

Platinum(0)- η^2 -1,2-(*E*)ditosylethene complexes bearing phosphine, isocyanide and *N*-heterocyclic carbene ligands: synthesis and cytotoxicity towards ovarian and breast cancer cells

Nicola Compagno¹, Rachele Piccolo¹, Enrica Bortolamiol¹, Nicola Demitri², Flavio Rizzolio^{1,3}, Fabiano Visentin^{1*} and Thomas Scattolin^{4*}

¹ Department of Molecular Sciences and Nanosystems Università Ca' Foscari Campus Scientifico
Via Torino 155, 30174, Venezia, Italy: nicola.compagno@unive.it (N.C.);

enrica.bortolamiol@unive.it (E.B.); flavio.rizzolio@unive.it (F.R.); fvise@unive.it (F.V.)

² Area Science Park Elettra-Sincrotrone Trieste, S.S. 14 Km 163.5 Basovizza, 34149, Trieste, Italy

³ Pathology Unit, Department of Molecular Biology and Translational Research Centro di
Riferimento Oncologico di Aviano (CRO) IRCCS via Franco Gallini 2, 33081, Aviano, Italy:
flavio.rizzolio@unive.it (F.R.)

⁴ Dipartimento di Scienze Chimiche, Università degli Studi di Padova, via Marzolo 1, 35131
Padova, Italy: thomas.scattolin@unipd.it (T.S)

* Correspondence: thomas.scattolin@unipd.it (T.S); fvise@unive.it (F.V.)

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NMR and IR spectra

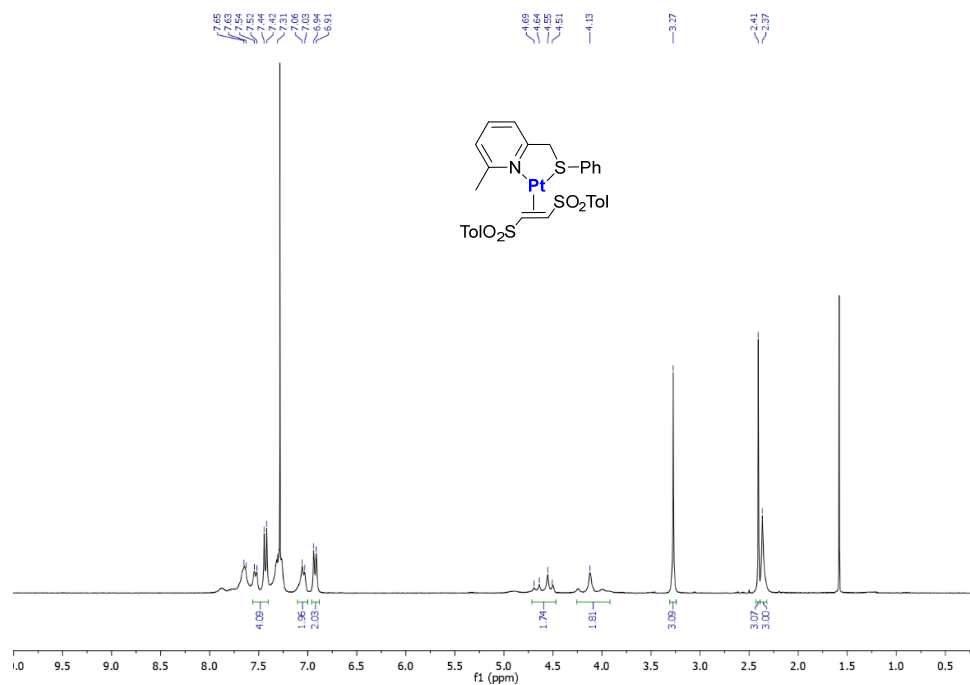


Figure S1. ¹H NMR spectrum of compound **1** in CDCl₃ at 298K

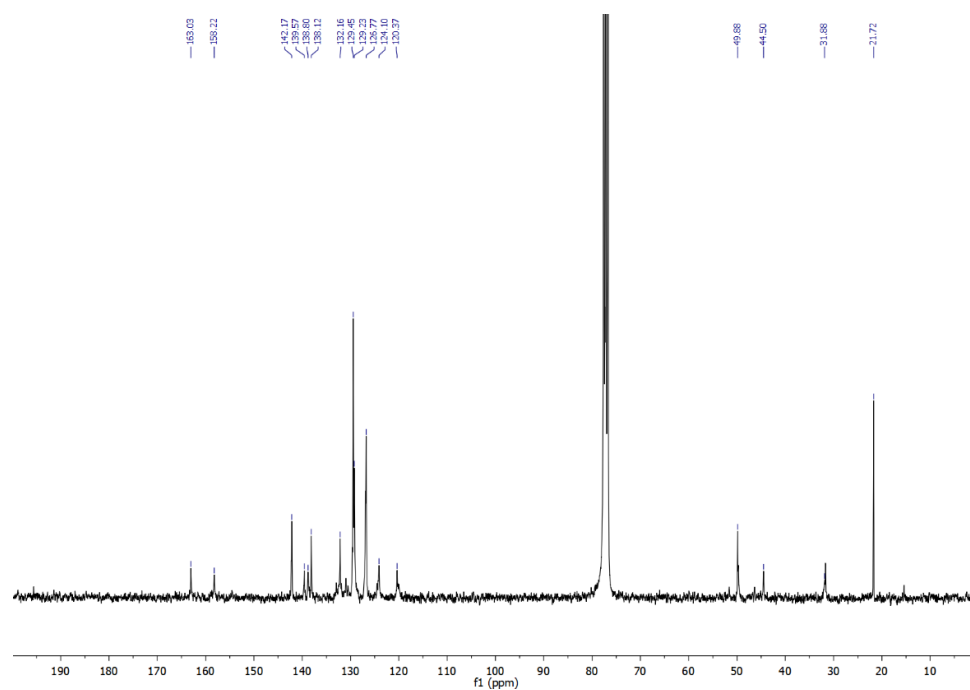


Figure S2. ¹³C{¹H} NMR spectrum of compound **1** in CDCl₃ at 298K

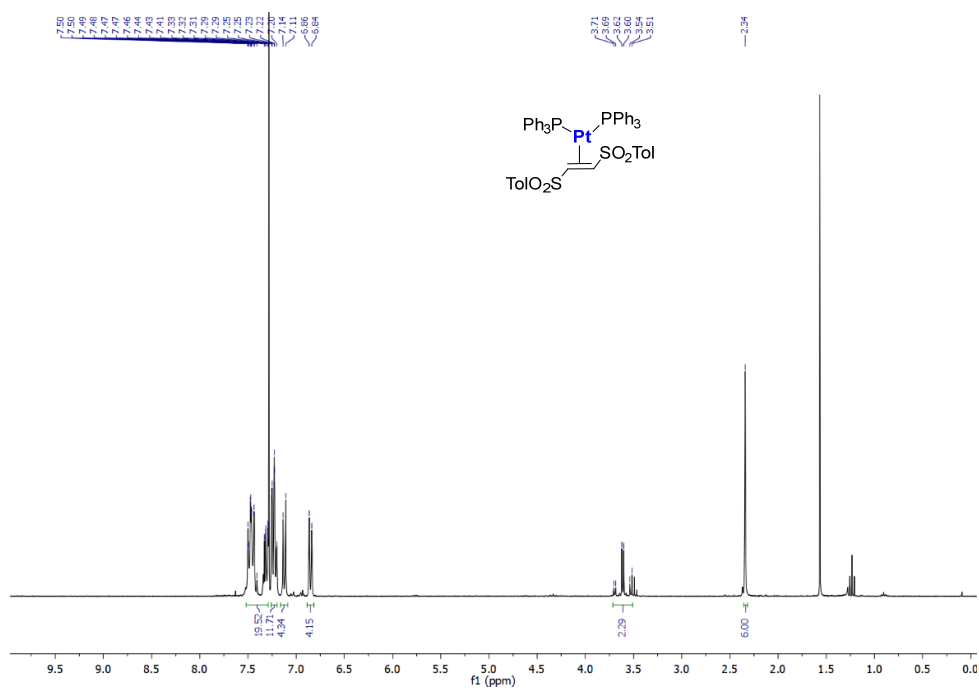


Figure S3. ¹H NMR spectrum of compound **2a** in CDCl₃ at 298K

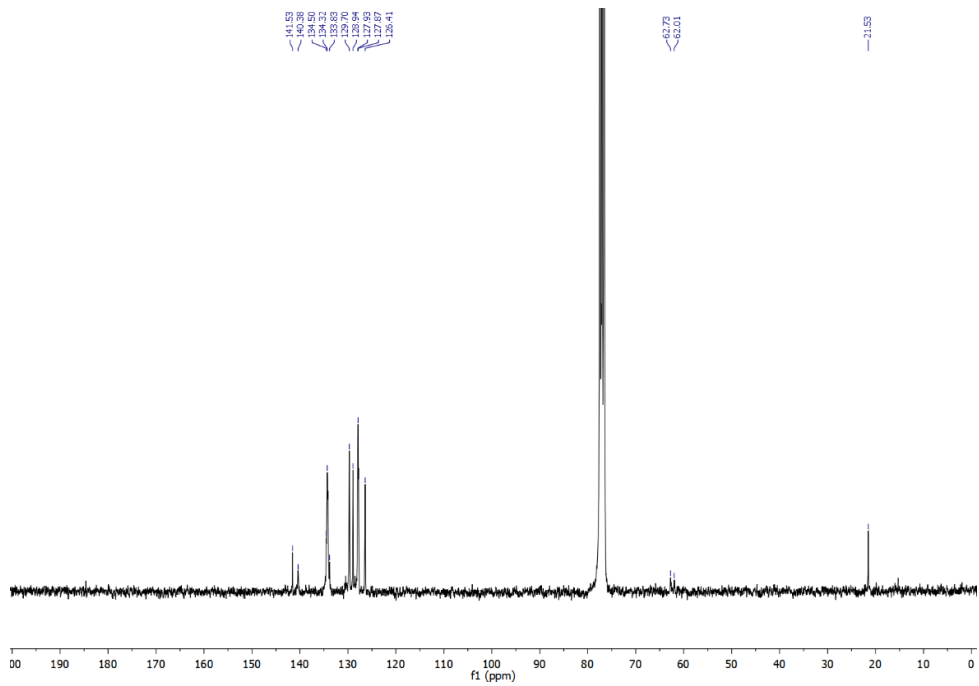
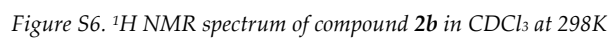
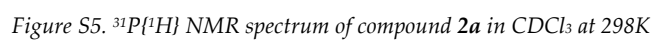


Figure S4. ¹³C{¹H} NMR spectrum of compound **2a** in CDCl₃ at 298K



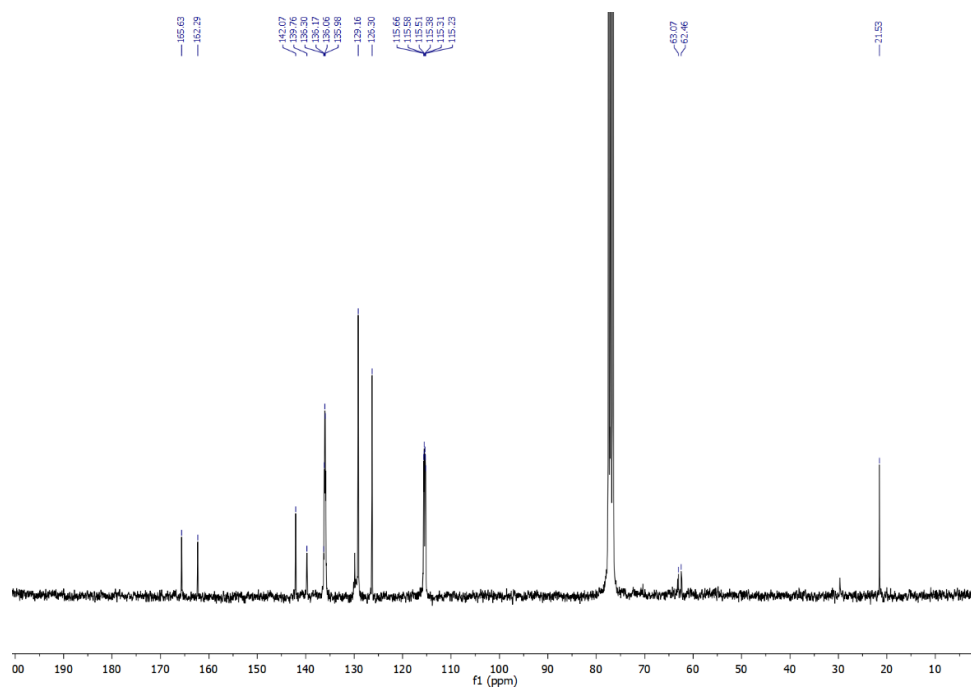


Figure S7. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of compound **2b** in CDCl_3 at 298K

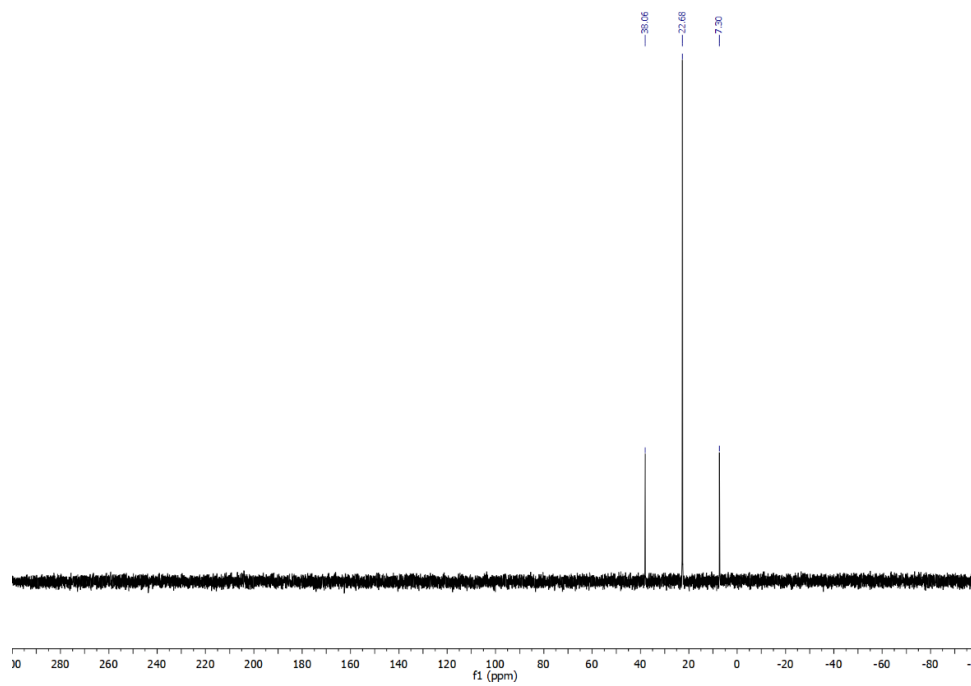


Figure S8. $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum of compound **2b** in CDCl_3 at 298K

