120.5

C(203)-C(202)-H(202)	120.5
C(203)-C(204)-C(205)	119.4(7)
C(203)-C(204)-H(204)	120.3
C(205)-C(204)-H(204)	120.3
C(9)-C(12)-H(12A)	109.5
C(9)-C(12)-H(12B)	109.5
H(12A)-C(12)-H(12B)	109.5
C(9)-C(12)-H(12C)	109.5
H(12A)-C(12)-H(12C)	109.5
H(12B)-C(12)-H(12C)	109.5
C(2)-C(3)-H(3A)	109.5
C(2)-C(3)-H(3B)	109.5
H(3A)-C(3)-H(3B)	109.5
C(2)-C(3)-H(3C)	109.5
H(3A)-C(3)-H(3C)	109.5
H(3B)-C(3)-H(3C)	109.5
C(101)-C(102)-C(103)	118.5(7)
C(101)-C(102)-H(102)	120.7
C(103)-C(102)-H(102)	120.7
C(104)-C(103)-C(102)	119.0(7)
C(104)-C(103)-H(103)	120.5
C(102)-C(103)-H(103)	120.5
C(5)-C(6)-H(6A)	109.5
C(5)-C(6)-H(6B)	109.5
H(6A)-C(6)-H(6B)	109.5
C(5)-C(6)-H(6C)	109.5
H(6A)-C(6)-H(6C)	109.5
H(6B)-C(6)-H(6C)	109.5

Symmetry transformations used to generate equivalent atoms:

Table S8. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **4.** The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Pt(1)	13(1)	15(1)	14(1)	0(1)	5(1)	-1(1)
P(1)	15(1)	14(1)	15(1)	1(1)	3(1)	-1(1)
P(2)	24(1)	23(1)	20(1)	1(1)	7(1)	1(1)
F(5)	61(4)	27(2)	38(3)	-3(2)	20(3)	3(3)
F(6)	28(2)	37(3)	35(3)	4(2)	15(2)	2(2)
F(2)	62(4)	46(3)	61(4)	-29(3)	30(3)	-24(3)
F(4)	75(4)	48(3)	33(3)	18(2)	5(3)	27(3)
F(1)	23(3)	79(4)	45(3)	8(3)	-6(2)	11(3)
F(3)	80(4)	44(3)	83(4)	-9(3)	65(4)	-17(3)
N(2)	16(3)	23(3)	19(3)	2(2)	5(2)	4(2)
N(1)	17(3)	20(3)	15(3)	0(2)	2(2)	0(2)
C(9)	20(3)	19(3)	18(3)	0(3)	3(3)	-4(3)
C(10)	26(4)	22(4)	23(4)	-1(3)	3(3)	-9(3)
C(11)	23(4)	29(4)	19(4)	1(3)	0(3)	-6(3)
C(2)	17(3)	17(3)	22(3)	2(3)	8(3)	2(3)
C(5)	17(3)	20(3)	16(3)	4(3)	4(3)	-3(3)
C(205)	15(3)	19(3)	22(4)	-1(3)	2(3)	1(3)
C(7)	24(4)	30(4)	23(4)	0(3)	5(3)	-10(3)
C(4)	13(3)	30(4)	29(4)	2(3)	9(3)	5(3)
C(8)	15(4)	35(4)	28(4)	5(3)	8(3)	4(3)
C(203)	20(4)	41(5)	16(4)	-1(3)	1(3)	9(3)
C(105)	26(4)	20(4)	13(3)	2(3)	5(3)	-5(3)
C(101)	20(3)	26(4)	19(3)	0(3)	4(3)	-3(3)
C(1)	17(3)	21(4)	26(4)	-1(3)	8(3)	7(3)
C(104)	24(4)	28(4)	24(4)	4(3)	9(3)	5(3)
C(201)	10(3)	33(4)	22(4)	5(3)	5(3)	-3(3)
C(202)	28(4)	37(4)	22(4)	4(3)	-2(3)	4(4)
C(204)	20(4)	31(4)	20(4)	-5(3)	4(3)	3(3)
C(12)	34(4)	21(4)	28(4)	-8(3)	5(3)	1(3)
C(3)	30(4)	25(4)	28(4)	4(3)	7(3)	4(3)
C(102)	36(4)	20(4)	26(4)	1(3)	12(3)	-5(3)

C(103)	41(5)	20(4)	31(4)	4(3)	13(4)	7(3)
C(6)	20(4)	32(4)	21(4)	7(3)	10(3)	-7(3)

Table S9. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^{-3}) for **4**.

	x	y	z	U(eq)
H(10A)	1331	1414	139	37
H(10B)	2410	694	583	37
H(10C)	1608	475	-322	37
H(11A)	2805	2352	-1304	37
H(11B)	1547	2393	-1072	37
H(11C)	1910	1437	-1473	37
H(205)	4340	4019	3016	24
H(7A)	5484	3724	1461	39
H(7B)	4812	4443	747	39
H(7C)	6204	4143	864	39
H(4A)	549	3721	387	36
H(4B)	1063	2669	694	36
H(4C)	782	2945	-240	36
H(8A)	6801	2605	666	38
H(8B)	5886	1788	186	38
H(8C)	5990	2001	1113	38
H(203)	3265	3376	4985	32
H(105)	6267	1549	2440	24
H(101)	3065	245	1980	26
H(1A)	2244	3865	1643	25
H(1B)	3512	4246	1522	25
H(104)	7266	82	2742	30
H(201)	2925	1442	3187	26
H(202)	2699	1818	4436	37
H(204)	4100	4473	4261	29
H(12A)	3495	283	-626	43
H(12B)	4369	671	213	43
H(12C)	4402	1168	-616	43
H(3A)	1801	4937	61	42
H(3B)	2075	4273	-625	42

