SUPPORTING INFORMATION FOR

Chalcogenourea derivatives of N-heterocyclic carbenes: synthesis of seleno, thio- and tello-urea compounds and selenoureas coordination to transition metals (Au, Ag and Cu)

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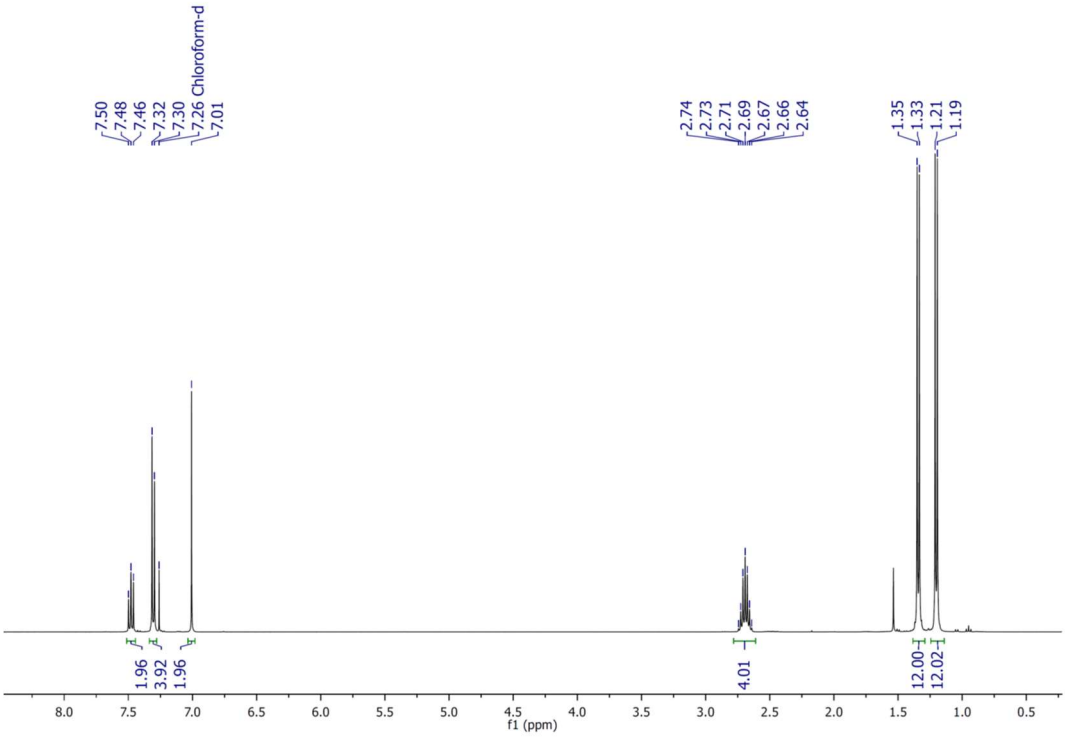
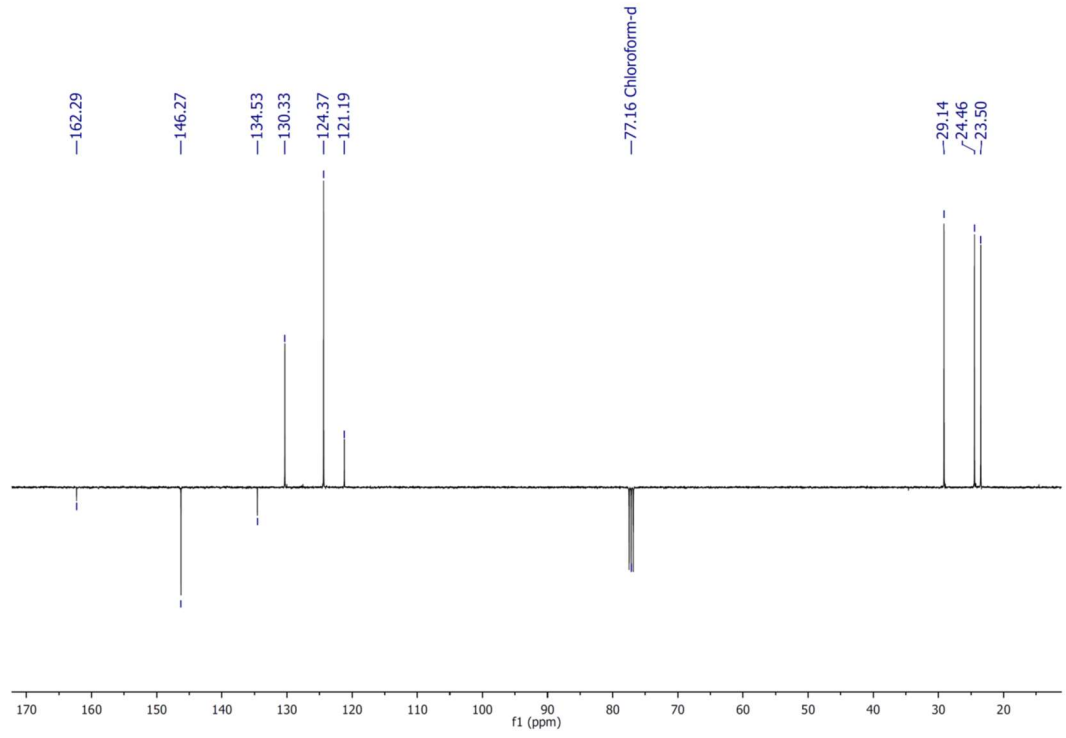
NMR spectra of the ligands

[Se(IPr)]

^{1}H NMR

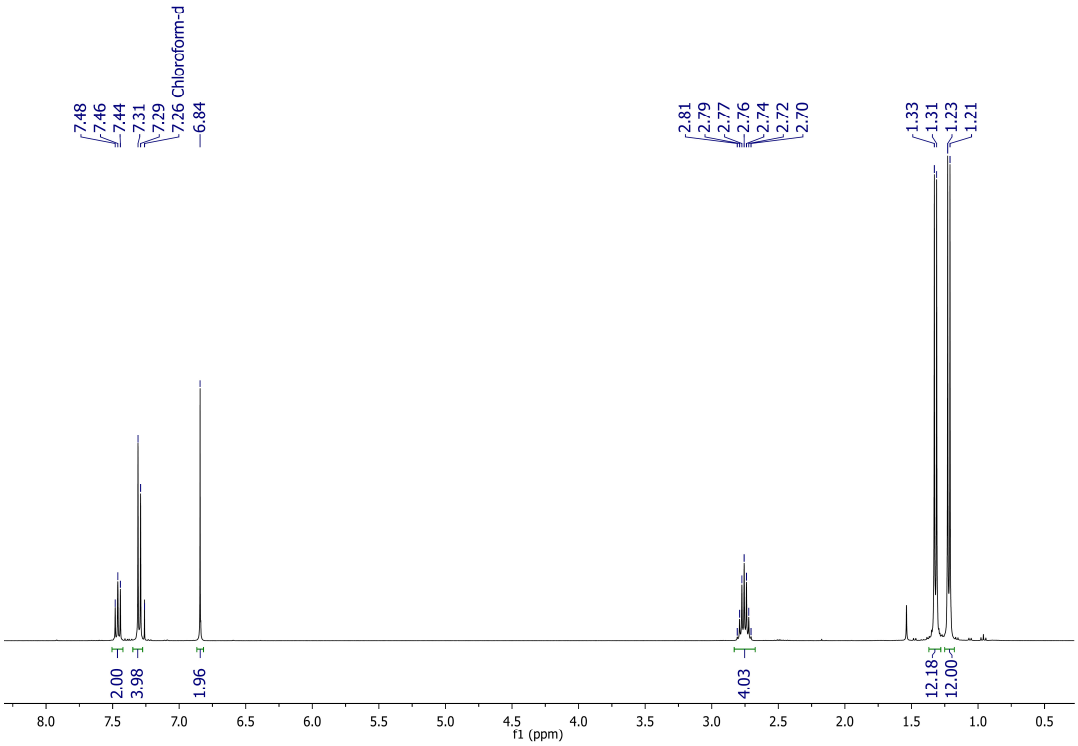


^{13}C{^{1}H} DEPT Q NMR



[S(IPr)]

^{1}H NMR



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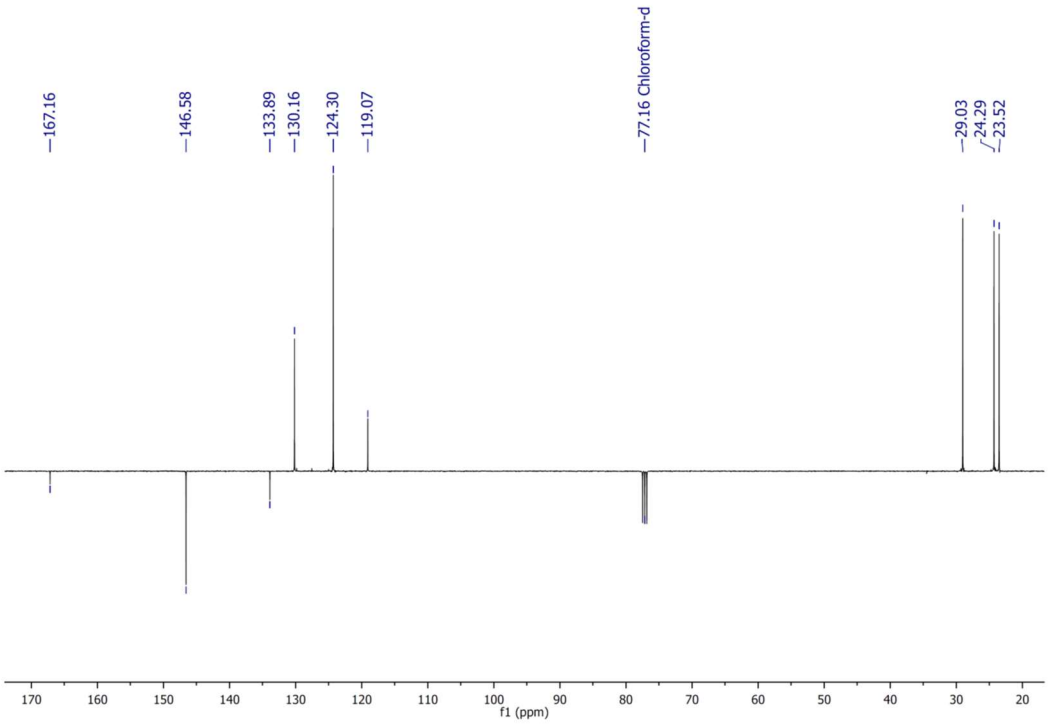
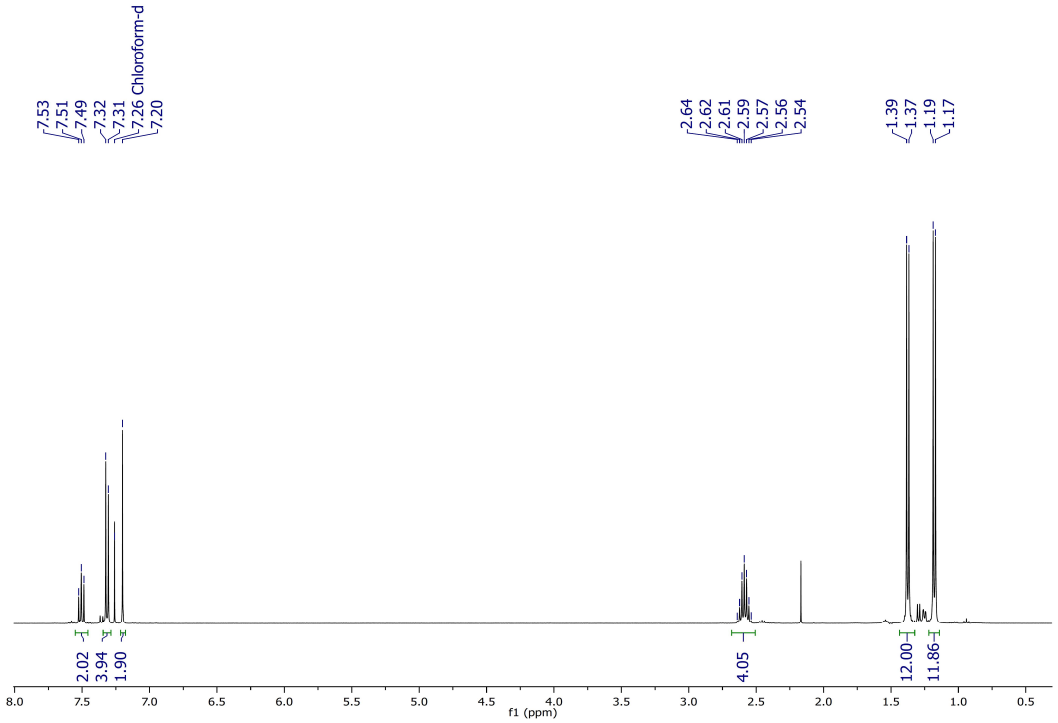


[Te(IPr)]

^{1}H NMR



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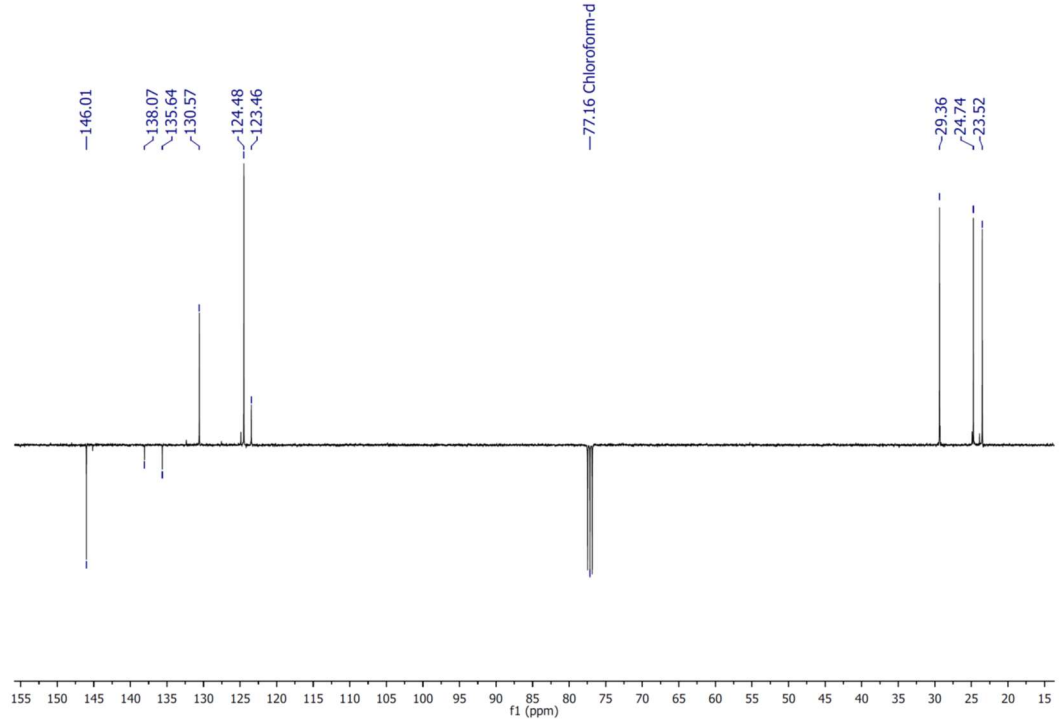
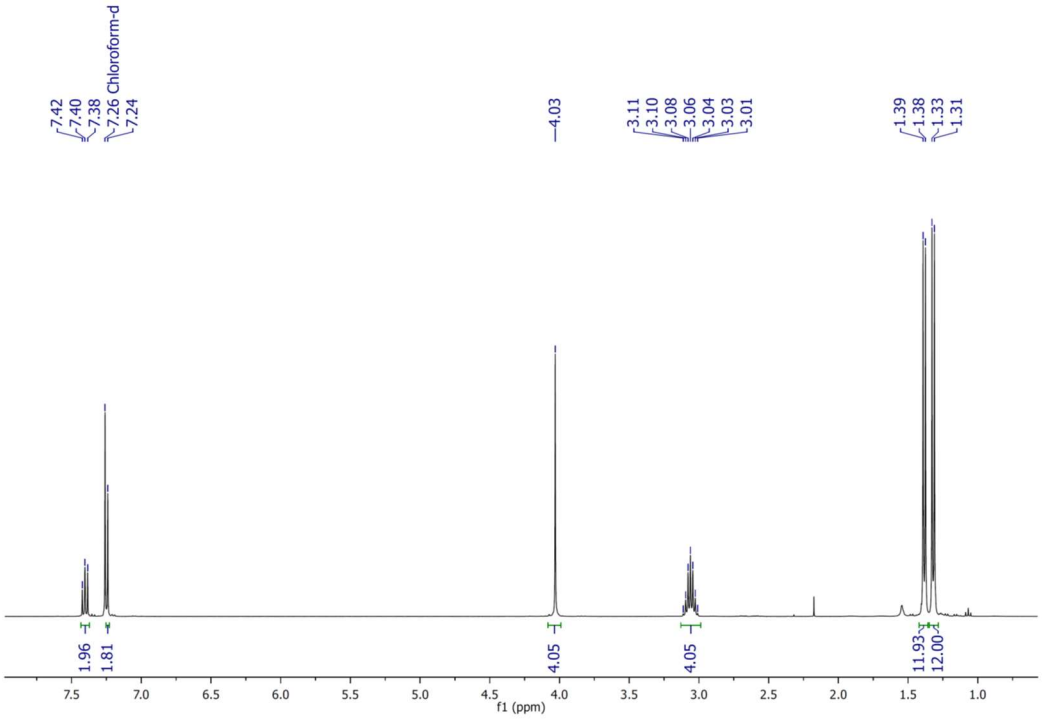


[Se(SIPr)]