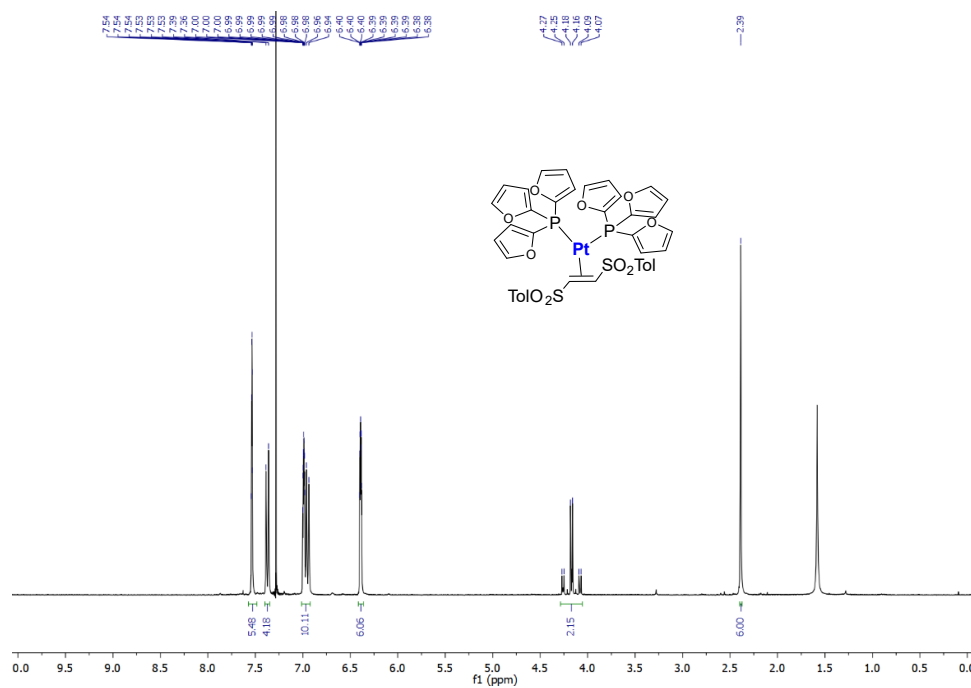


Figure S9. ¹H NMR spectrum of compound **2c** in CDCl₃ at 298K

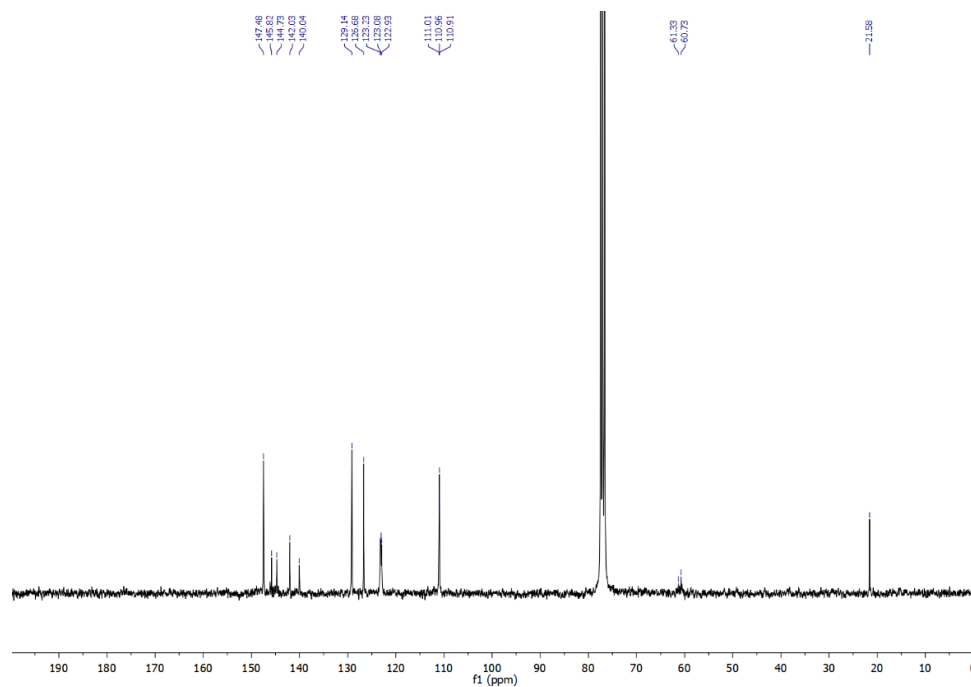


Figure S10. ¹³C{¹H} NMR spectrum of compound **2c** in CDCl₃ at 298K

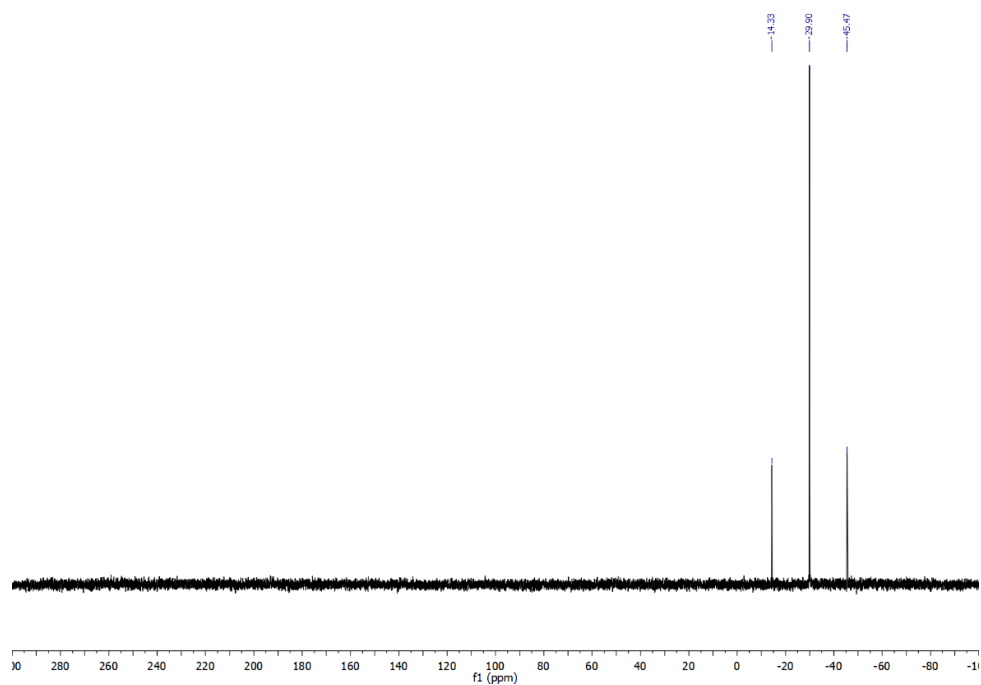


Figure S11. $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum of compound **2c** in CDCl_3 at 298K

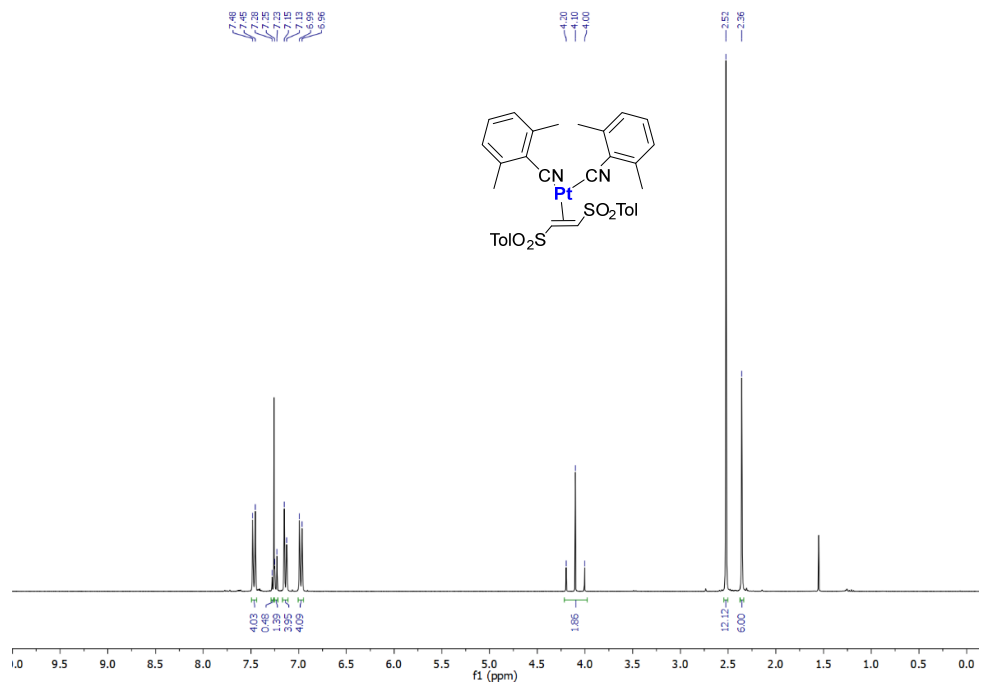


Figure S12. ^1H NMR spectrum of compound **3a** in CDCl_3 at 298K

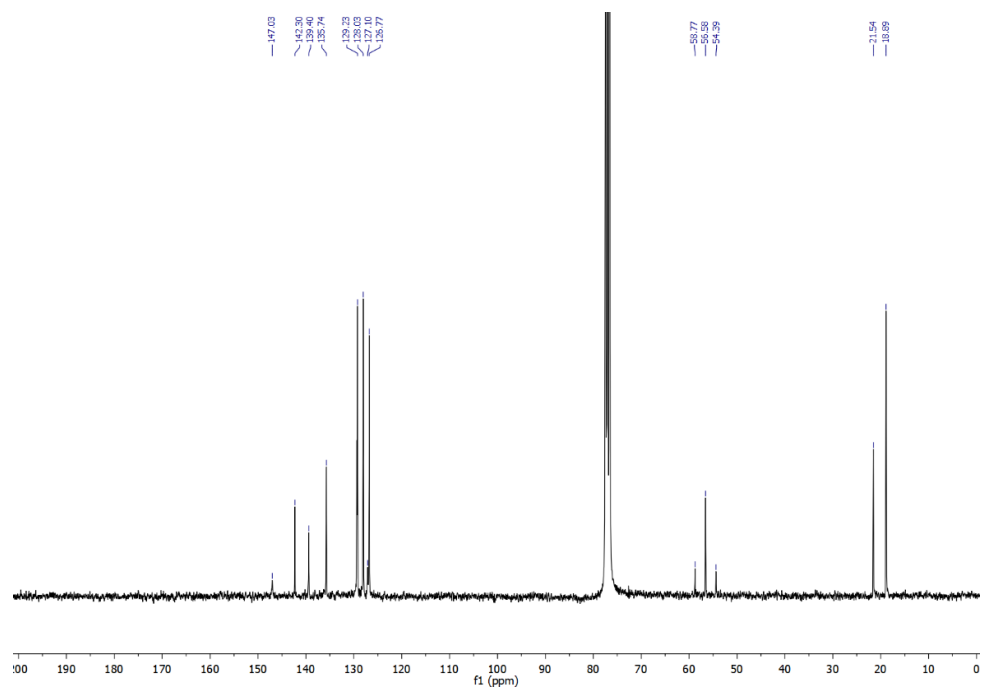


Figure S13. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of compound **3a** in CDCl_3 at 298K

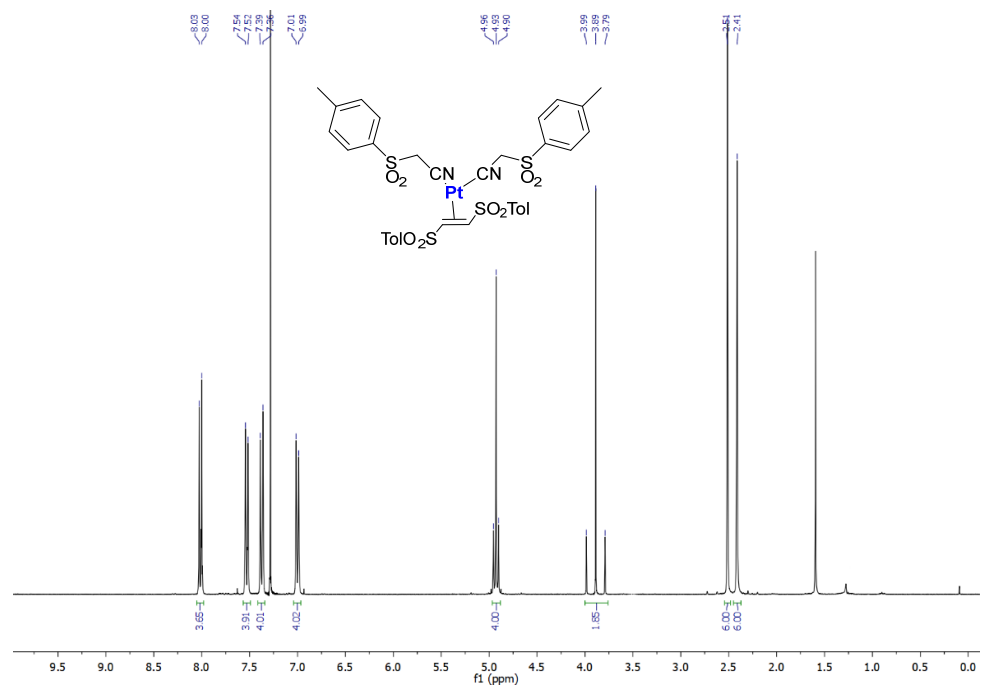


Figure S14. ^1H NMR spectrum of compound **3b** in CDCl_3 at 298K

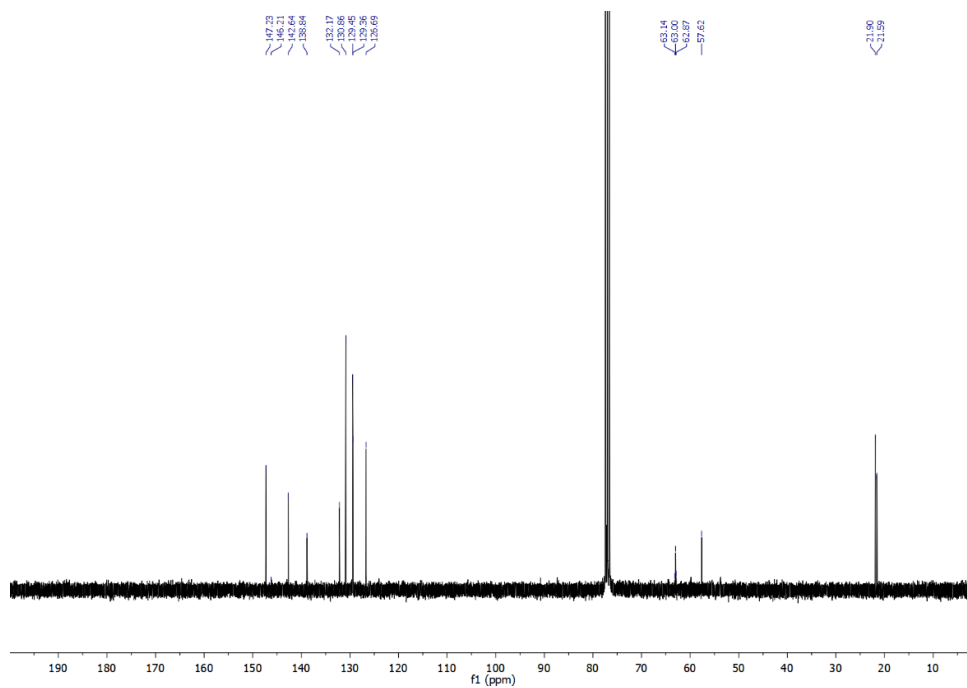


Figure S15. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of compound **3b** in CDCl_3 at 298K