H(3C)	3181	4732	65	42
H(102)	3988	-1244	2306	32
H(103)	6129	-1343	2669	36
H(6A)	4152	3804	-719	35
H(6B)	4693	2783	-887	35
H(6C)	5591	3678	-574	35

Table S10. Torsion angles [°] for **4.**

C(1)-Pt(1)-P(1)-C(9)	-131.9(4)
N(2)-Pt(1)-P(1)-C(9)	-133.7(7)
N(1)-Pt(1)-P(1)-C(9)	48.3(3)
C(1)-Pt(1)-P(1)-C(5)	95.1(3)
N(2)-Pt(1)-P(1)-C(5)	93.3(7)
N(1)-Pt(1)-P(1)-C(5)	-84.7(3)
C(1)-Pt(1)-P(1)-C(2)	-16.6(3)
N(2)-Pt(1)-P(1)-C(2)	-18.3(7)
N(1)-Pt(1)-P(1)-C(2)	163.6(3)
C(1)-Pt(1)-N(2)-C(205)	-44.9(6)
N(1)-Pt(1)-N(2)-C(205)	134.9(5)
P(1)-Pt(1)-N(2)-C(205)	-43.3(10)
C(1)-Pt(1)-N(2)-C(201)	128.1(6)
N(1)-Pt(1)-N(2)-C(201)	-52.1(6)
P(1)-Pt(1)-N(2)-C(201)	129.7(6)
C(1)-Pt(1)-N(1)-C(101)	-93(5)
N(2)-Pt(1)-N(1)-C(101)	90.9(6)
P(1)-Pt(1)-N(1)-C(101)	-89.7(5)
C(1)-Pt(1)-N(1)-C(105)	84(5)
N(2)-Pt(1)-N(1)-C(105)	-91.8(5)
P(1)-Pt(1)-N(1)-C(105)	87.6(5)
C(5)-P(1)-C(9)-C(11)	-77.5(6)
C(2)-P(1)-C(9)-C(11)	47.9(6)
Pt(1)-P(1)-C(9)-C(11)	149.9(4)
C(5)-P(1)-C(9)-C(10)	161.0(5)
C(2)-P(1)-C(9)-C(10)	-73.6(5)
Pt(1)-P(1)-C(9)-C(10)	28.4(6)
C(5)-P(1)-C(9)-C(12)	45.2(6)
C(2)-P(1)-C(9)-C(12)	170.6(5)
Pt(1)-P(1)-C(9)-C(12)	-87.5(5)
C(9)-P(1)-C(2)-C(3)	-93.3(6)
C(5)-P(1)-C(2)-C(3)	31.8(7)
Pt(1)-P(1)-C(2)-C(3)	142.2(6)
C(9)-P(1)-C(2)-C(4)	36.5(6)

C(5)-P(1)-C(2)-C(4)	161.5(5)
Pt(1)-P(1)-C(2)-C(4)	-88.1(5)
C(9)-P(1)-C(2)-C(1)	145.2(4)
C(5)-P(1)-C(2)-C(1)	-89.7(5)
Pt(1)-P(1)-C(2)-C(1)	20.7(4)
C(9)-P(1)-C(5)-C(7)	174.3(5)
C(2)-P(1)-C(5)-C(7)	48.2(6)
Pt(1)-P(1)-C(5)-C(7)	-46.8(5)
C(9)-P(1)-C(5)-C(8)	-70.2(6)
C(2)-P(1)-C(5)-C(8)	163.7(5)
Pt(1)-P(1)-C(5)-C(8)	68.7(5)
C(9)-P(1)-C(5)-C(6)	52.3(6)
C(2)-P(1)-C(5)-C(6)	-73.9(6)
Pt(1)-P(1)-C(5)-C(6)	-168.9(5)
C(201)-N(2)-C(205)-C(204)	-0.5(10)
Pt(1)-N(2)-C(205)-C(204)	172.9(5)
C(101)-N(1)-C(105)-C(104)	1.9(10)
Pt(1)-N(1)-C(105)-C(104)	-175.6(5)
C(105)-N(1)-C(101)-C(102)	-0.9(10)
Pt(1)-N(1)-C(101)-C(102)	176.5(6)
C(3)-C(2)-C(1)-Pt(1)	-148.2(5)
C(4)-C(2)-C(1)-Pt(1)	91.0(5)
P(1)-C(2)-C(1)-Pt(1)	-23.3(4)
N(2)-Pt(1)-C(1)-C(2)	-159.7(4)
N(1)-Pt(1)-C(1)-C(2)	24(5)
P(1)-Pt(1)-C(1)-C(2)	20.8(4)
N(1)-C(105)-C(104)-C(103)	-1.2(11)
C(205)-N(2)-C(201)-C(202)	-0.3(11)
Pt(1)-N(2)-C(201)-C(202)	-173.4(6)
N(2)-C(201)-C(202)-C(203)	1.1(12)
C(204)-C(203)-C(202)-C(201)	-1.1(11)
C(202)-C(203)-C(204)-C(205)	0.3(11)
N(2)-C(205)-C(204)-C(203)	0.5(11)
N(1)-C(101)-C(102)-C(103)	-0.8(12)
C(105)-C(104)-C(103)-C(102)	-0.6(12)
C(101)-C(102)-C(103)-C(104)	1.5(12)

Symmetry transformations used to generate equivalent atoms: