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MDPI

Supporting Information

for

Coupling of Thiazole-2-Amines with Isocyanide Ligands in *bis*-(Isocyanide) Platinum Complex: A New Type of Reactivity

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X-ray Diffraction Details

Table S1. Crystal data and structure refinement for **4a**, **4b**, and **5a**

Identification code	**4a** (yug102)	**4b** (yug102-2)	**5a** (yor019)
Empirical formula	$C_{39}H_{38}Cl_2N_6Pt_2S$	$C_{40}H_{39}Cl_5N_6Pt_2S$	$C_{41}H_{41}Cl_5N_6Pt_2S$
Formula weight	1083.89	1203.26	1217.29
Temperature/K	100(2)	100(2)	100(2)
Crystal system	triclinic	monoclinic	monoclinic
Space group	P-1	$P2_1/c$	$P2_1/c$
a/Å	7.6428(2)	8.13876(12)	14.4775(2)
b/Å	8.2736(4)	18.8975(3)	18.7218(3)
c/Å	30.3466(11)	27.7978(4)	15.7573(3)
α/°	86.354(3)	90	90
β/°	88.298(3)	96.0606(13)	94.769(2)
γ/°	84.719(3)	90	90
Volume/Å^3	1906.35(13)	4251.47(11)	4256.15(12)
Z	2	4	4
ϱ_{calc}g/cm^3	1.888	1.880	1.900
μ/mm^{-1}	7.562	6.974	15.763
F(000)	1040.0	2312.0	2344.0
Crystal size/mm^3	0.15 × 0.1 × 0.1	0.15 × 0.12 × 0.1	0.2 × 0.15 × 0.15
Radiation	Mo Kα (λ = 0.71073)	MoKα (λ = 0.71073)	CuKα (λ = 1.54184)
2Θ range for data collection/°	5.054 to 49.996	5.222 to 54.998	6.126 to 134.996
Index ranges	-9 ≤ h ≤ 9, -8 ≤ k ≤ 9, -36 ≤ l ≤ 31	-10 ≤ h ≤ 10, -24 ≤ k ≤ 24, -36 ≤ l ≤ 36	-17 ≤ h ≤ 17, -22 ≤ k ≤ 21, -18 ≤ l ≤ 18
Reflections collected	12848	86216	28850
Independent reflections	6675 [R_{int} = 0.0338, R_{sigma} = 0.0495]	9760 [R_{int} = 0.0363, R_{sigma} = 0.0188]	7670 [R_{int} = 0.0664, R_{sigma} = 0.0484]
Data/restraints/parameters	6675/0/459	9760/0/495	7670/0/505
Goodness-of-fit on F^2	1.135	1.287	1.038

Final R indexes [I>=2σ (I)]	R_1 = 0.0337, wR_2 = 0.0619	R_1 = 0.0278, wR_2 = 0.0595	R_1 = 0.0425, wR_2 = 0.1131
Final R indexes [all data]	R_1 = 0.0416, wR_2 = 0.0643	R_1 = 0.0302, wR_2 = 0.0603	R_1 = 0.0455, wR_2 = 0.1158
Largest diff. peak/hole / e $Å^{-3}$	2.09/-2.28	1.48/-2.02	1.97/-1.97
Flack parameter	n/a	n/a	n/a
CCDC number	2214271	2212279	2212276

Table S2. Crystal data and structure refinement for **5b**, **6**, and **7**

Identification code	**5b** (yor21)	**6** (asm232)	**7** (yor024)
Empirical formula	$C_{41}H_{41}Cl_5N_6Pt_2S$	$C_{25}H_{29}Cl_3N_6OPtS_2$	$C_{30}H_{32}Cl_{13}N_6PtS_2$
Formula weight	1217.29	795.10	1196.67
Temperature/K	100(2)	100(2)	100.01(10)
Crystal system	orthorhombic	monoclinic	orthorhombic
Space group	$P2_12_12_1$	$P2_1/n$	Pbca
a/Å	8.11247(5)	11.9674(3)	14.2834(3)
b/Å	20.40385(10)	16.2090(5)	23.4916(4)
c/Å	26.31527(14)	16.0375(5)	26.8793(4)
α/°	90	90	90
β/°	90	108.421(3)	90
γ/°	90	90	90
Volume/$Å^3$	4355.85(4)	2951.53(15)	9019.1(3)
Z	4	4	8
$\varrho_{calc}g/cm^3$	1.856	1.789	1.763
μ/mm^{-1}	15.402	5.198	14.034
F(000)	2344.0	1560.0	4680.0
Crystal size/mm^3	0.6 × 0.5 × 0.3	0.1 × 0.1 × 0.1	0.12 × 0.12 × 0.1
Radiation	CuKα (λ = 1.54184)	MoKα (λ = 0.71073)	CuKα (λ = 1.54184)
2Θ range for data collection/°	5.48 to 139.99	5.11 to 54.996	6.576 to 155.088
Index ranges	-9 ≤ h ≤ 9, -24 ≤ k ≤ 24, -32 ≤ l ≤ 32	-15 ≤ h ≤ 12, -19 ≤ k ≤ 21, -20 ≤ l ≤ 20	-18 ≤ h ≤ 17, -29 ≤ k ≤ 29, -33 ≤ l ≤ 18
Reflections collected	110650	13267	35479
Independent reflections	8247 [R_{int} = 0.0653, R_{sigma} = 0.0230]	6781 [R_{int} = 0.0399, R_{sigma} = 0.0737]	9208 [R_{int} = 0.0641, R_{sigma} = 0.0543]
Data/restraints/parameters	8247/0/505	6781/0/342	9208/0/475
Goodness-of-fit on F^2	1.044	1.027	1.085
Final R indexes [I>=2σ (I)]	R_1 = 0.0241, wR_2 = 0.0580	R_1 = 0.0425, wR_2 = 0.0783	R_1 = 0.0441, wR_2 = 0.1161