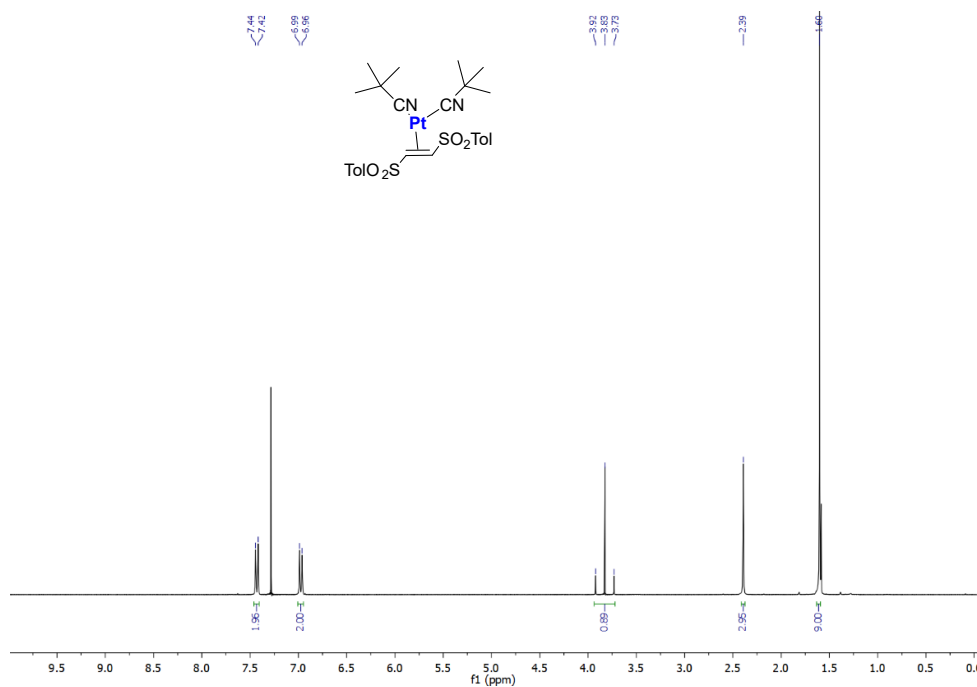


Figure S16. ^1H NMR spectrum of compound **3c** in CDCl_3 at 298K

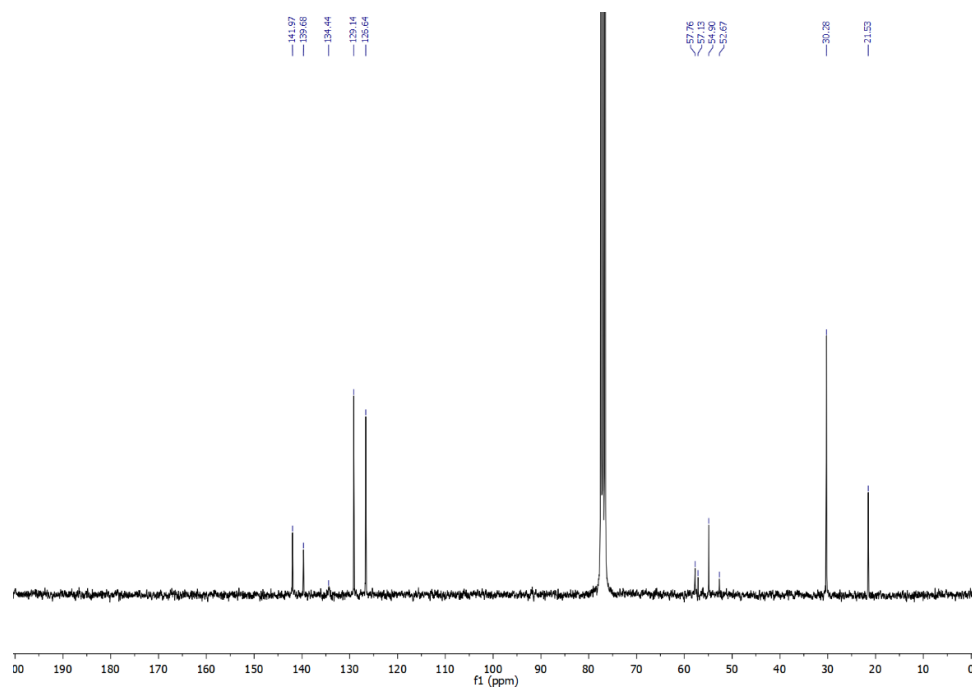


Figure S17. ¹³C(¹H) NMR spectrum of compound **3c** in CDCl₃ at 298K

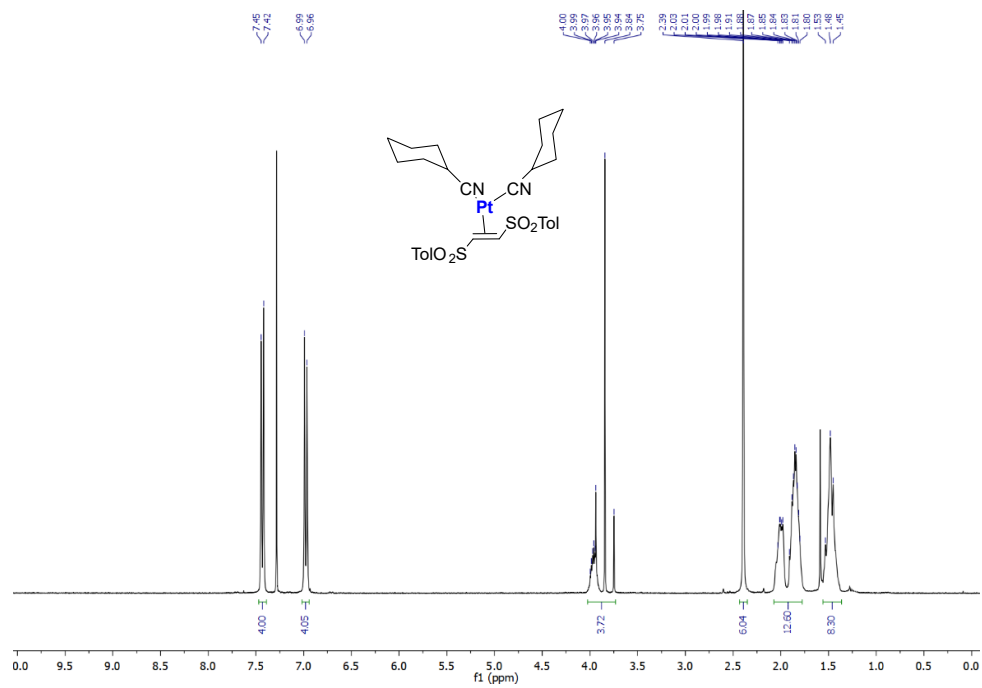


Figure S18. ¹H NMR spectrum of compound **3d** in CDCl₃ at 298K

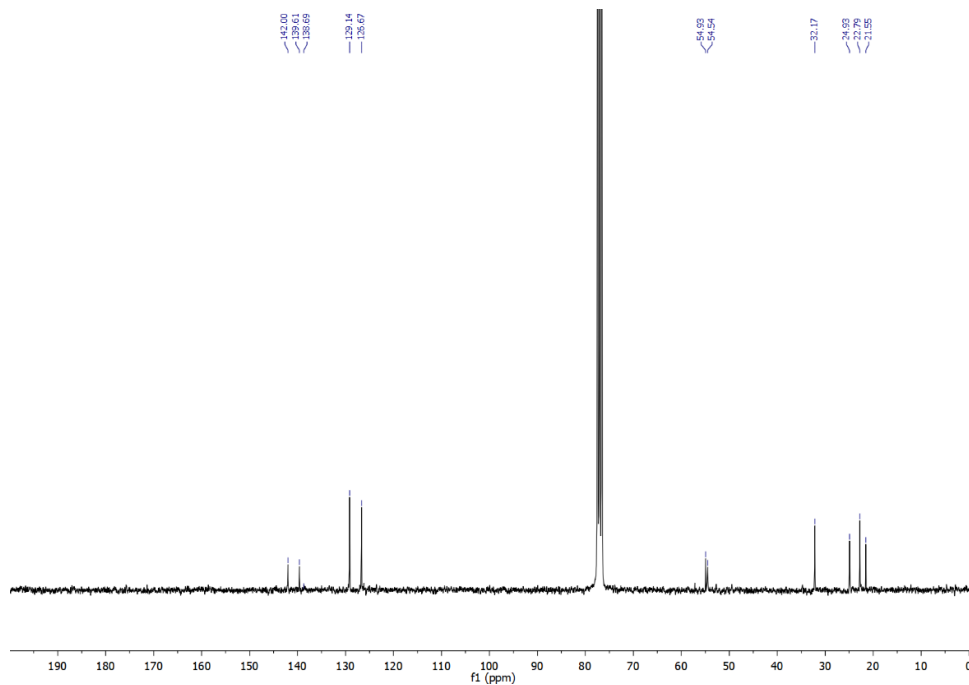


Figure S19. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of compound **3d** in CDCl_3 at 298K

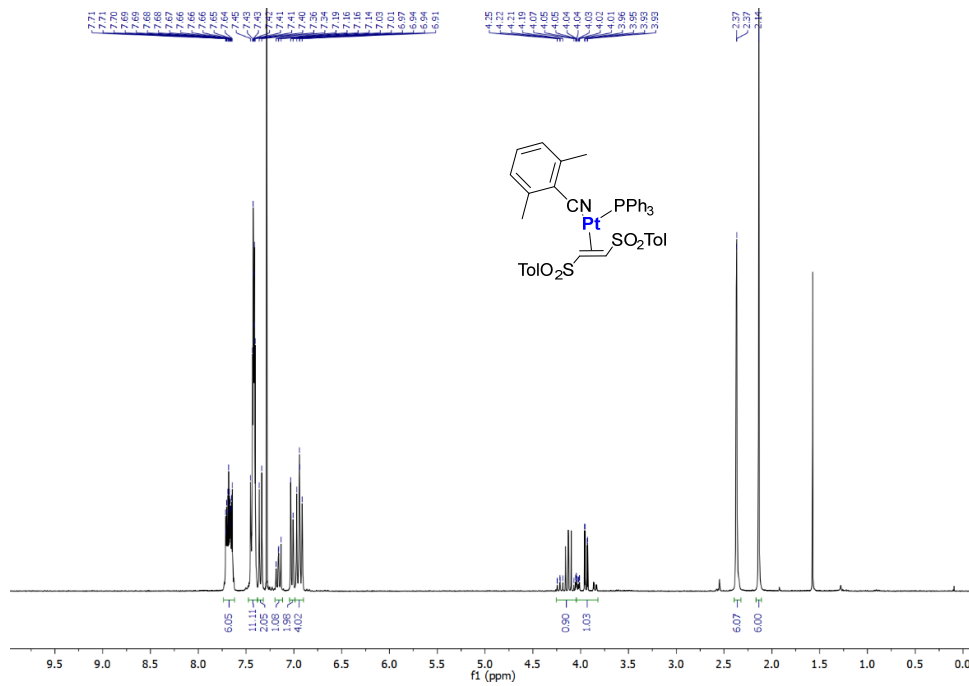


Figure S20. ^1H NMR spectrum of compound **4a** in CDCl_3 at 298K

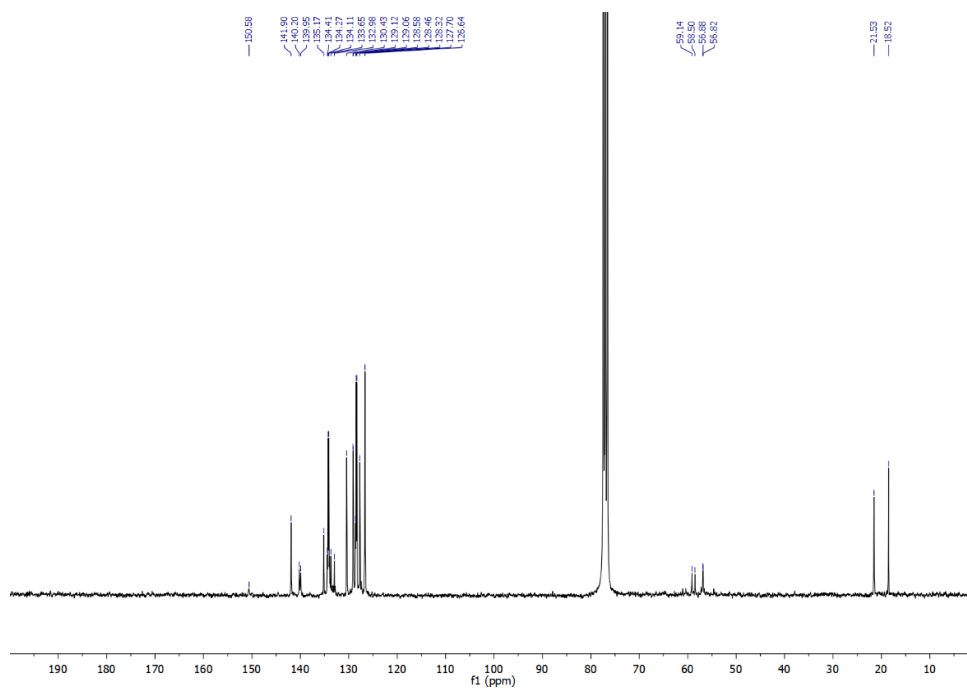


Figure S21. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of compound **4a** in CDCl_3 at 298K