^{1}H NMR



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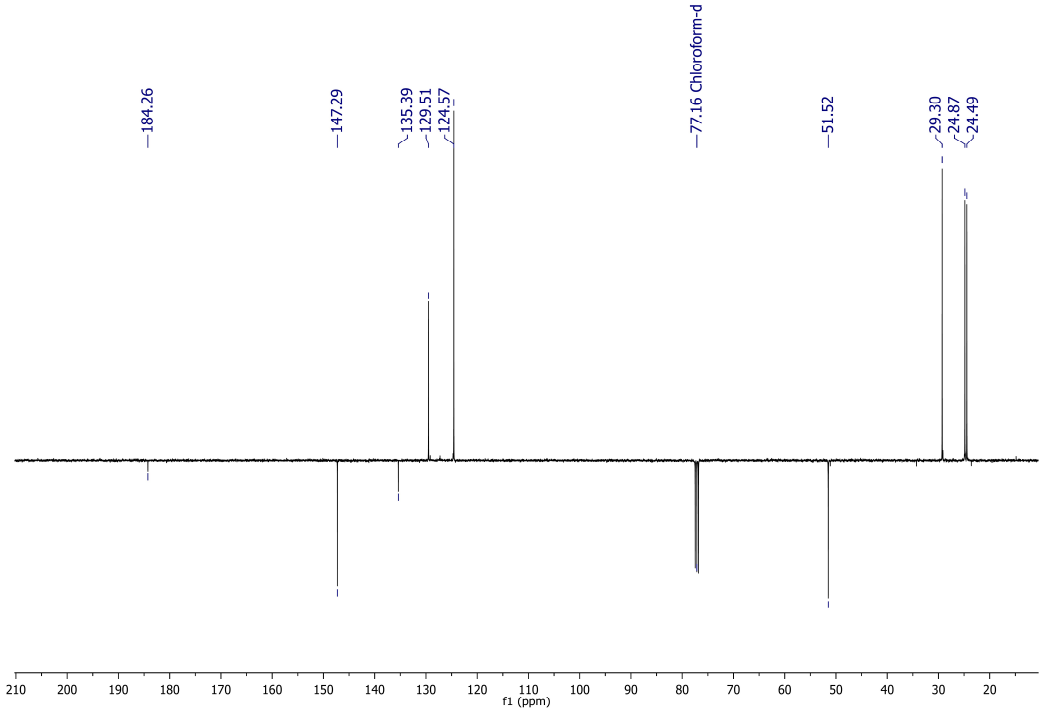
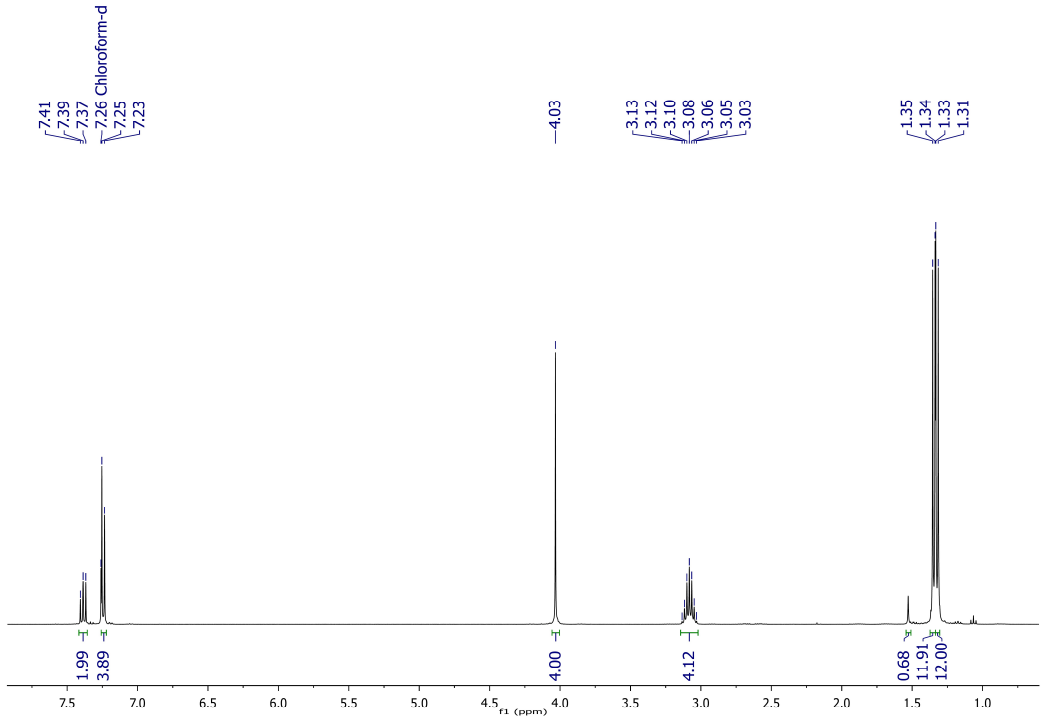


[S(SIPr)]

^{1}H NMR



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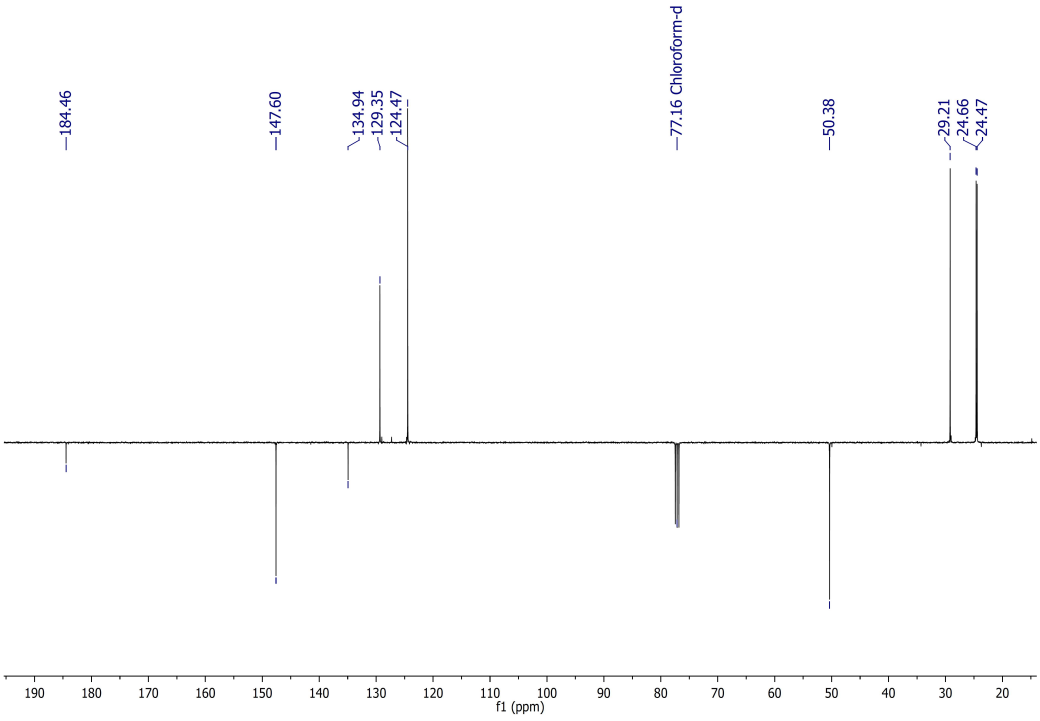
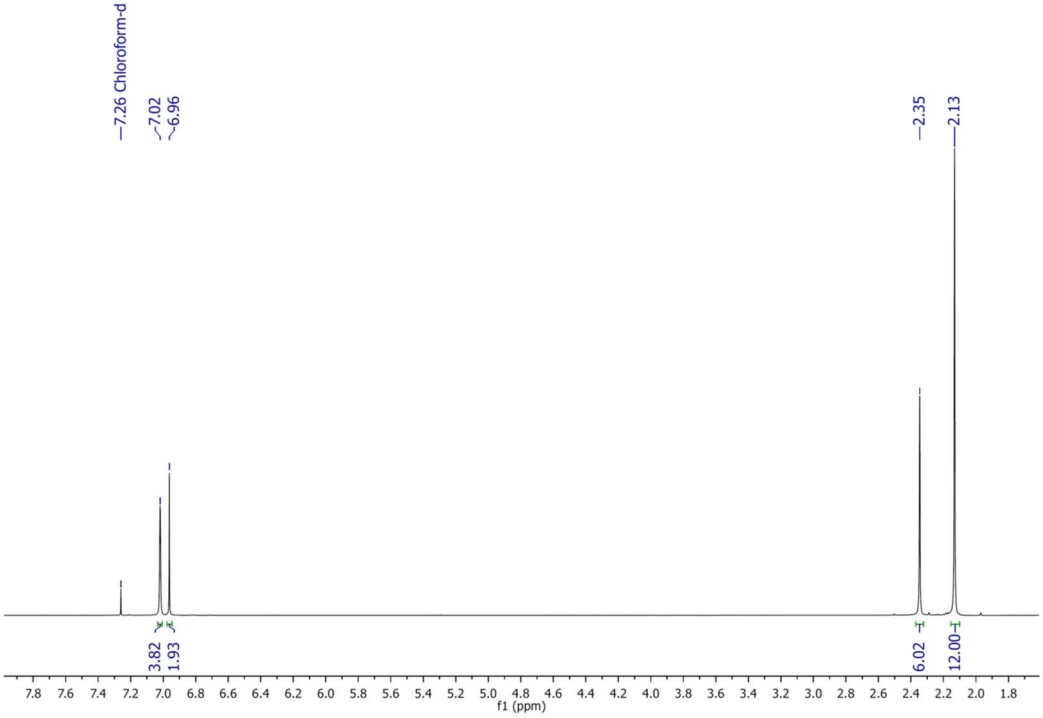


[Se(IMes)]

^{1}H NMR



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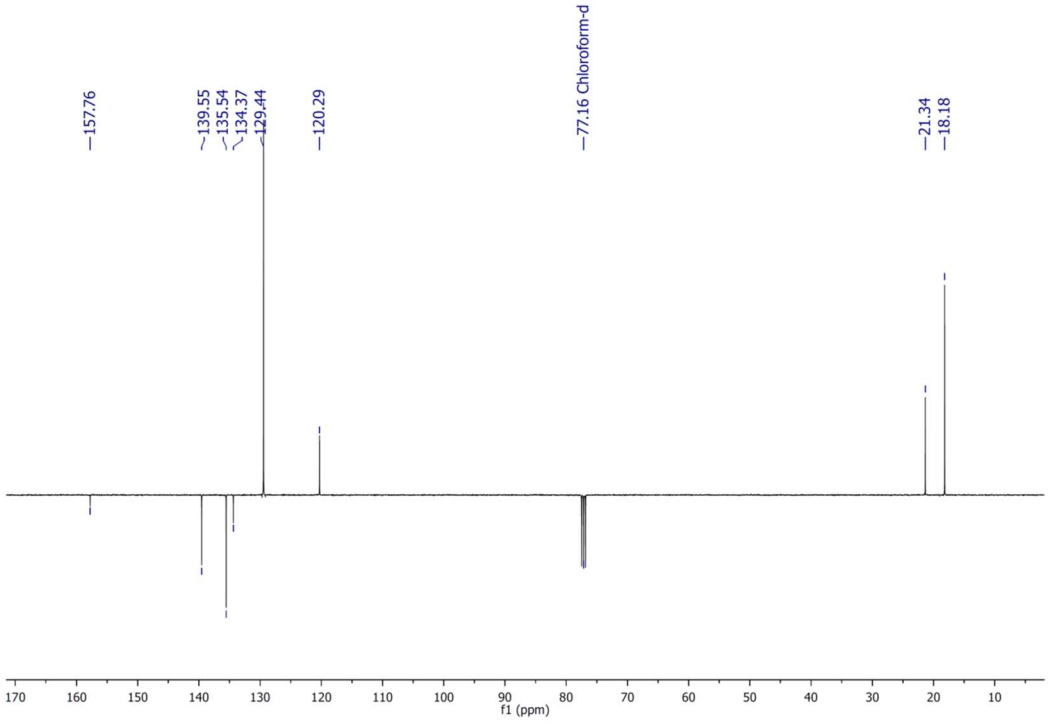
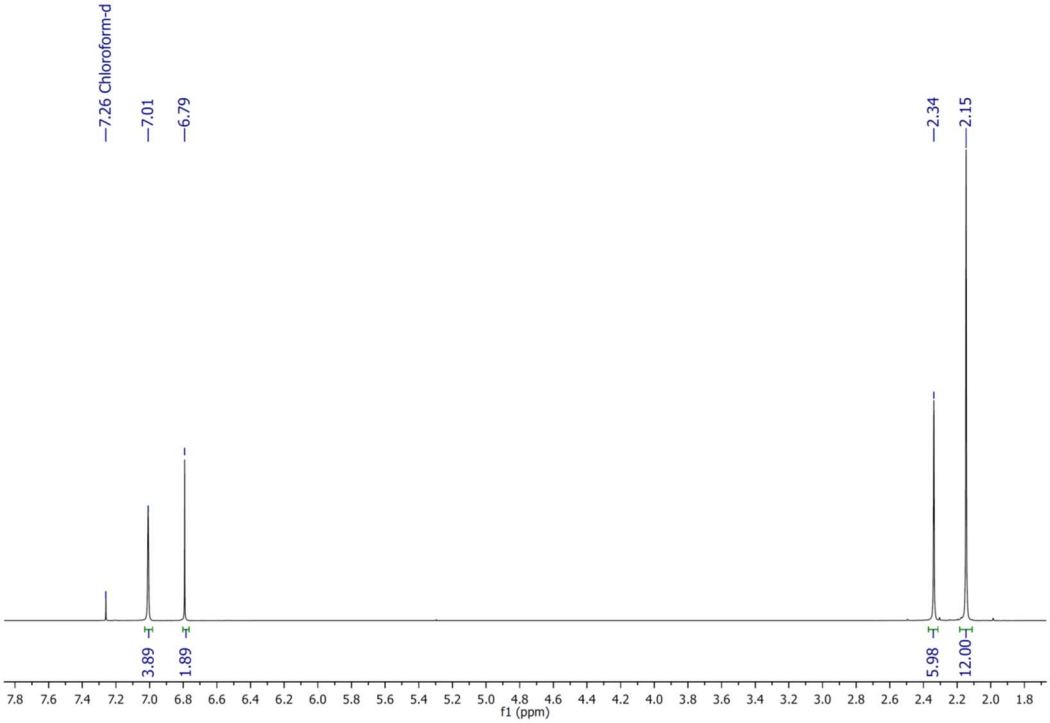
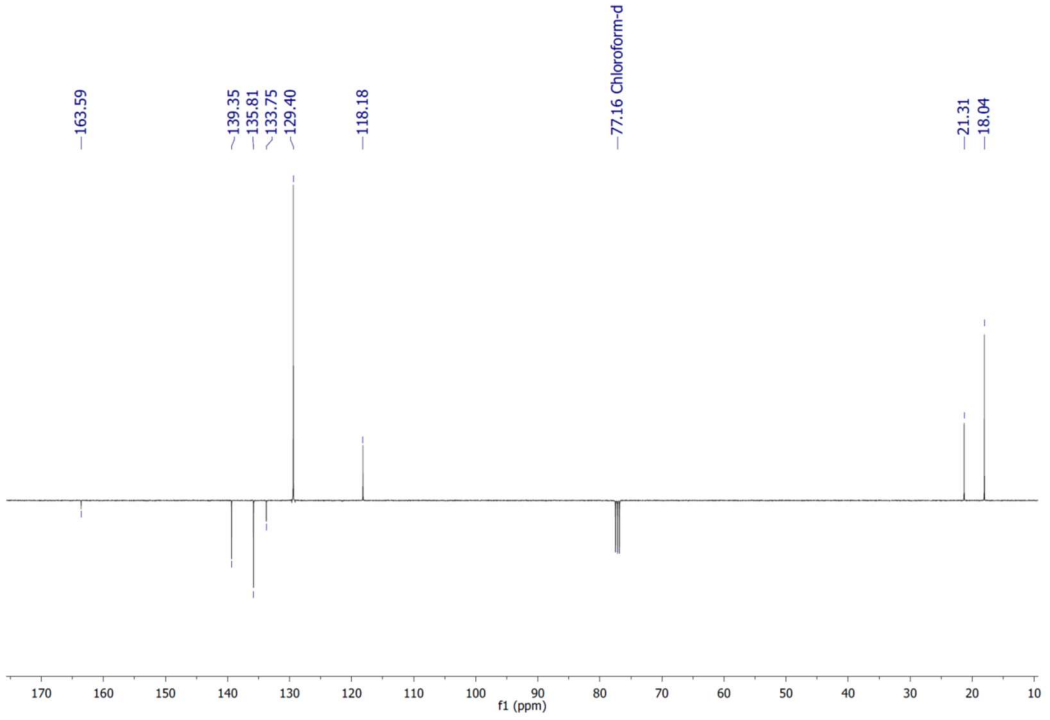


[S(IMes)]

^{1}H NMR

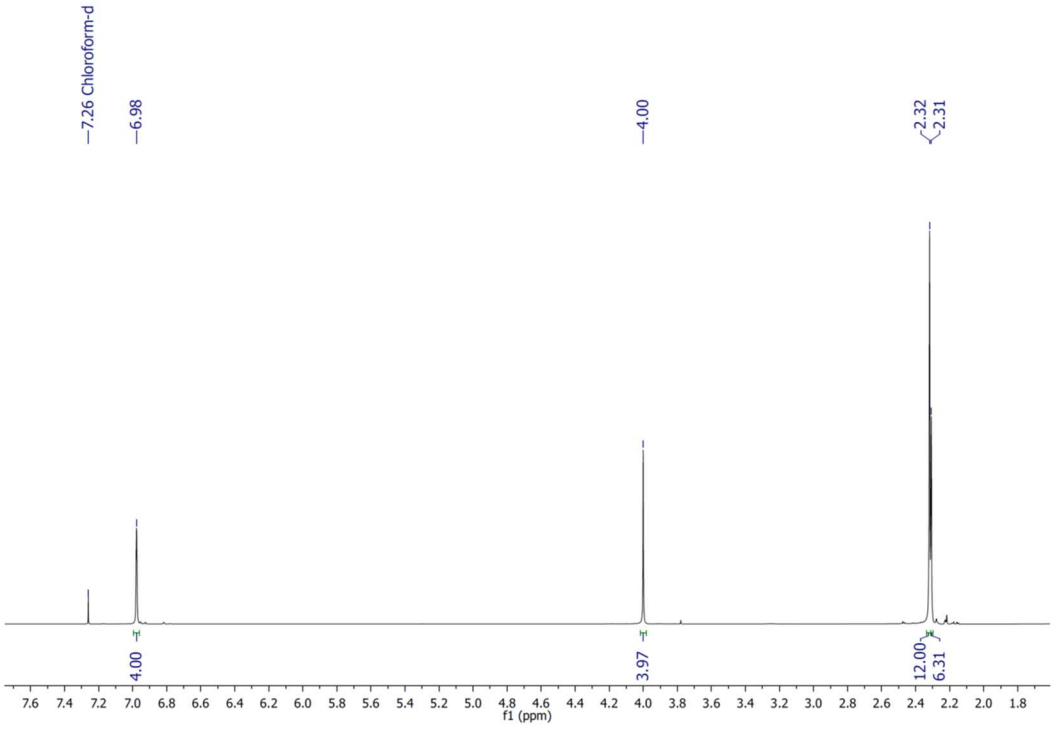


^{13}C{^{1}H} DEPT Q NMR

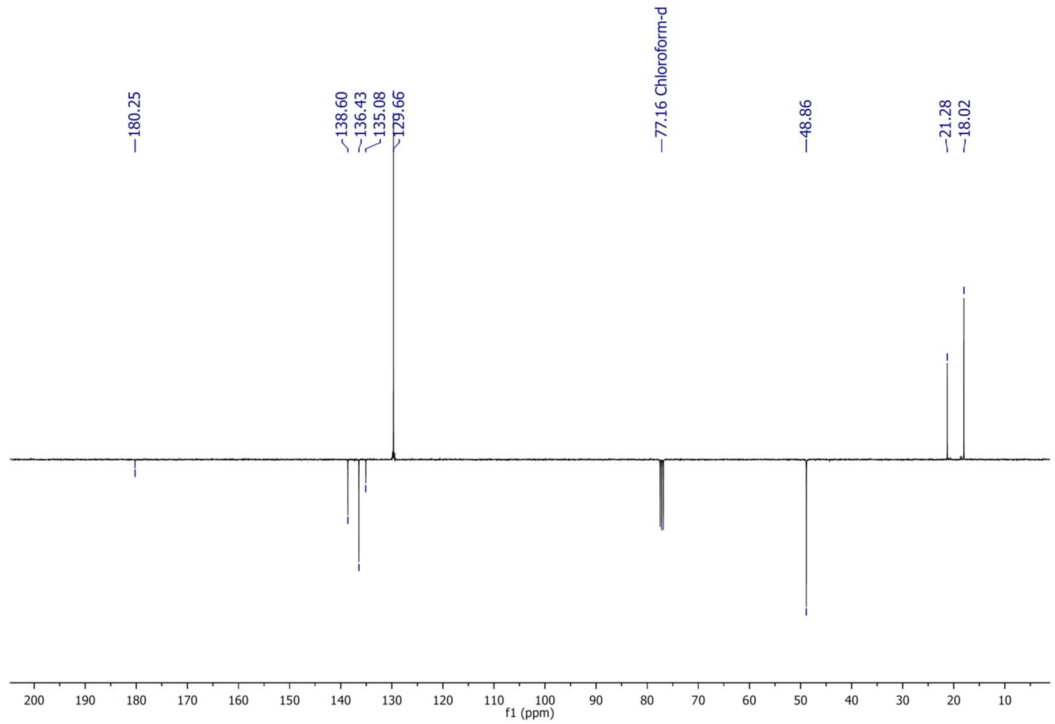


[Se(SIMes)]

^{1}H NMR

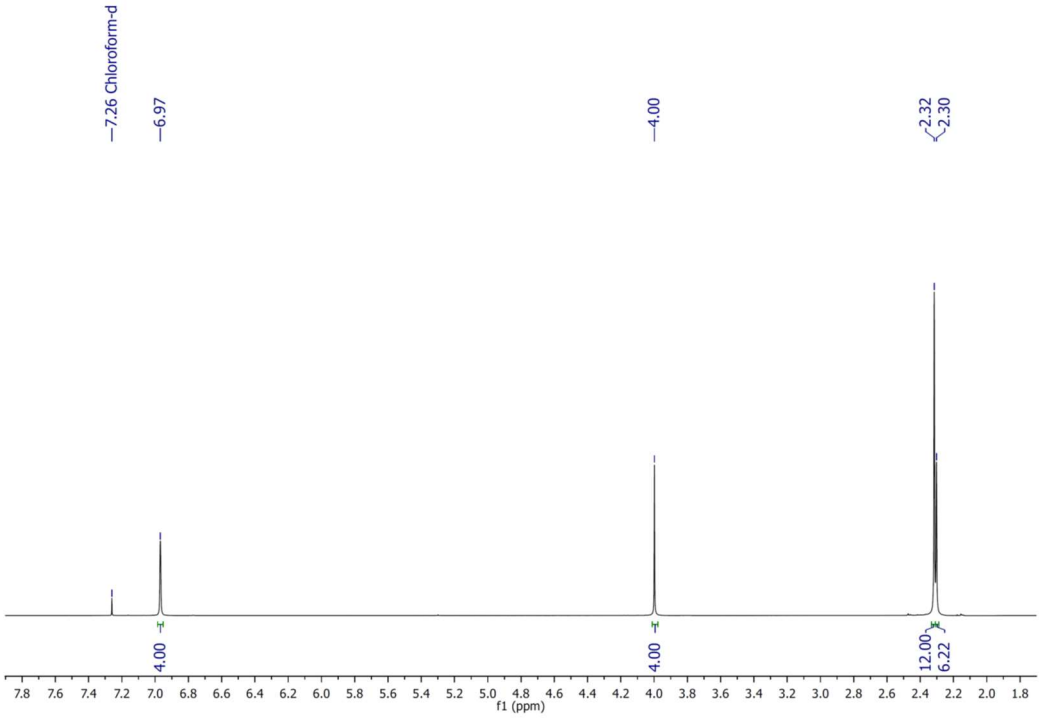


^{13}C{^{1}H} DEPT Q NMR

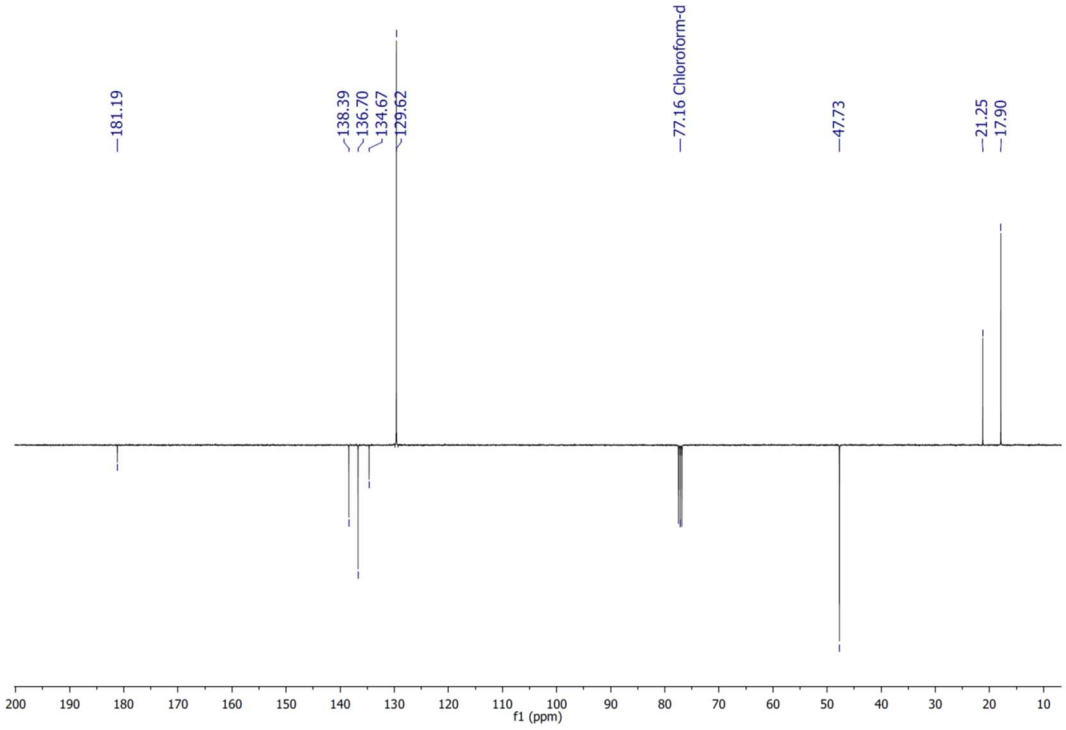


[S(SIMes)]