Final R indexes [all data]	R_1 = 0.0248, wR_2 = 0.0584	R_1 = 0.0694, wR_2 = 0.0899	R_1 = 0.0526, wR_2 = 0.1216
Largest diff. peak/hole / e Å^{-3}	0.84/-1.17	2.53/-1.12	2.02/-2.02
Flack parameter	-0.034(5)	n/a	n/a
CCDC number	2212278	2212275	2212277

NMR Spectra

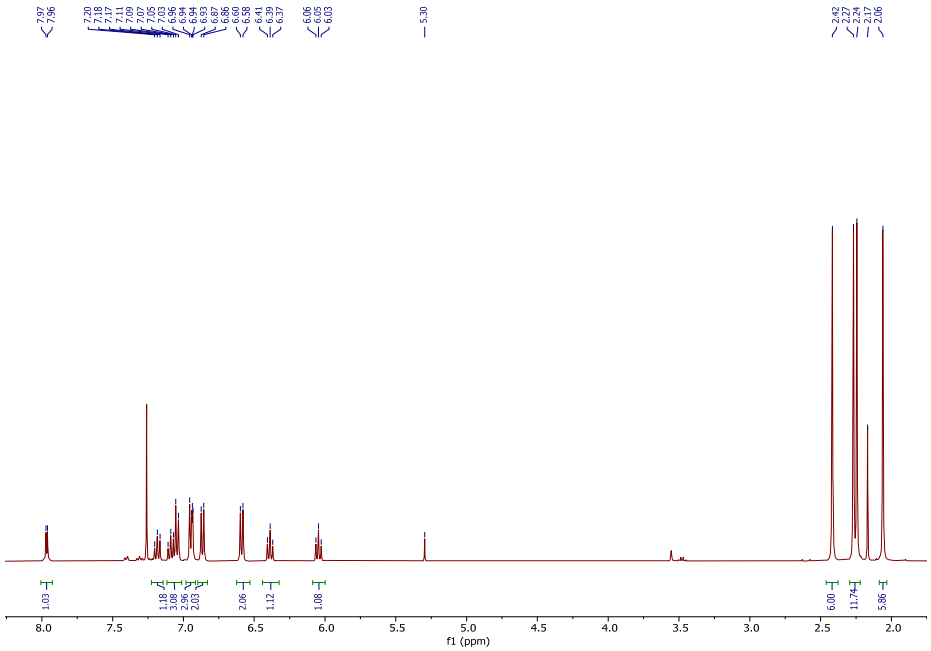

Figure S1. The ^{1}H NMR spectrum of **4a** in $CDCl_3$.

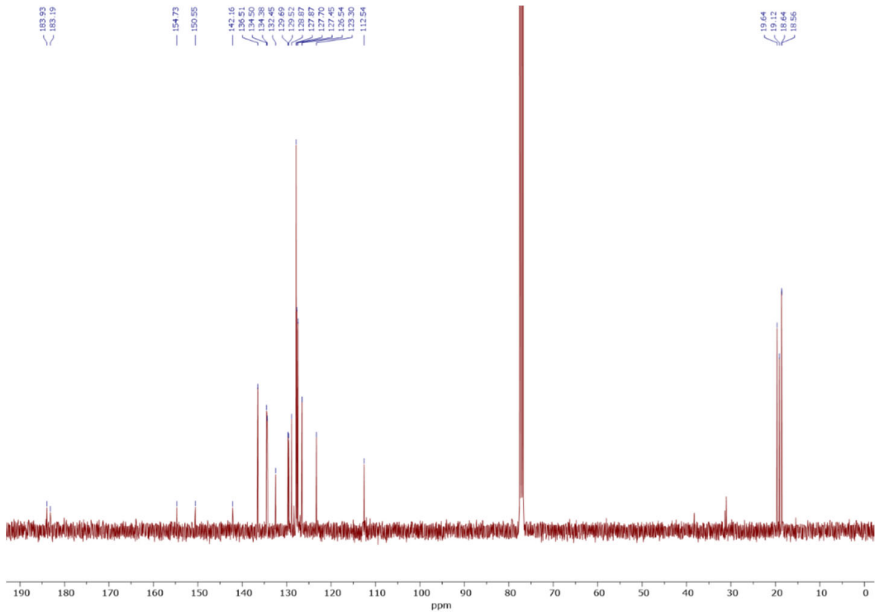

Figure S2. The ^{13}C NMR spectrum of **4a** in $CDCl_3$.