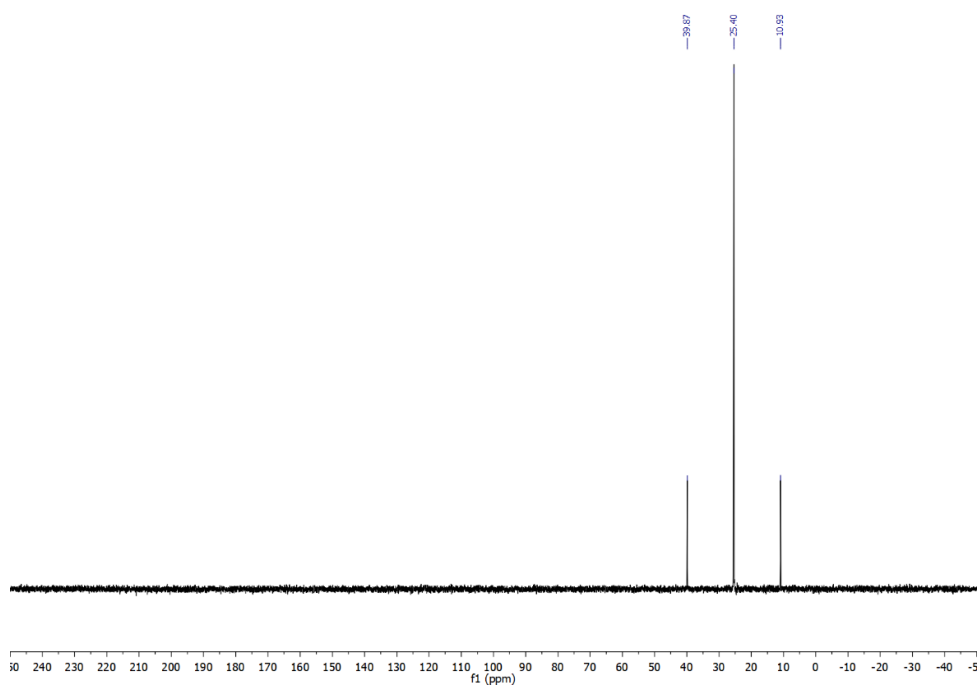


Figure S22. $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum of compound **4a** in CDCl_3 at 298K

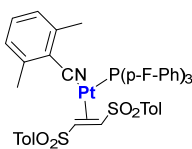
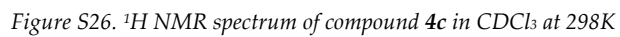
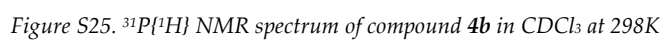
[illegible]

Figure S24. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of compound **4b** in CDCl_3 at 298K



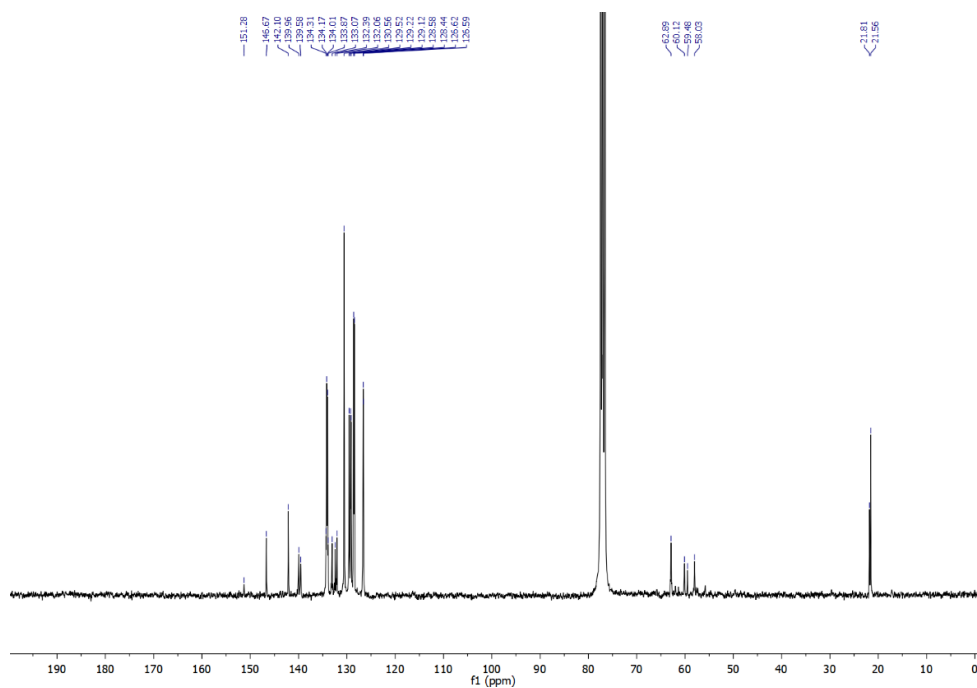


Figure S27. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of compound **4c** in CDCl_3 at 298K

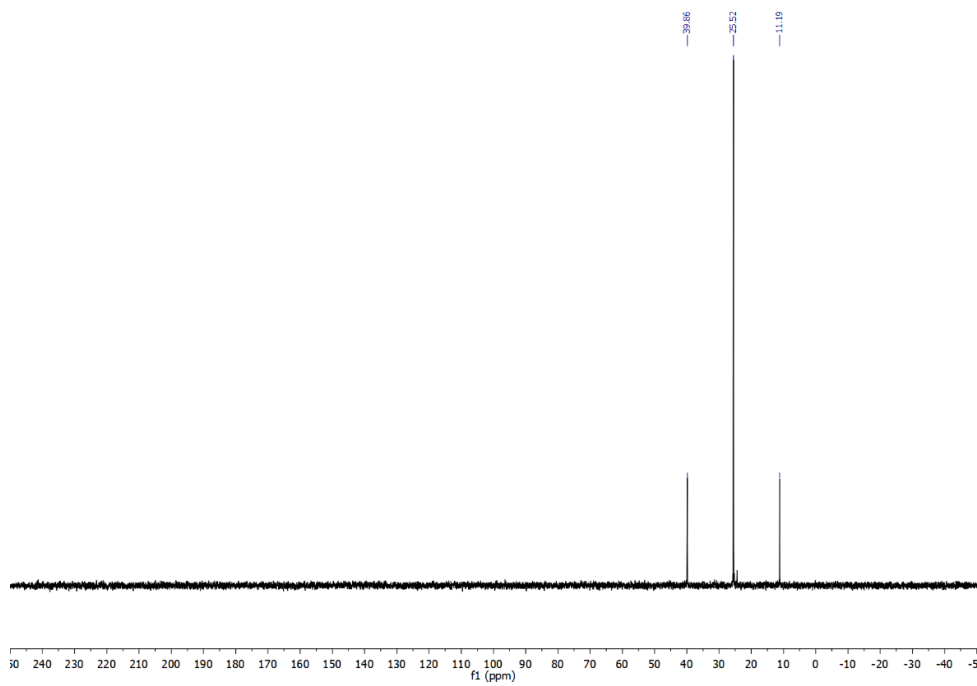
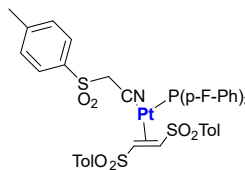


Figure S28. $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum of compound **4c** in CDCl_3 at 298K



166.03
162.69
150.79
148.86
142.28
139.35
138.45
137.72
132.72
130.61
129.25
128.82
128.07
125.89
123.46
116.10
115.98
115.02
69.01
66.65
62.03
56.30
21.84
21.56
21.59

Figure S30. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of compound **4d** in CDCl_3 at 298K

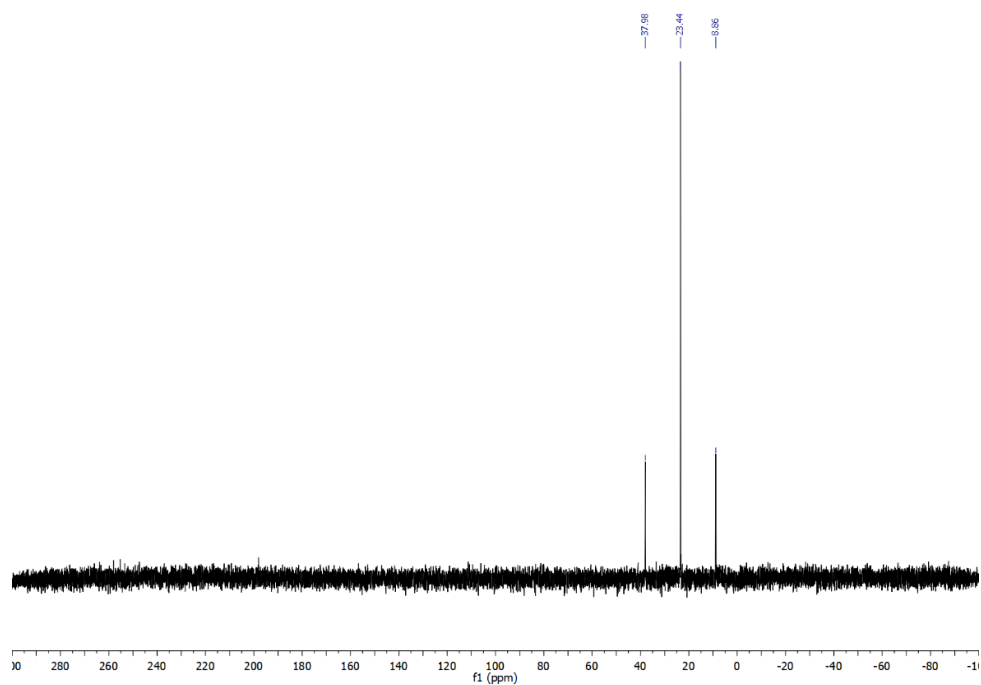


Figure S31. $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum of compound **4d** in CDCl_3 at 298K

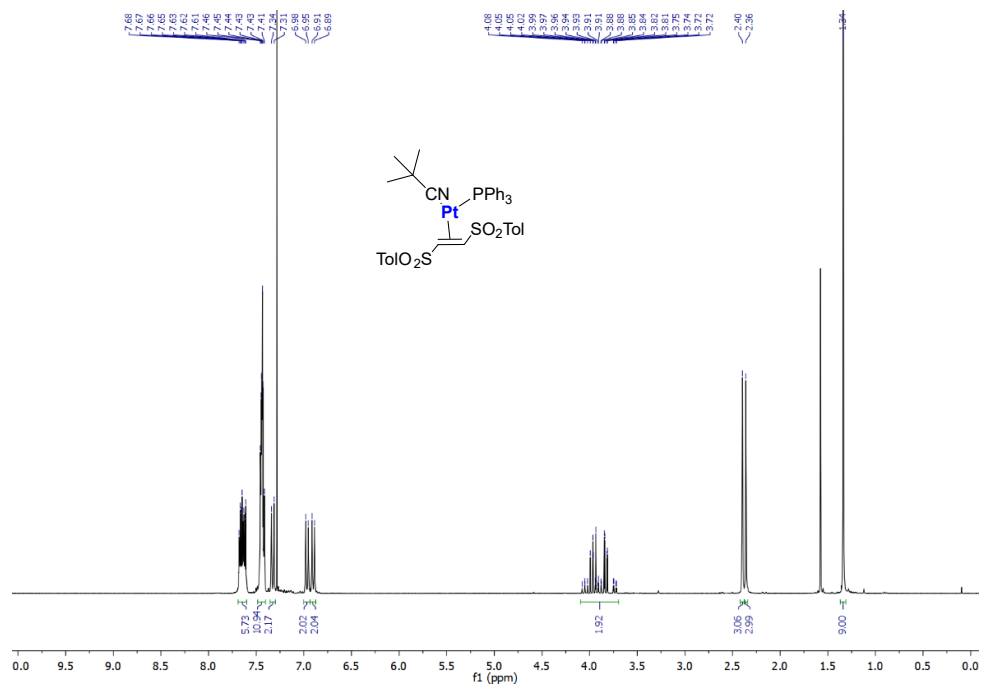


Figure S32. ^1H NMR spectrum of compound **4e** in CDCl_3 at 298K

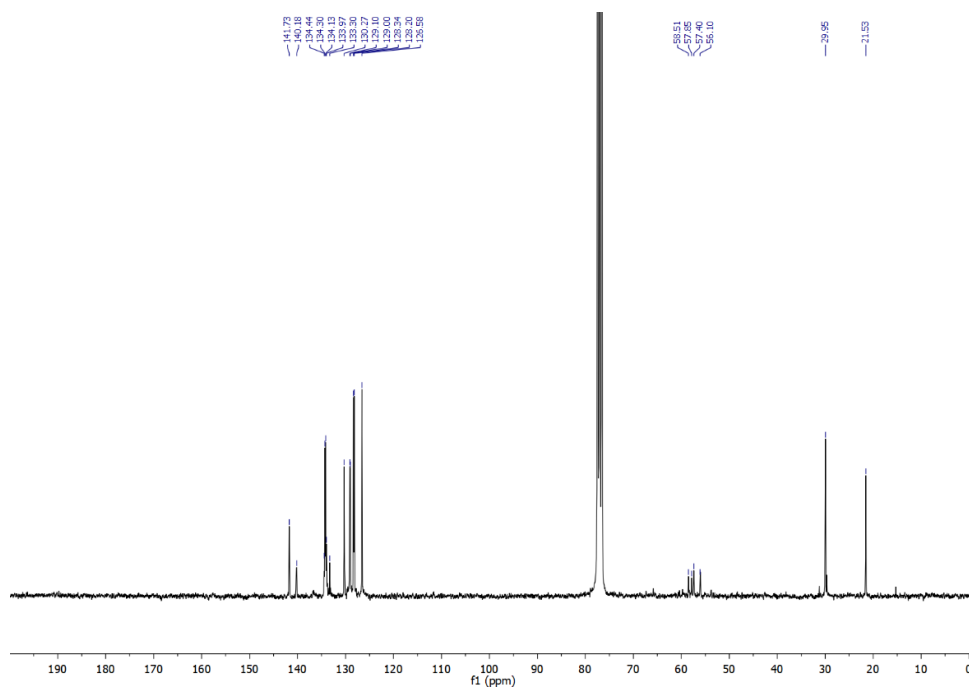


Figure S33. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of compound **4e** in CDCl_3 at 298K

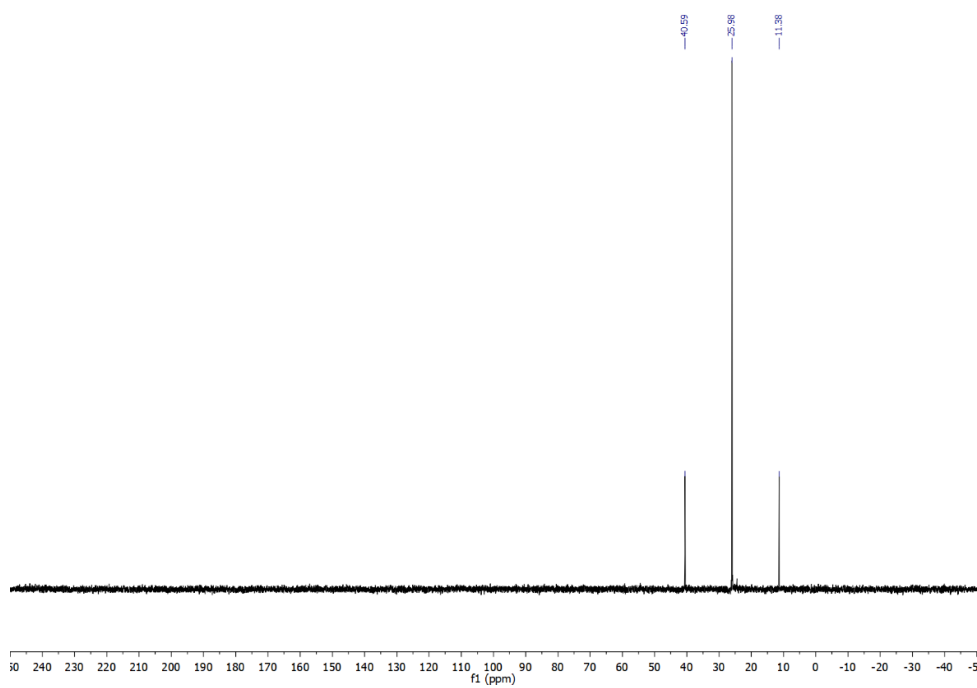


Figure S34. $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum of compound **4e** in CDCl_3 at 298K

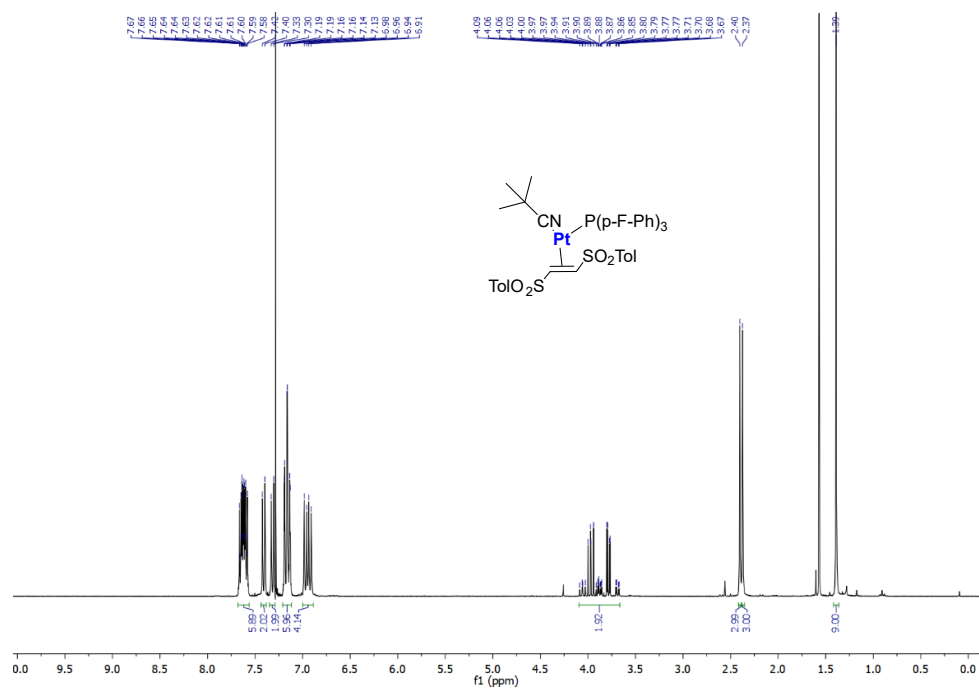


Figure S35. ¹H NMR spectrum of compound **4f** in CDCl₃ at 298K

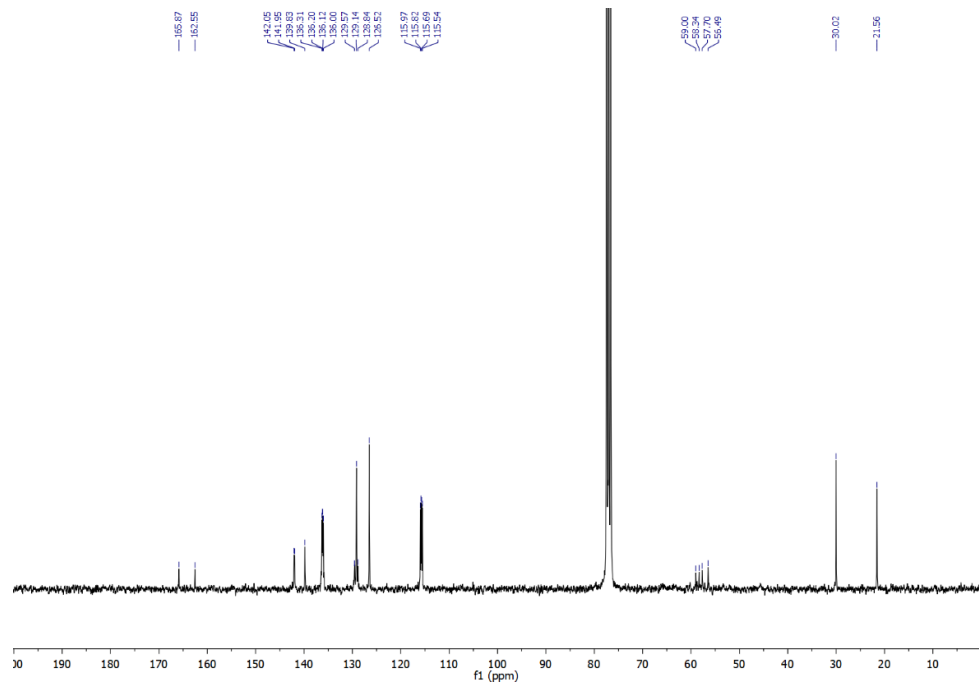


Figure S36. ¹³C[¹H] NMR spectrum of compound **4f** in CDCl₃ at 298K

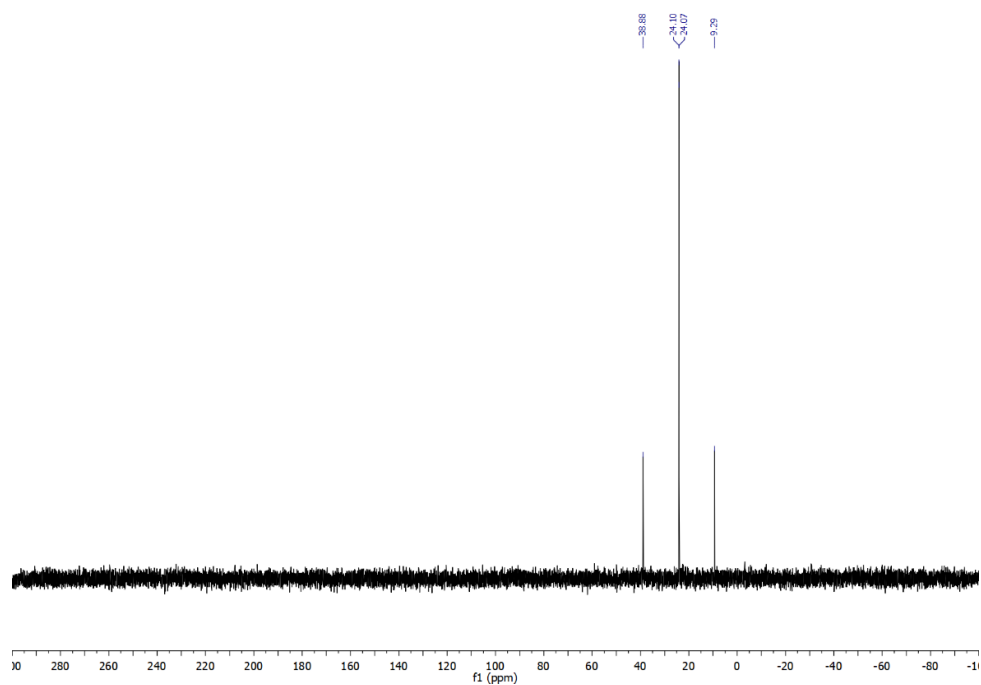


Figure S37. $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum of compound **4f** in CDCl_3 at 298K

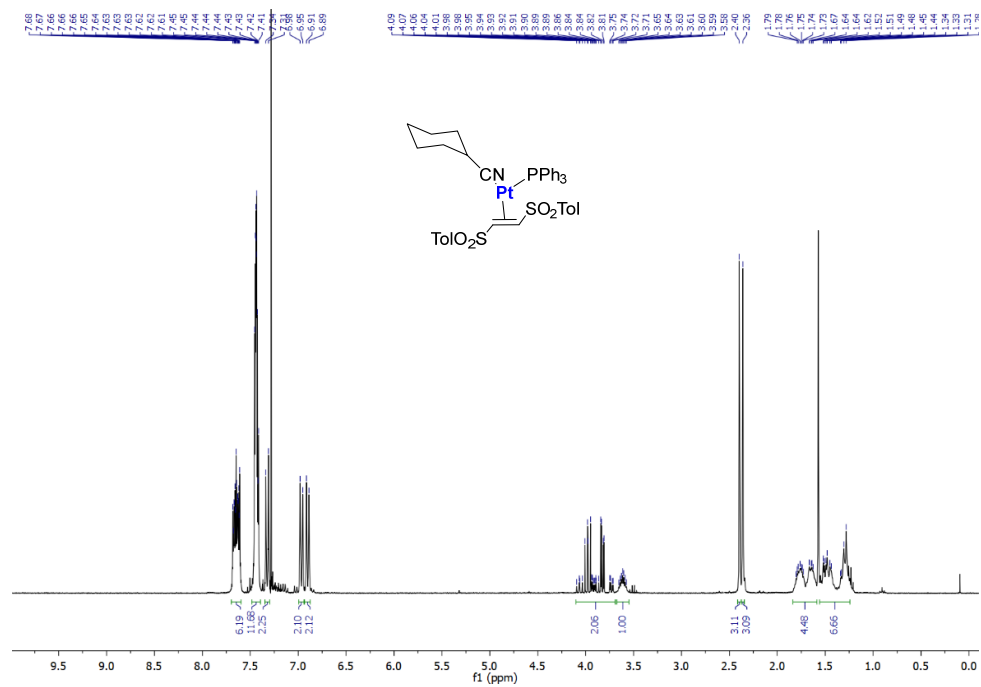


Figure S38. ^1H NMR spectrum of compound **4g** in CDCl_3 at 298K

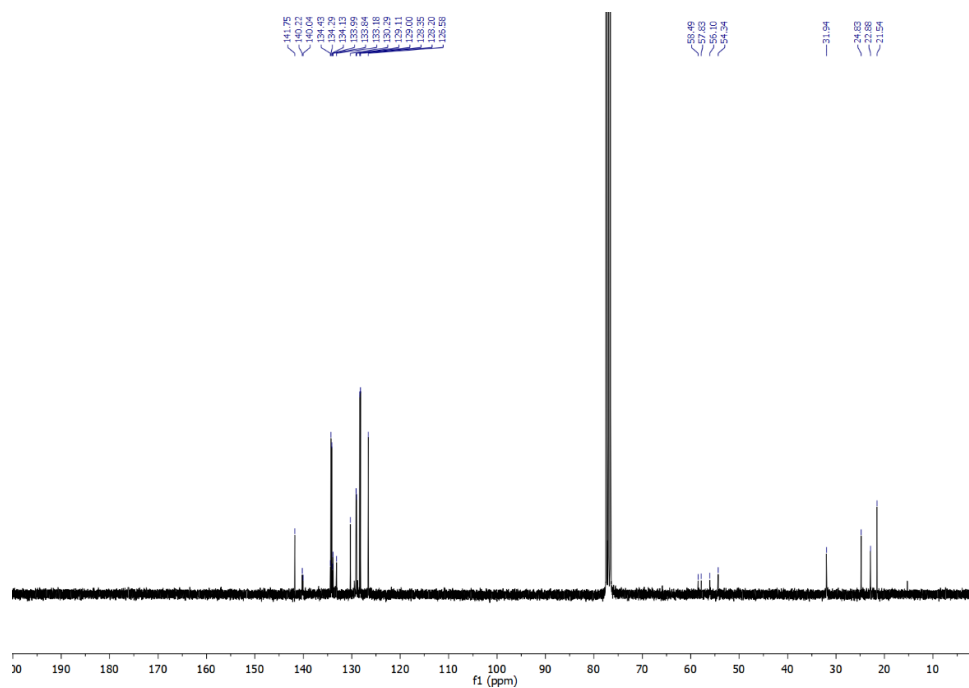


Figure S39. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of compound **4g** in CDCl_3 at 298K

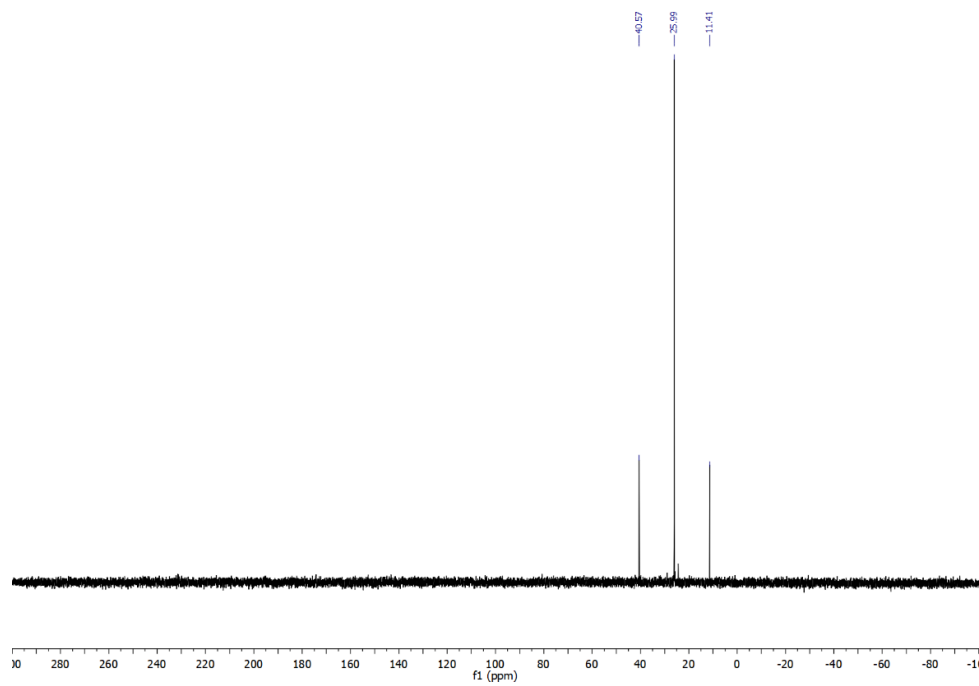


Figure S40. $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum of compound **4g** in CDCl_3 at 298K

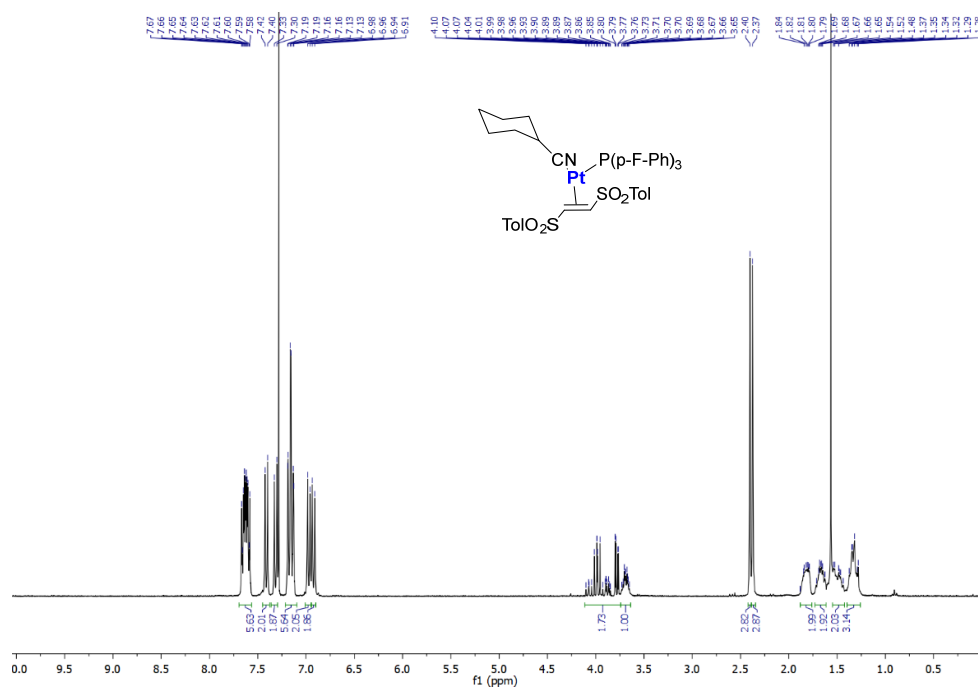


Figure S41. ¹H NMR spectrum of compound **4h** in CDCl₃ at 298K

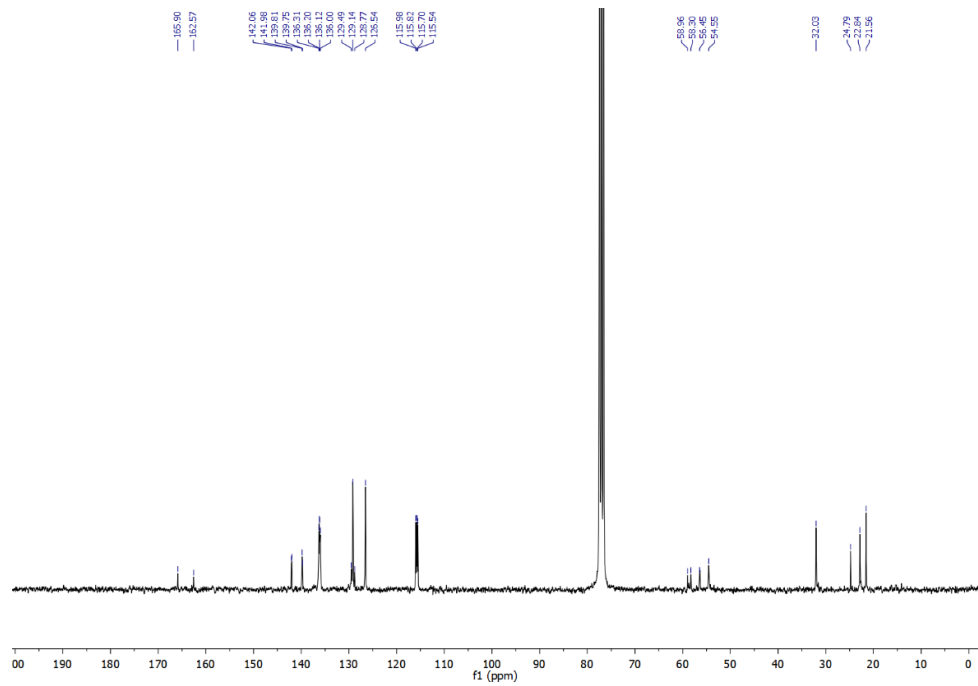


Figure S42. ¹³C[¹H] NMR spectrum of compound **4h** in CDCl₃ at 298K

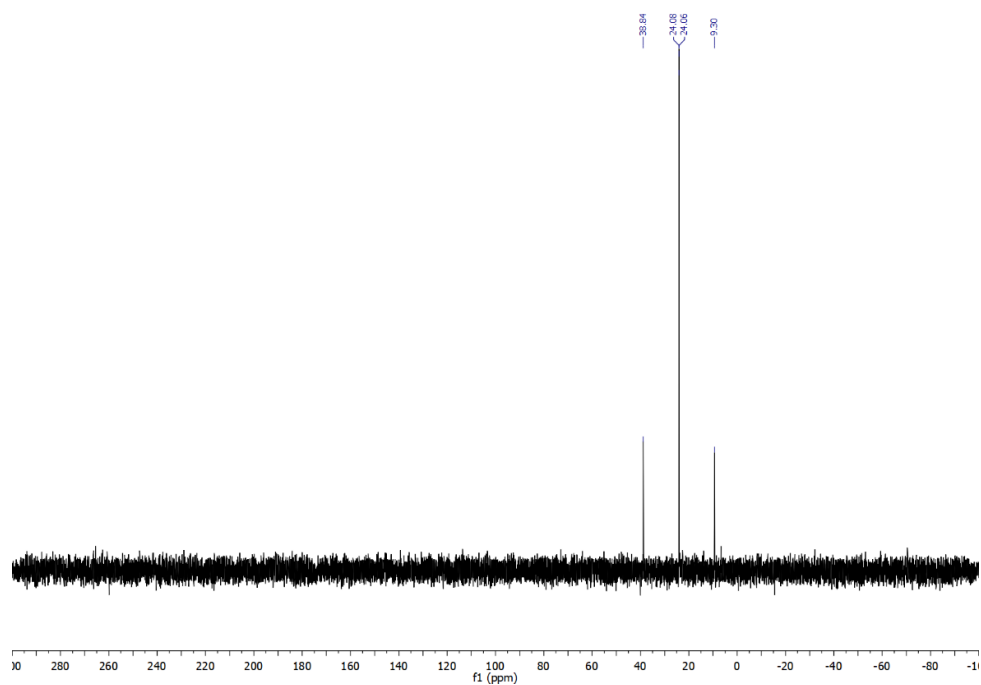


Figure S43. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of compound **4h** in CDCl_3 at 298K

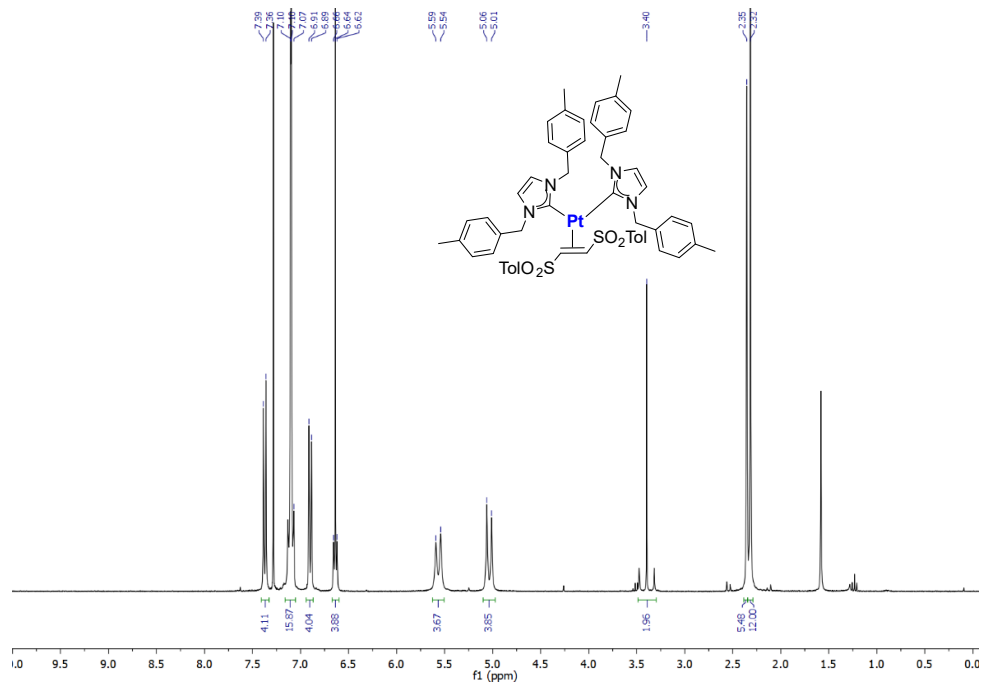


Figure S44. ^1H NMR spectrum of compound **6a** in CDCl_3 at 298K

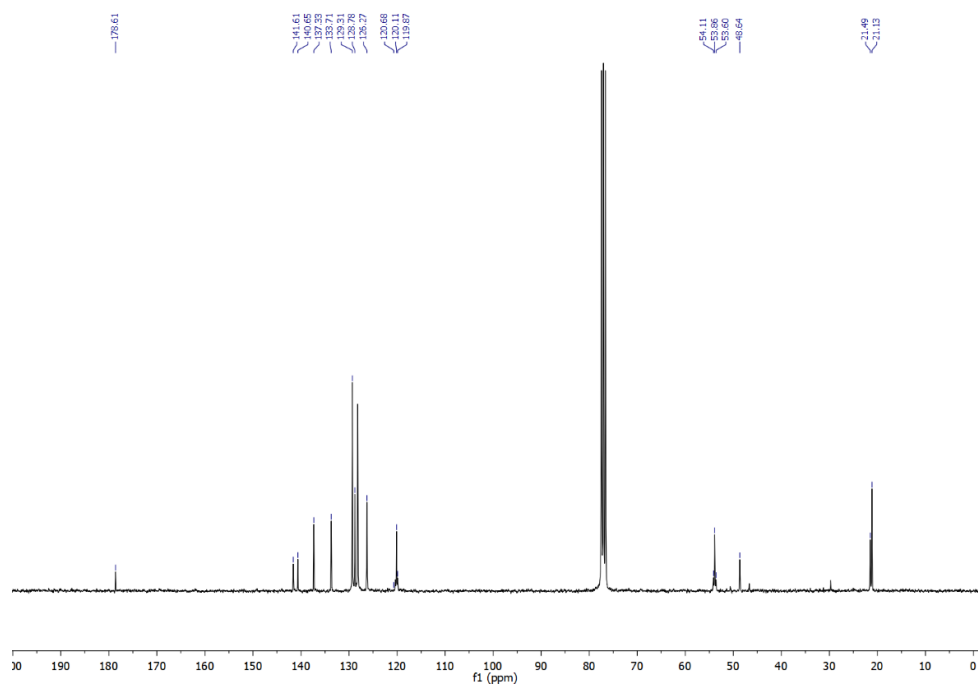


Figure S45. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of compound **6a** in CDCl_3 at 298K