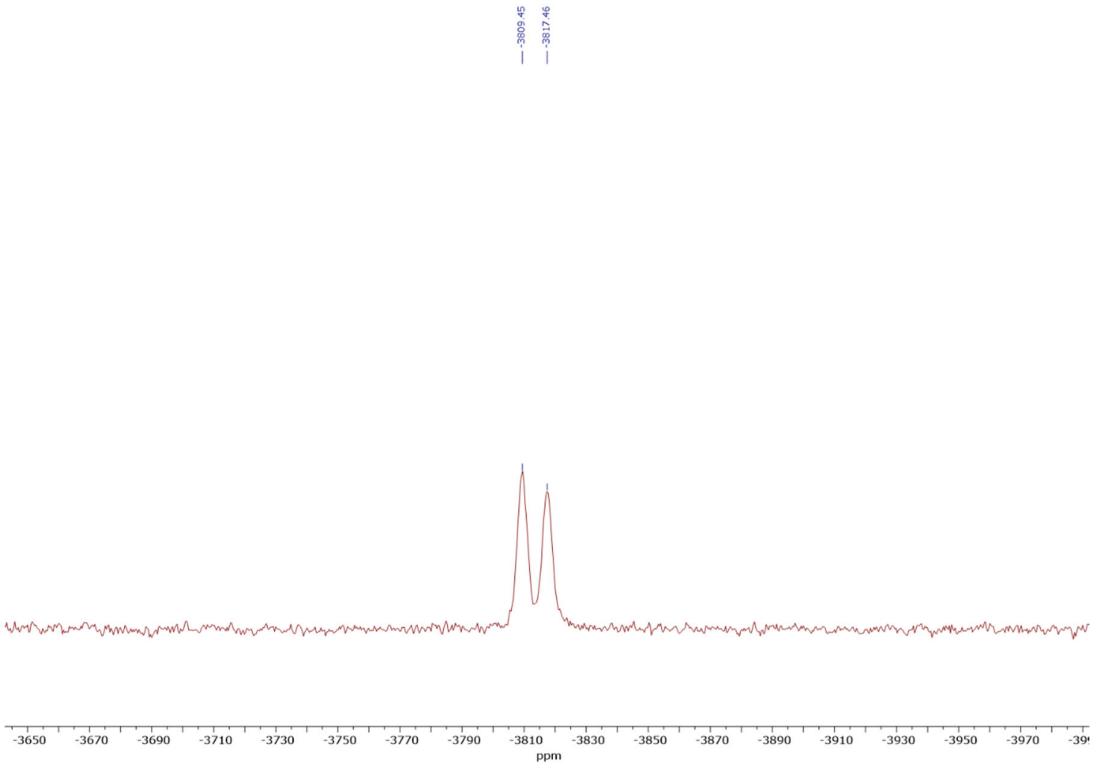

Figure S3. The ^{195}Pt spectrum of **4a** in $CDCl_3$.

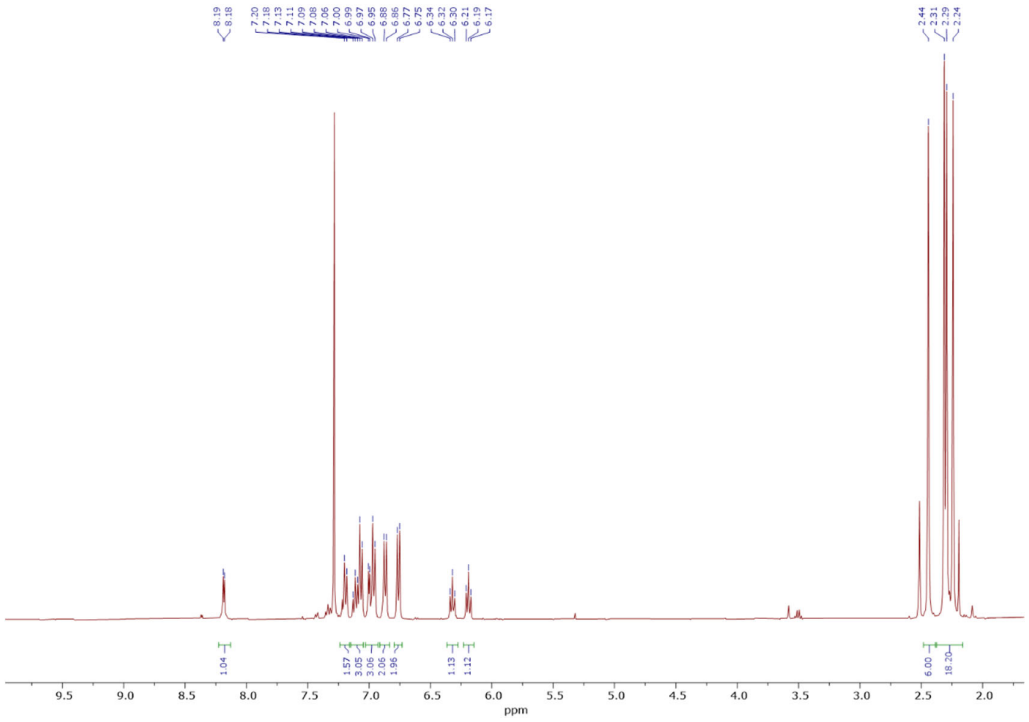

Figure S4. The ^{1}H NMR spectrum of **4b** in $CDCl_3$.