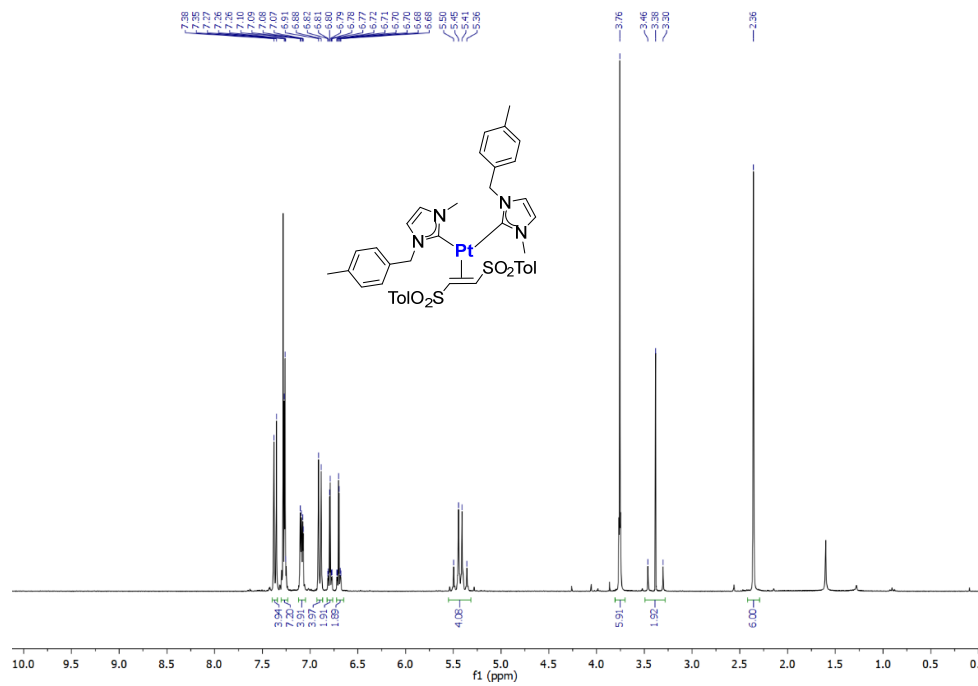


Figure S46. ^1H NMR spectrum of compound **6b** in CDCl_3 at 298K

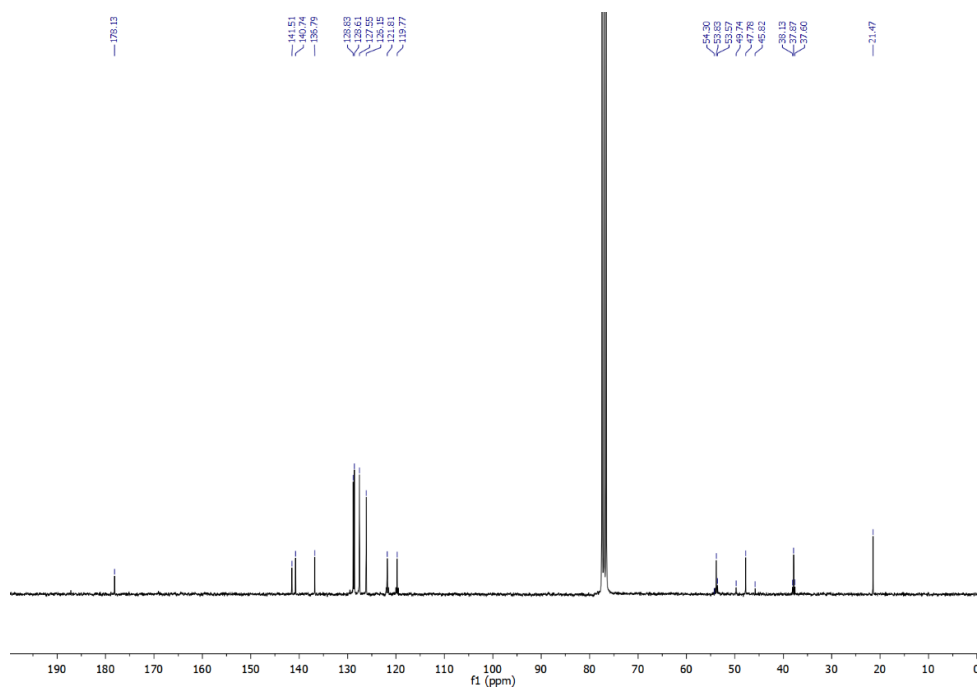


Figure S47. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of compound **6b** in CDCl_3 at 298K

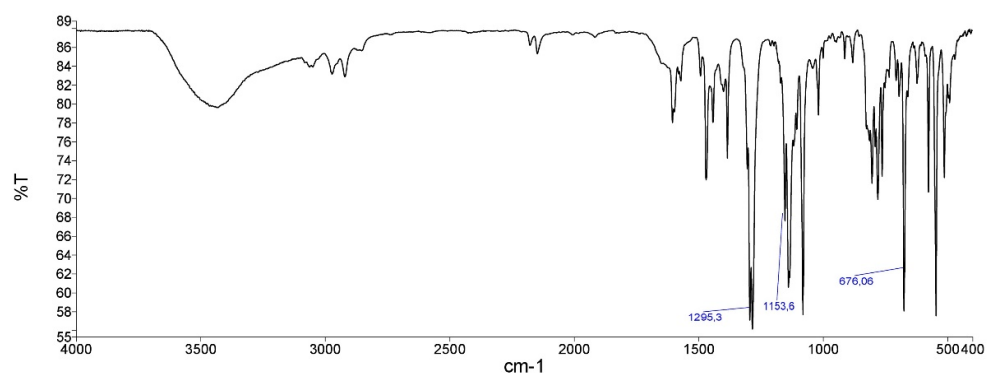


Figure S48. IR spectrum of compound **1**

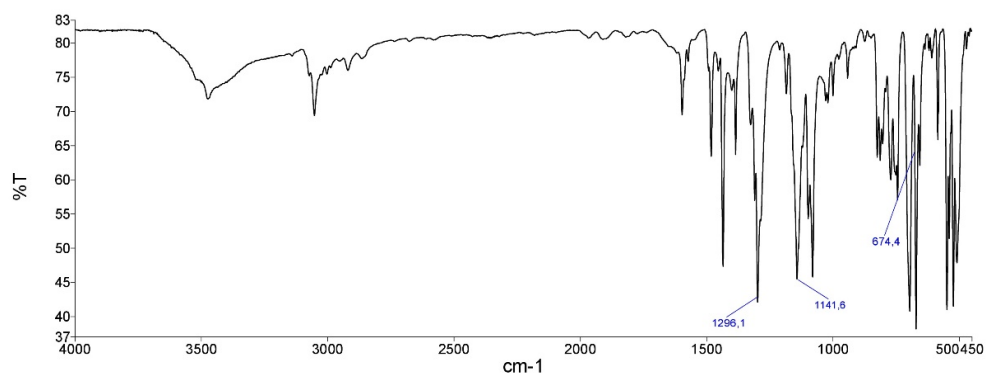


Figure S49. IR spectrum of compound 2a

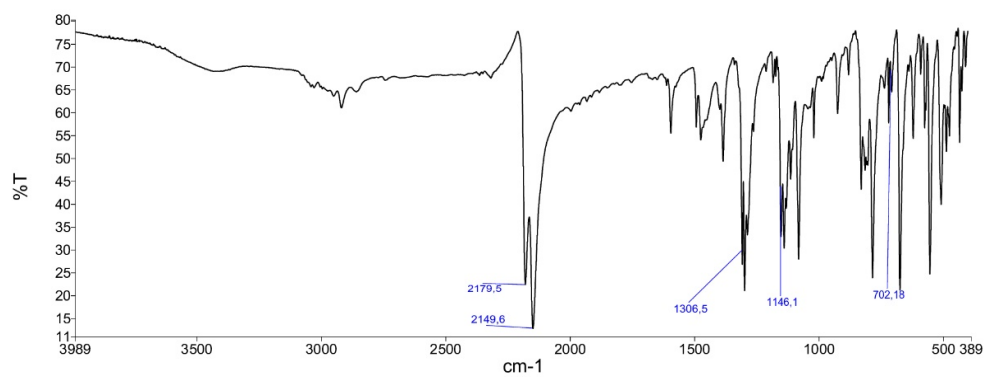


Figure S50. IR spectrum of compound 3a

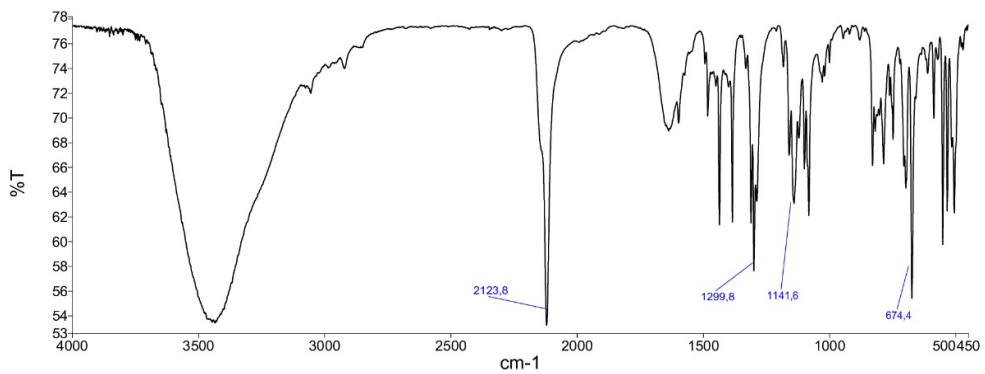


Figure S51. IR spectrum of compound 4a

X-ray diffraction analysis - Structural characterization

Table S1. Crystallographic data.

Compound	3a@100 K	3b@100 K	2a@100 K
Formula	PtC ₃₄ H ₃₄ N ₂ O ₄ S ₂	PtC ₃₄ H ₃₄ N ₂ O ₈ S ₄	PtC ₅₂ H ₄₆ O ₄ P ₂ S ₂ · ¹ / ₄ C ₄ H ₁₀ O· ¹ / ₄ CH ₂ Cl ₂
M/g·mol ⁻¹	793.84	921.96	1095.54
Space group	<i>P</i> 2 ₁ / <i>c</i>	<i>P</i> -1	<i>P</i> -1
Crystal system	Monoclinic	Triclinic	Triclinic
<i>a</i> /Å	15.496(3)	10.295(2)	14.660(3)
<i>b</i> /Å	9.010(2)	13.985(3)	17.981(4)
<i>c</i> /Å	23.067(5)	14.334(3)	18.585(4)
α /°	90	62.54(3)	101.57(3)
β /°	101.56(3)	80.47(3)	96.12(3)
γ /°	90	75.95(3)	98.80(3)
<i>V</i> /Å ³	3155.2(11)	1773.1(8)	4695.1(18)
<i>Z</i>	4	2	4
T/K	100(2)	100(2)	100(2)
<i>D</i> _c /g·cm ⁻³	1.671	1.727	1.550
<i>F</i> (000)	1576	916	2203
μ /mm ⁻¹	3.232	2.966	2.251
Measured Reflections	60938	64502	223791
Unique Reflections	10435	12650	41421
<i>R</i> _{int}	0.0397	0.0568	0.0645
Obs. Refl.ns [<i>I</i> ≥2σ(<i>I</i>)]	9184	12023	39404
θ_{\min} – θ_{\max} /°	1.17 – 27.12	1.46 – 28.01	0.99 – 31.13
<i>hkl</i> ranges	-22,22; -13,13; -33,33	-15,15; -21,21; -21,21	-23,23; -29,29; -30,30
<i>R</i> (<i>F</i> ²) (Obs.Refl.ns)	0.0289	0.0215	0.0295
<i>wR</i> (<i>F</i> ²) (All Refl.ns)	0.0767	0.0538	0.0737
No. Variables	394	446	1193
Goodness of fit	1.105	1.038	1.050
$\Delta\rho_{\max}$; $\Delta\rho_{\min}$ /e·Å ⁻³	2.26; -2.39	1.35; -2.52	2.36; -2.22
CCDC Deposition N.	2323081	2323083	2323084

Compound	2a@298 K	4b@100 K	6b@100 K
Formula	PtC ₅₂ H ₄₆ O ₄ P ₂ S ₂ · ¹ / ₄ C ₄ H ₁₀ O· ¹ / ₄ CH ₂ Cl ₂	PtC ₄₃ H ₃₇ F ₃ NO ₄ PS ₂	PtC ₃₈ H ₄₀ N ₄ O ₄ S ₂
M/g·mol ⁻¹	1095.54	978.91	875.95
Space group	<i>P</i> -1	<i>P</i> 1	<i>P</i> -1
Crystal system	Triclinic	Triclinic	Triclinic
<i>a</i> /Å	14.754(3)	11.488(2)	10.808(2)
<i>b</i> /Å	18.270(4)	14.203(3)	11.808(2)
<i>c</i> /Å	18.705(4)	14.404(3)	15.799(3)
α /°	101.72(3)	62.21(3)	74.17(3)
β /°	95.88(3)	75.71(3)	70.02(3)
γ /°	98.88(3)	74.35(3)	76.02(3)
<i>V</i> /Å ³	4830.9(18)	1981.8(9)	1798.5(8)
<i>Z</i>	4	2	2
T/K	298(2)	100(2)	100(2)
<i>D</i> _c /g·cm ⁻³	1.506	1.640	1.618
<i>F</i> (000)	2203	972	876
μ /mm ⁻¹	2.188	2.618	2.843
Measured Reflections	232518	70256	17625
Unique Reflections	40702	31365	5731
<i>R</i> _{int}	0.0492	0.0420	0.0476
Obs. Refl.ns [<i>I</i> ≥2σ(<i>I</i>)]	34524	29616	5440
θ_{\min} – θ_{\max} /°	0.98 – 31.83	1.41 – 30.00	1.17 – 27.12
<i>hkl</i> ranges	-24,24; -29,29; -29,29	-18,18; -22,22; -23,23	-12,12; -13,13; -18,18

R(F ²) (Obs.Refl.ns)	0.0343	0.0277	0.0260
wR(F ²) (All Refl.ns)	0.0940	0.0628	0.0636
No. Variables	1150	1000	446
Goodness of fit	1.055	1.109	1.074
$\Delta\rho_{\max}$; $\Delta\rho_{\min}/\text{e}\cdot\text{\AA}^{-3}$	1.07; -2.53	1.90; -2.40	2.35; -1.56
CCDC Deposition N.	2323085	2323087	2323082

Table S2. Selected platinum distances and angles for **3a** at 100 K.

3a (100 K) - PtC₃₄H₃₄N₂O₄S₂			
Distances	(Å)	Angles	(°)
Pt_1-C1_2	2.073(2)	C1_2-Pt_1-C2_2	41.9(1)
Pt_1-C2_2	2.057(2)	C2_2-Pt_1-C_3	107.6(1)
Pt_1-C_3	1.957(3)	C_3-Pt_1-C_4	98.5(1)
Pt_1-C_4	1.962(3)	C1_2-Pt_1-C_4	112.0(1)
C1_2=C2_2	1.476(4)	Pd Ave.- C=C-S Planes ^a	88.4(7)

^aAverage angle among the mean metal coordination plane and the olefinic one (defined as the plane that contains the C=C and non-H atoms directly bound).