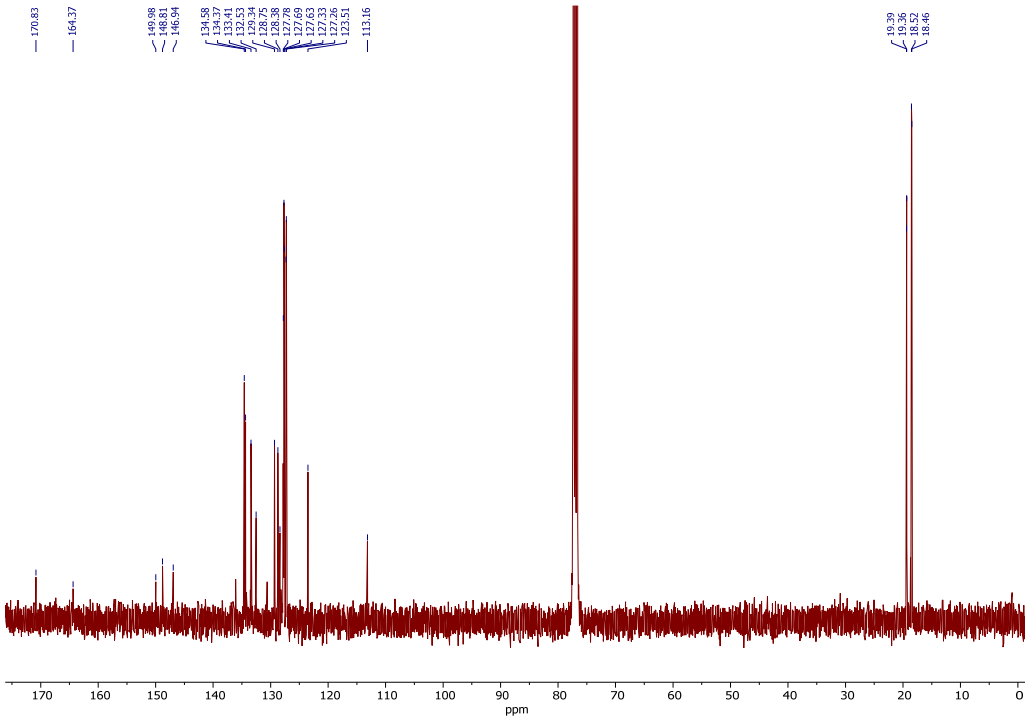

Figure S5. The ^{13}C NMR spectrum of **4b** in $CDCl_3$.

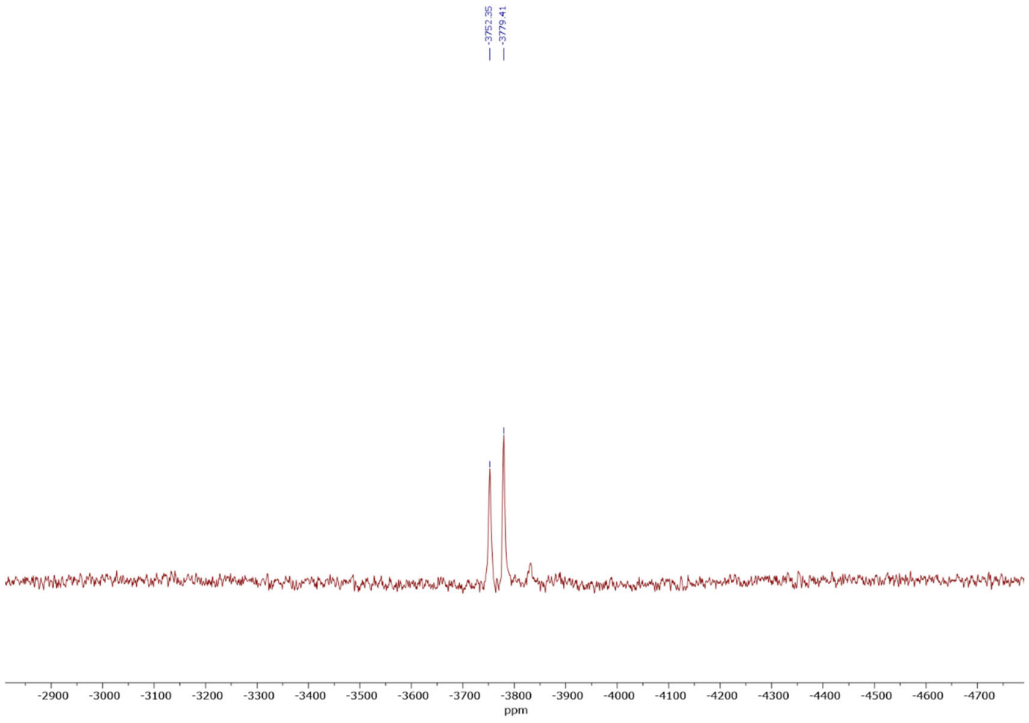

Figure S6. The ^{195}Pt NMR spectrum of **4b** in $CDCl_3$.

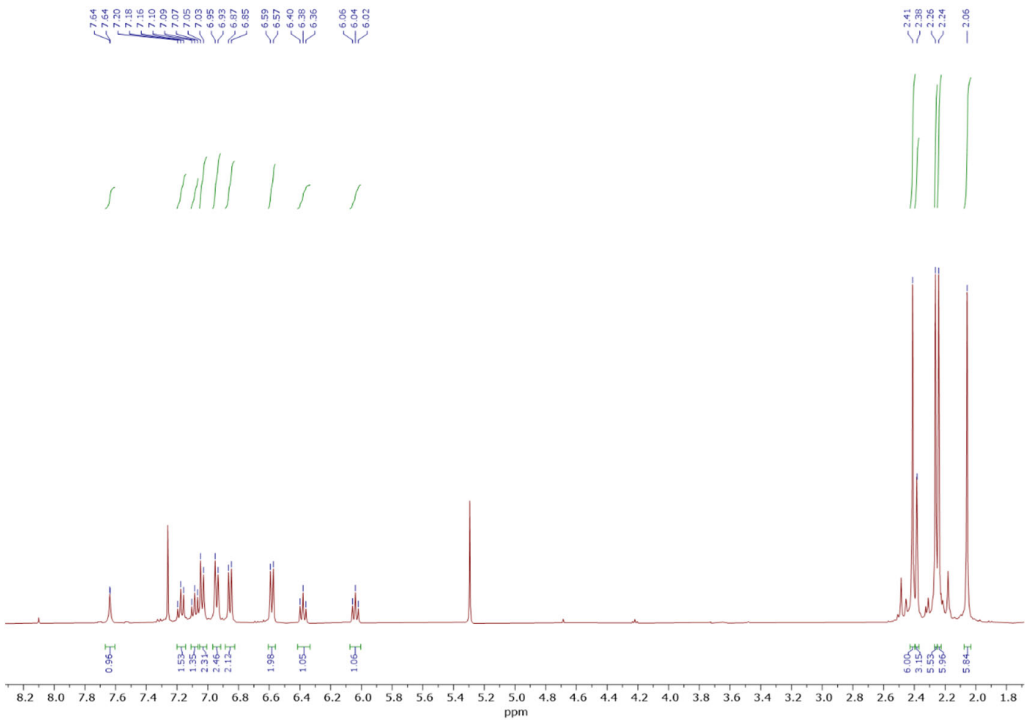

Figure S7. The ^{1}H NMR spectrum of **5a** in $CDCl_3$.

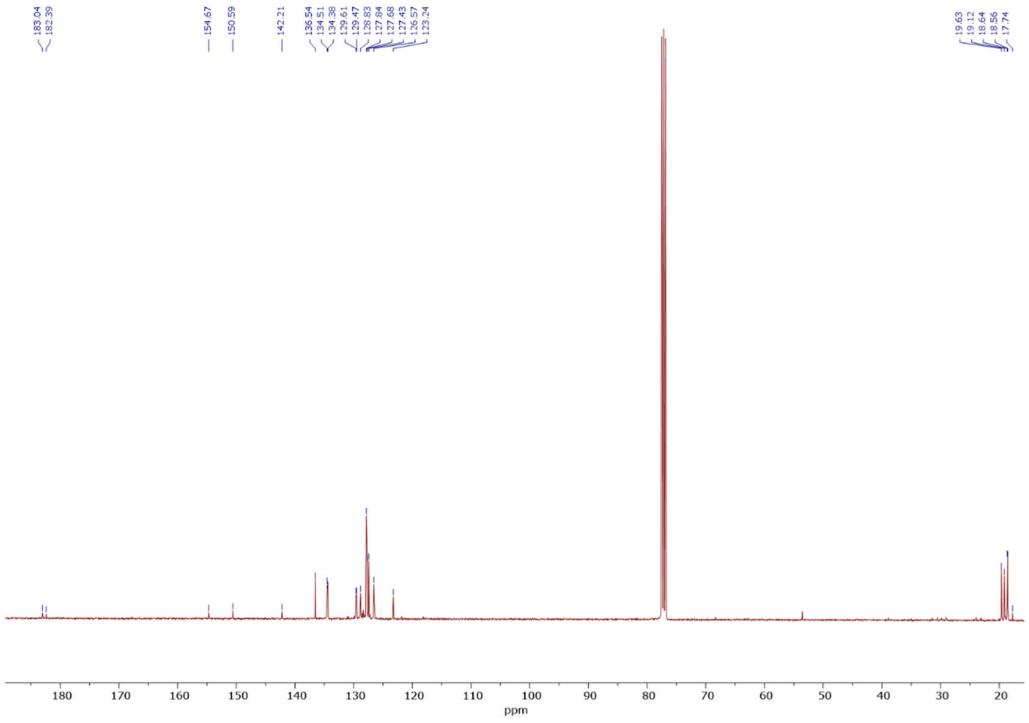

Figure S8. The ^{13}C NMR spectrum of **5a** in $CDCl_3$.

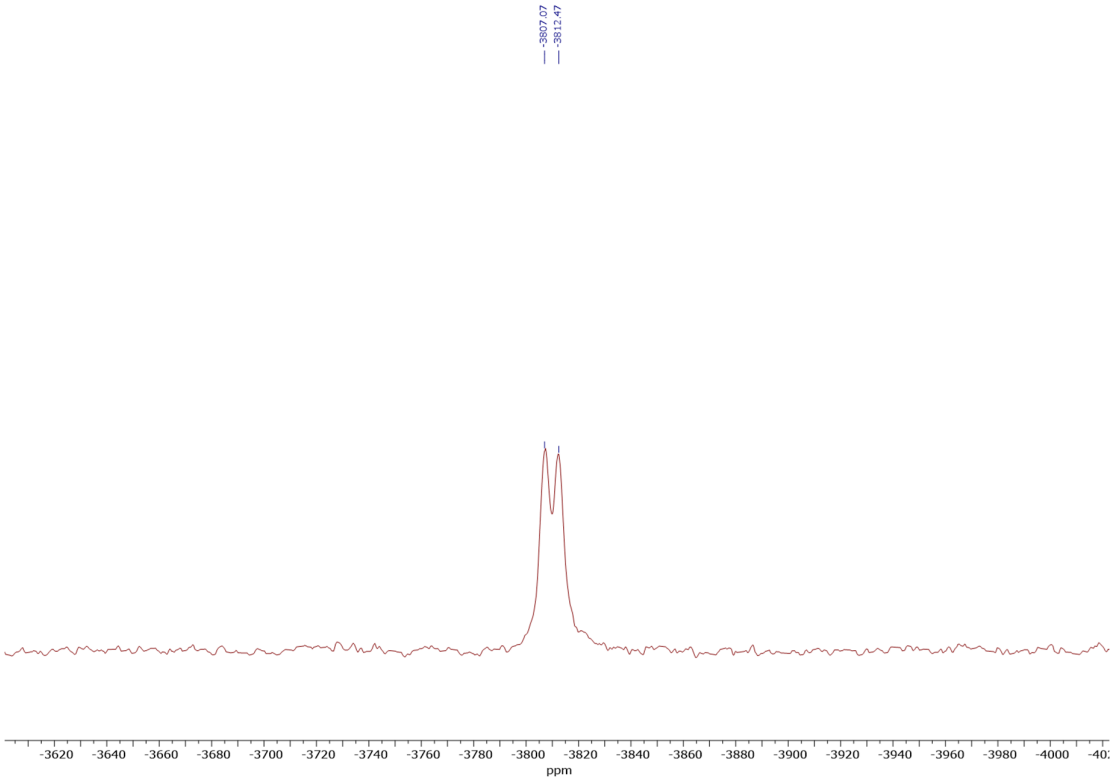

Figure S9. The ^{195}Pt NMR spectrum of **5a** in $CDCl_3$.

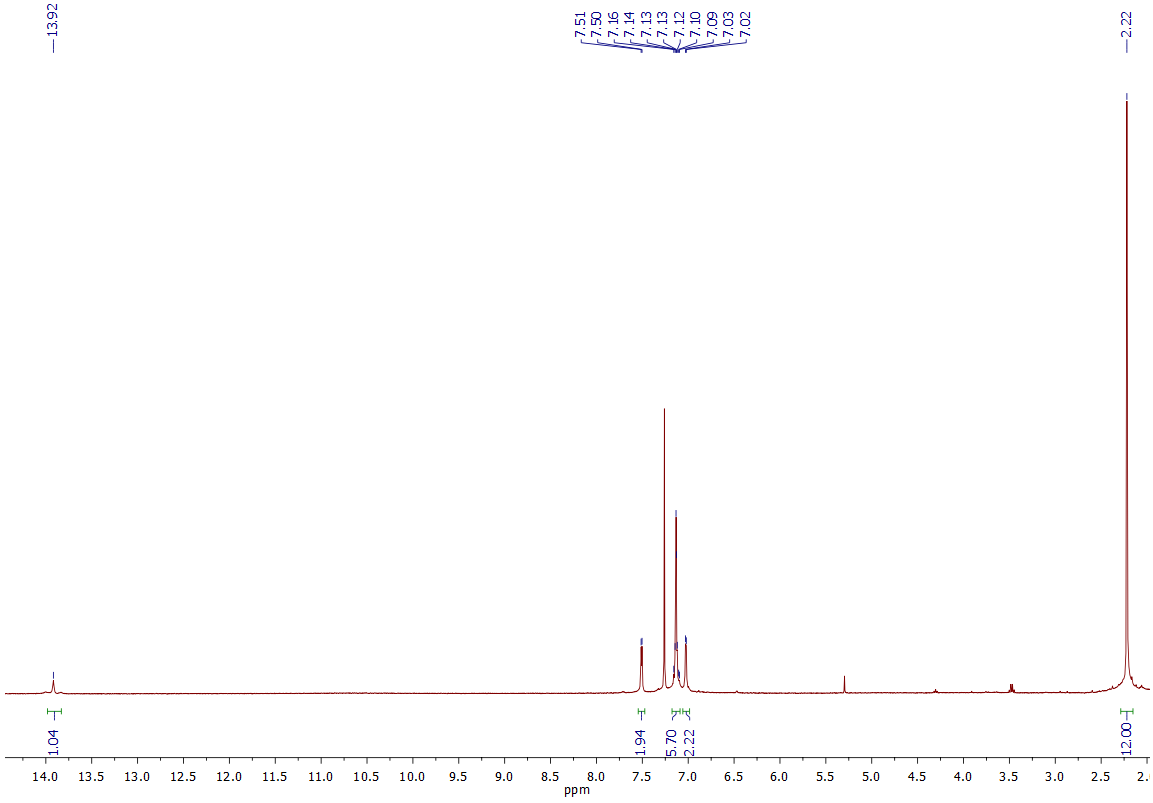

Figure S10. The ^{1}H NMR spectrum of **6** in $CDCl_3$.

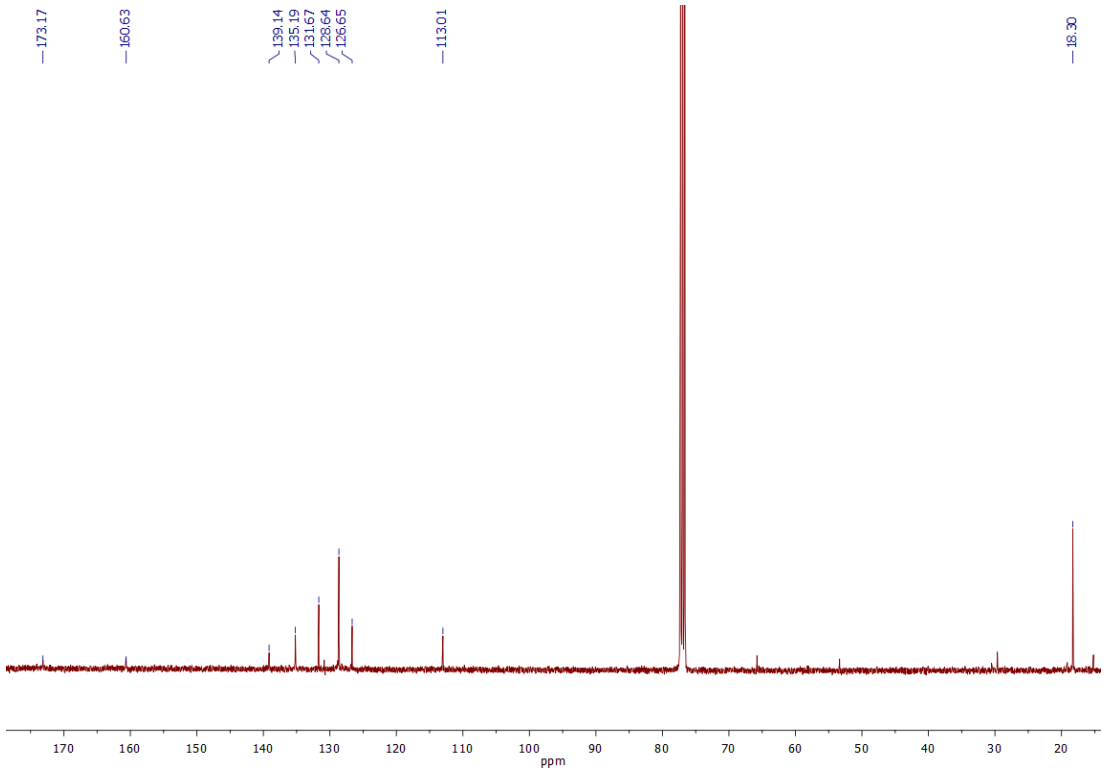

Figure S11. The ^{13}C NMR spectrum of **6** in $CDCl_3$.