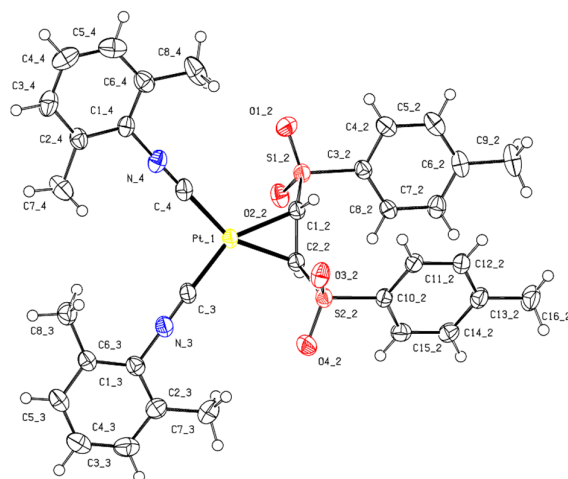
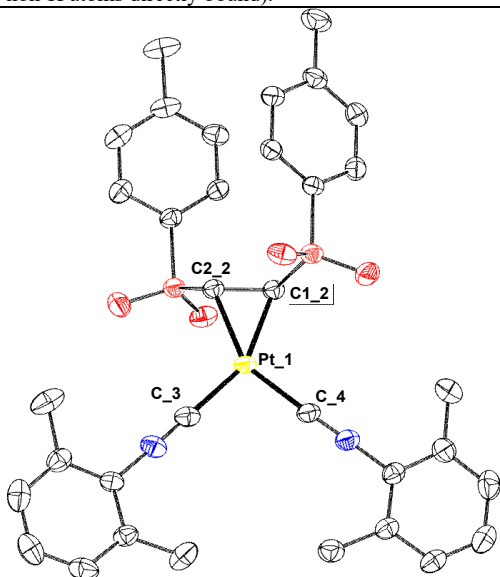


Table S3. Selected platinum distances and angles for **3b** at 100 K.

3b (100 K) - PtC₃₄H₃₄N₂O₈S₄			
Distances	(Å)	Angles	(°)
Pt_1-C1_2	2.076(2)	C1_2-Pt_1-C2_2	41.38(6)
Pt_1-C2_2	2.060(2)	C2_2-Pt_1-C_3	104.87(7)
Pt_1-C_3	1.948(2)	C_3-Pt_1-C_4	102.90(8)
Pt_1-C_4	1.968(2)	C1_2-Pt_1-C_4	110.80(7)
C1_2=C2_2	1.462(2)	Pd Ave.- C=C-S Planes ^a	89.0(5)

^aAverage angle among the mean metal coordination plane and the olefinic one (defined as the plane that contains the C=C and non-H atoms directly bound).

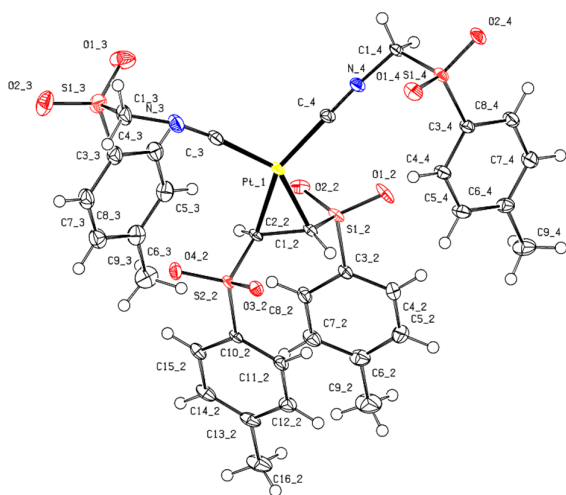
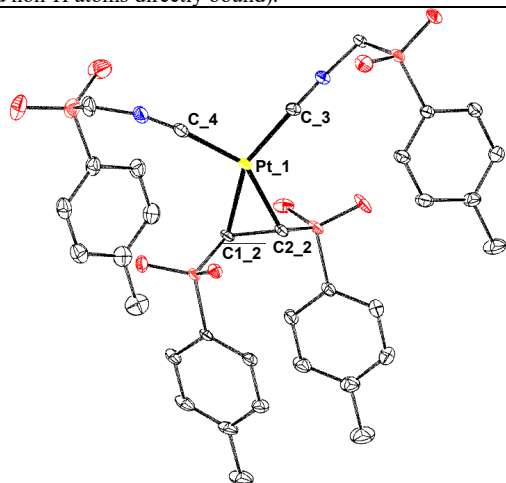


Table S4. Selected platinum distances and angles for **2a** at 100 K.

2a (100 K) - PtC₅₂H₄₆O₄P₂S₂

Molecule 1				Molecule 2			
Distances	(Å)	Angles	(°)	Distances	(Å)	Angles	(°)
Pt_11-C1_12	2.090(2)	C1_12-Pt_11-C2_12	40.99(8)	Pt_21-C1_22	2.104(2)	C1_22-Pt_21-C2_22	40.85(7)
Pt_11-C2_12	2.070(2)	C2_12-Pt_11-P_13	106.85(6)	Pt_21-C2_22	2.060(2)	C2_22-Pt_21-P_23	101.74(5)
Pt_11-P_13	2.288(1)	P_13-Pt_11-P_14	106.74(2)	Pt_21-P_23	2.284(1)	P_23-Pt_21-P_24	107.8(1)
Pt_11-P_14	2.283(1)	C1_12-Pt_11-P_14	106.21(6)	Pt_21-P_24	2.286(4)	C1_22-Pt_21-P_24	109.8(1)
C1_12=C2_12	1.457(3)	Pd Ave.- C=C-S Planes ^a	89.1(2)	C1_22=C2_22	1.453(2)	Pd Ave.- C=C-S Planes ^a	88.9(4)

^aAverage angle among the mean metal coordination plane and the olefinic one (defined as the plane that contains the C=C and non-H atoms directly bound).

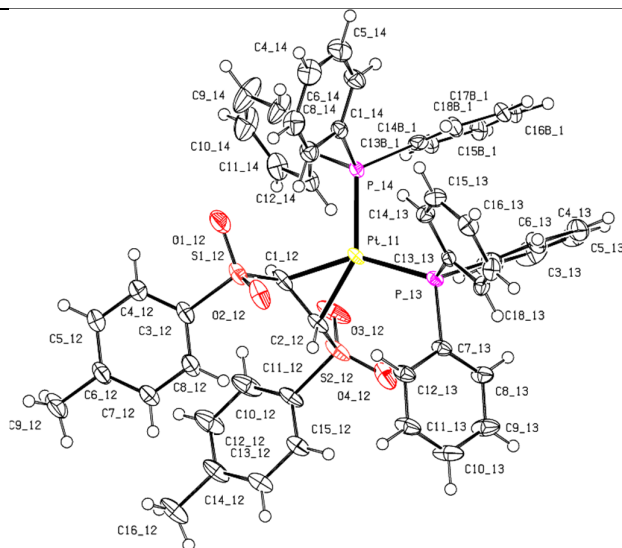
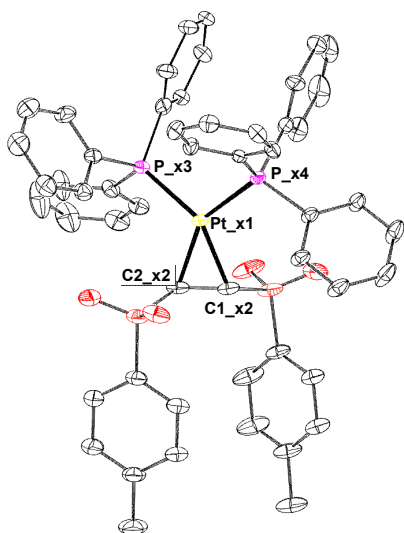


Table S5. Selected platinum distances and angles for **2a** at 298 K.

2a (298 K) - PtC ₅₂ H ₄₆ O ₄ P ₂ S ₂							
Molecule 1				Molecule 2			
Distances	(Å)	Angles	(°)	Distances	(Å)	Angles	(°)
Pt_11-C1_12	2.094(3)	C1_12-Pt_11-C2_12	40.9(1)	Pt_21-C1_22	2.099(2)	C1_22-Pt_21-C2_22	40.88(9)
Pt_11-C2_12	2.067(2)	C2_12-Pt_11-P_13	106.68(7)	Pt_21-C2_22	2.063(2)	C2_22-Pt_21-P_23	102.10(7)
Pt_11-P_13	2.292(1)	P_13-Pt_11-P_14	107.04(3)	Pt_21-P_23	2.290(1)	P_23-Pt_21-P_24	107.8(2)
Pt_11-P_14	2.287(1)	C1_12-Pt_11-P_14	106.30(7)	Pt_21-P_24	2.295(9)	C1_22-Pt_21-P_24	109.6(2)
C1_12=C2_12	1.453(3)	Pd Ave.- C=C-S Planes ^a	89.8(6)	C1_22=C2_22	1.454(3)	Pd Ave.- C=C-S Planes ^a	88.8(7)

^aAverage angle among the mean metal coordination plane and the olefinic one (defined as the plane that contains the C=C and non-H atoms directly bound).

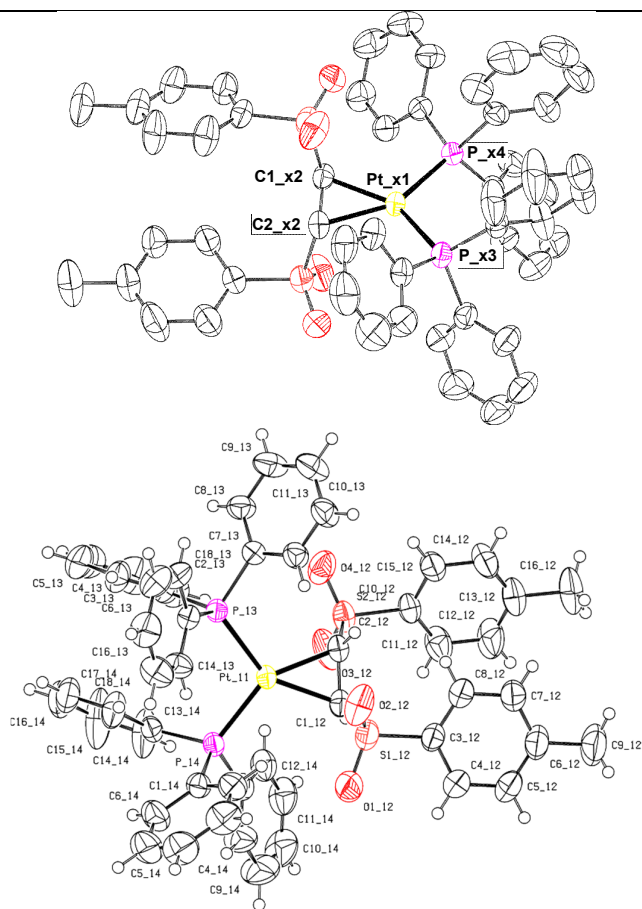


Table S6. Selected platinum distances and angles for **4b** at 100 K.

4b (100 K) - PtC ₄₃ H ₃₇ F ₃ NO ₄ PS ₂							
Molecule 1				Molecule 2			
Distances	(Å)	Angles	(°)	Distances	(Å)	Angles	(°)
Pt_11-C1_12	2.073(4)	C1_12-Pt_11-C2_12	41.2(2)	Pt_21-C1_22	2.077(3)	C1_22-Pt_21-C2_22	41.2(2)
Pt_11-C2_12	2.081(4)	C2_12-Pt_11-C_13	108.9(2)	Pt_21-C2_22	2.078(4)	C2_22-Pt_21-C_23	109.8(2)
Pt_11-C_13	1.942(3)	C_13-Pt_11-P_14	101.5(1)	Pt_21-C_23	1.941(3)	C_23-Pt_21-P_24	99.1(1)
Pt_11-P_14	2.305(1)	C1_12-Pt_11-P_14	108.5(1)	Pt_21-P_24	2.289(1)	C1_22-Pt_21-P_24	110.5(1)
C1_12=C2_12	1.461(5)	Pd Ave.- C=C-S Planes ^a	87.2(6)	C1_22=C2_22	1.462(5)	Pd Ave.- C=C-S Planes ^a	83.5(3)

^aAverage angle among the mean metal coordination plane and the olefinic one (defined as the plane that contains the C=C and non-H atoms directly bound).

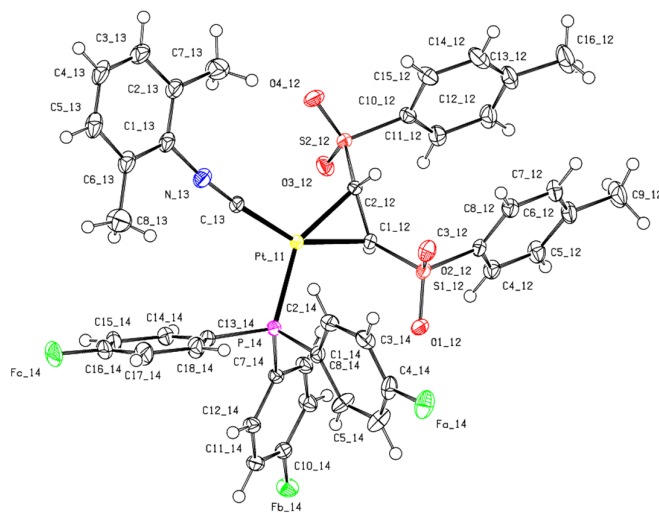
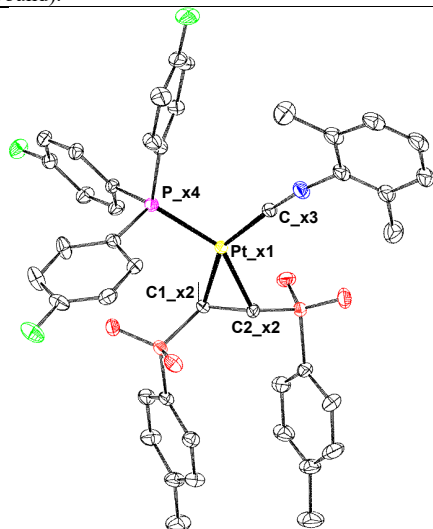


Table S7. Selected platinum distances and angles
for **6b** at 100 K.

6b (100 K) - PtC₃₈H₄₀N₄O₄S₂			
Distances	(Å)	Angles	(°)
Pt_1-C1_2	2.064(5)	C1_2-Pt_1-C2_2	42.0(2)
Pt_1-C2_2	2.078(5)	C2_2-Pt_1-C1_4	109.2(2)
Pt_1-C1_3	2.020(5)	C1_3-Pt_1-C1_4	99.3(2)
Pt_1-C1_4	2.007(4)	C1_2-Pt_1-C1_3	109.5(2)
C1_2=C2_2	1.486(5)	Pd Ave.- C=C-S Planes ^a	86.2(3)
		Pd Ave.- NHC Planes ^b	73.8(3)

^aAverage angle among the mean metal coordination plane and the olefinic one (defined as the plane that contains the C=C and non-H atoms directly bound).
^bAverage angle among the mean metal coordination plane and the NHC ones (defined as the plane that contains the C=C and non-H atoms directly bound).