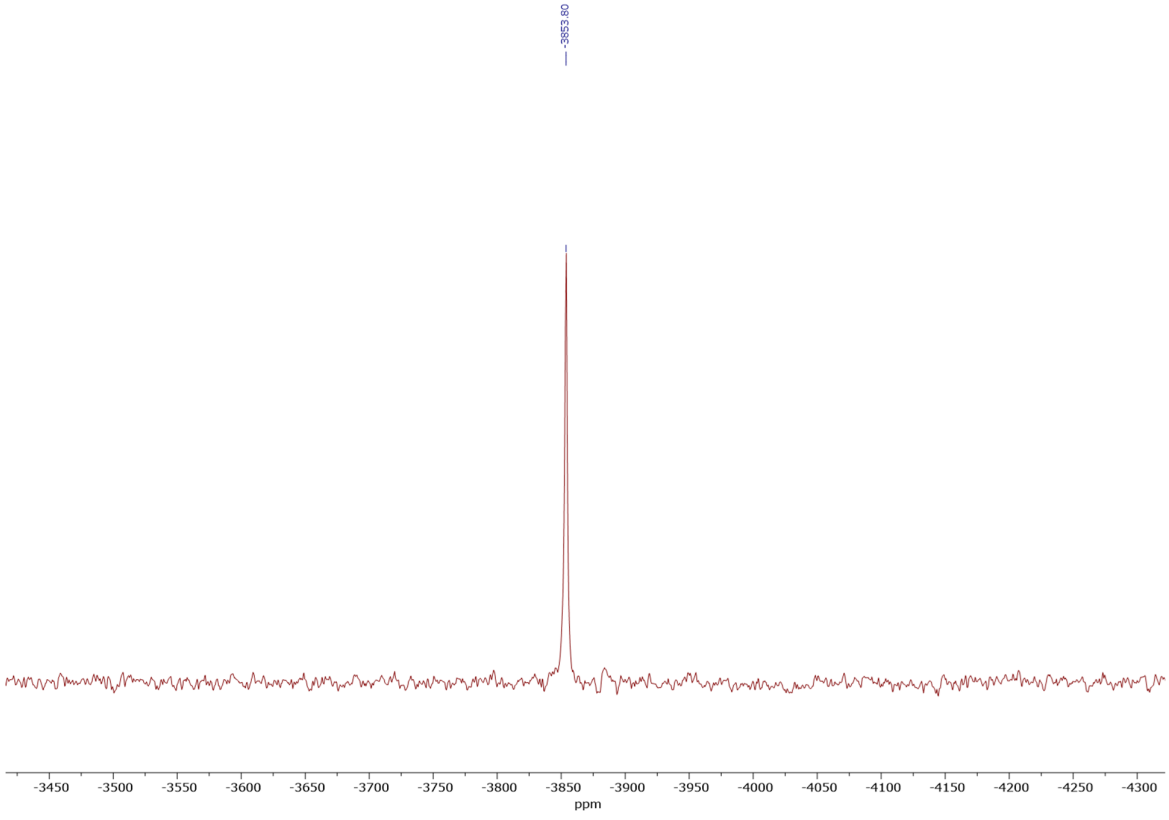

Figure S12. The ^{195}Pt NMR spectrum of **6** in $CDCl_3$.

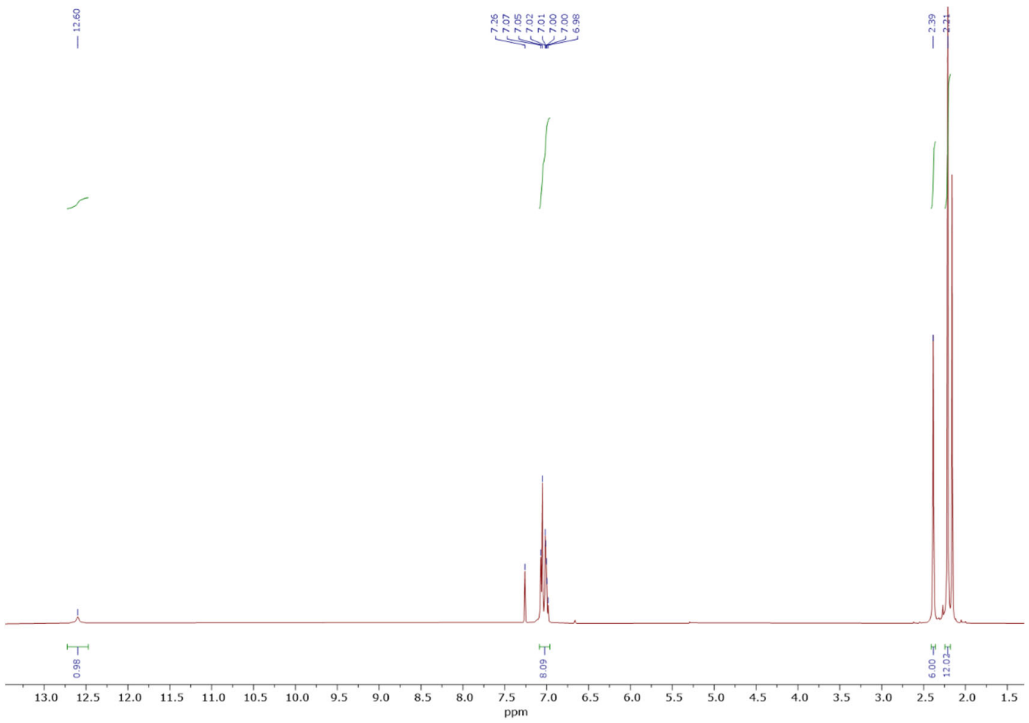

Figure S13. The ^{1}H NMR spectrum of **7**•Acetone in $CDCl_3$.

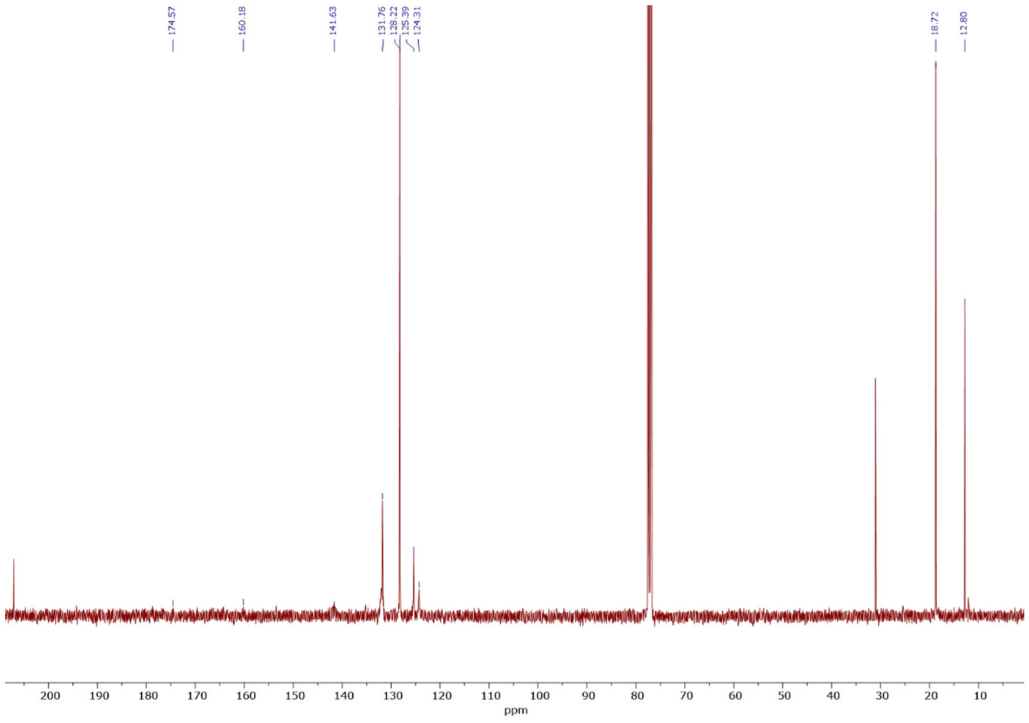

Figure S14. The ^{13}C NMR spectrum of **7**•Acetone in $CDCl_3$.

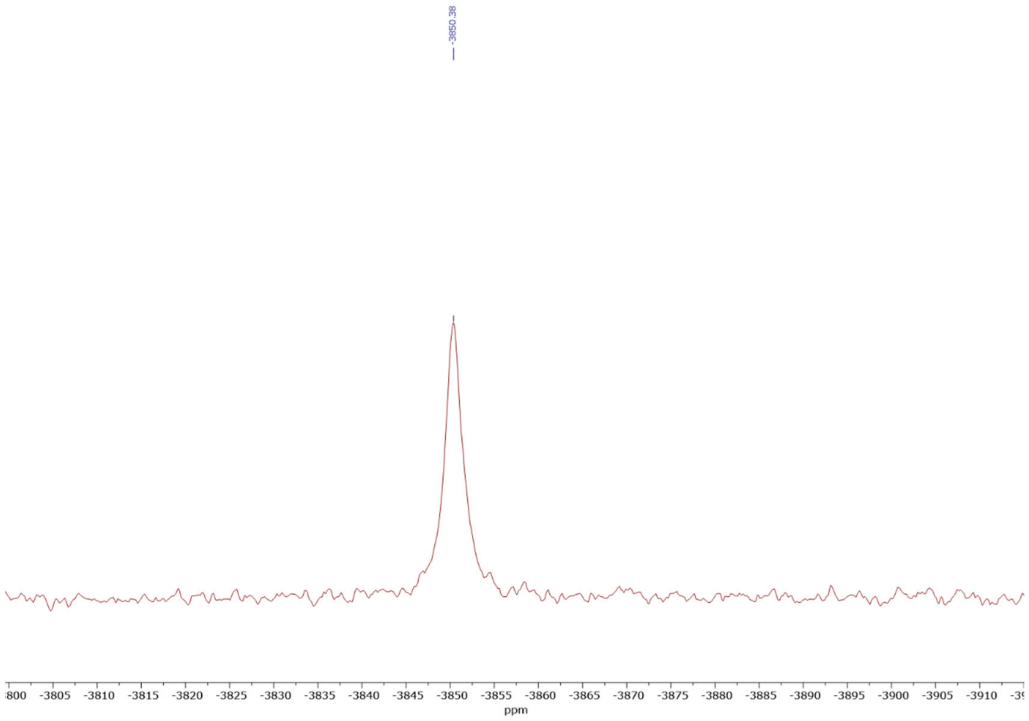

Figure S15. The ^{195}Pt NMR spectrum of **7**•Acetone in $CDCl_3$.