^{1}H NMR

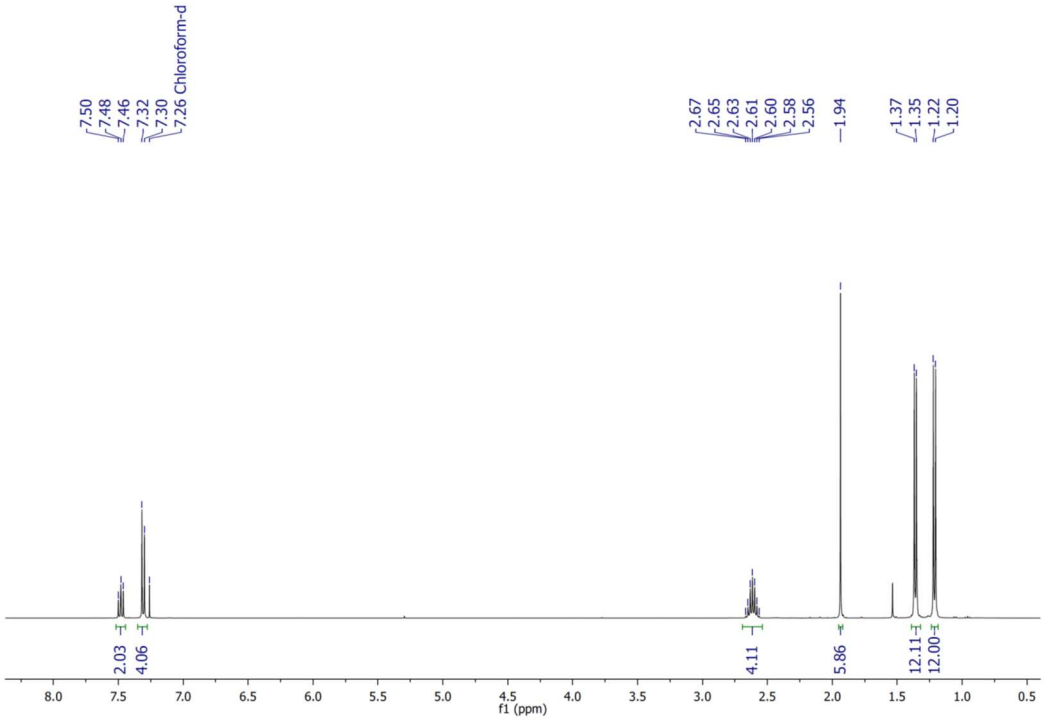


^{13}C{^{1}H} DEPT Q NMR

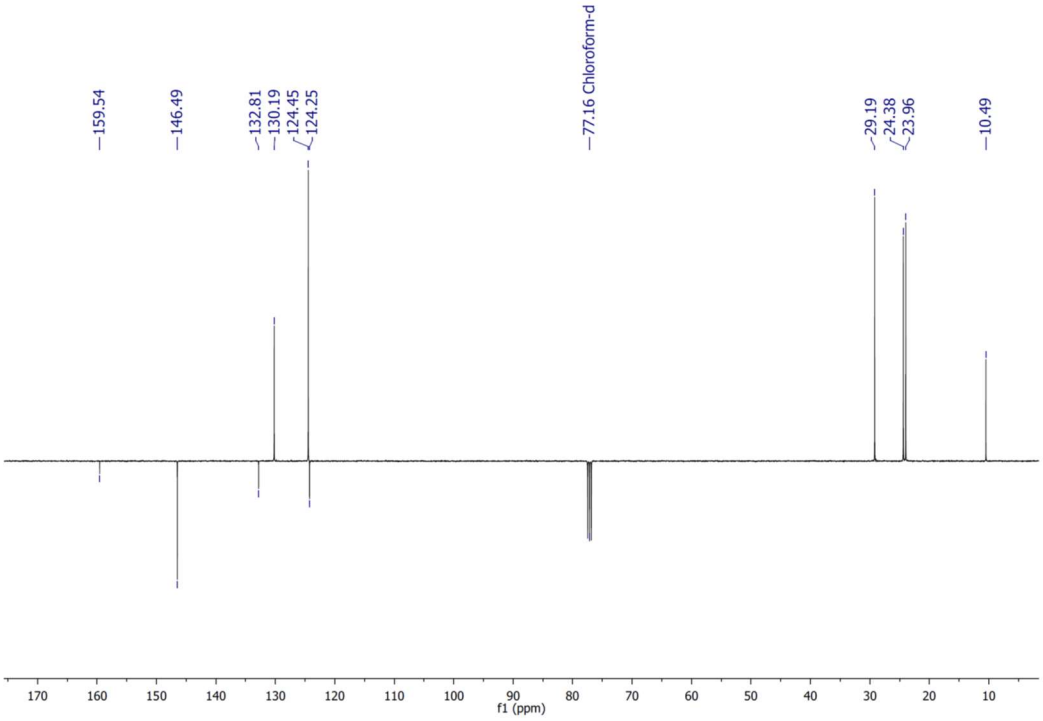


[Se(IPr^{Me})]

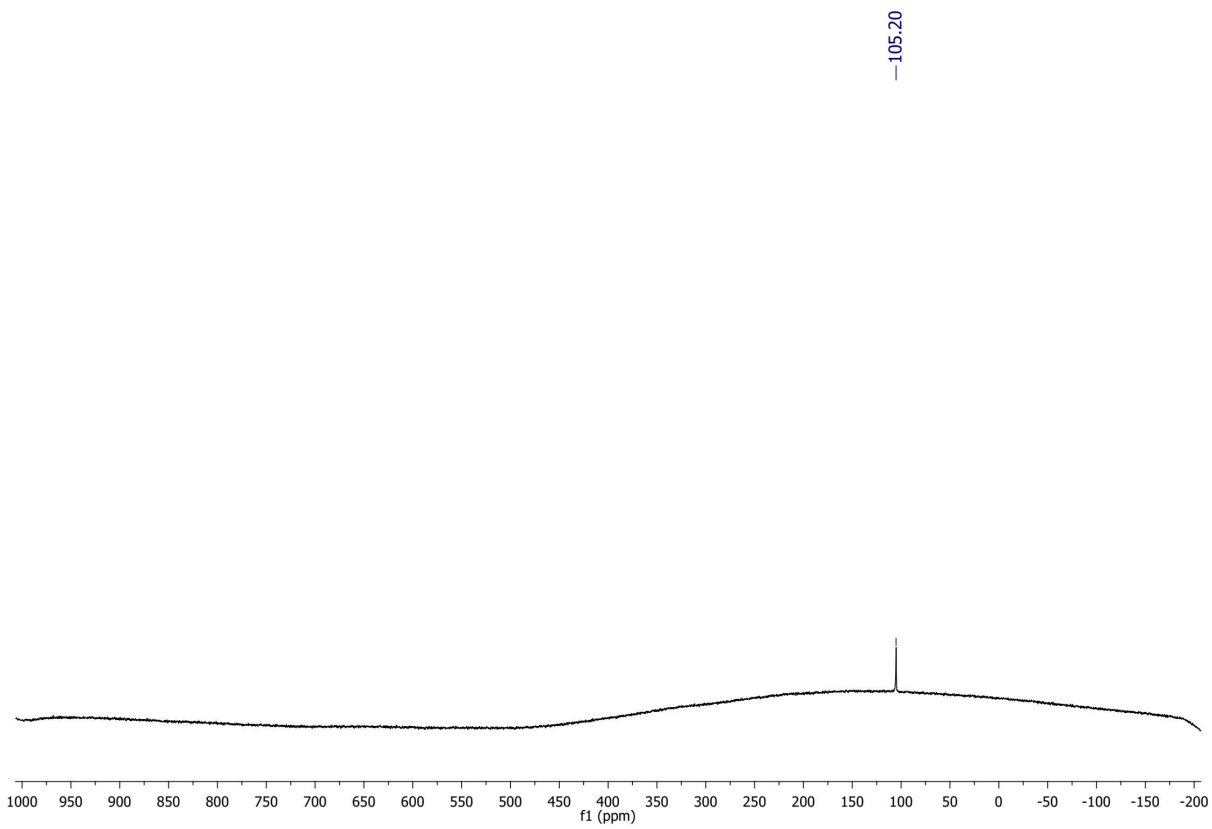
^{1}H NMR



^{13}C{^{1}H} DEPT Q NMR

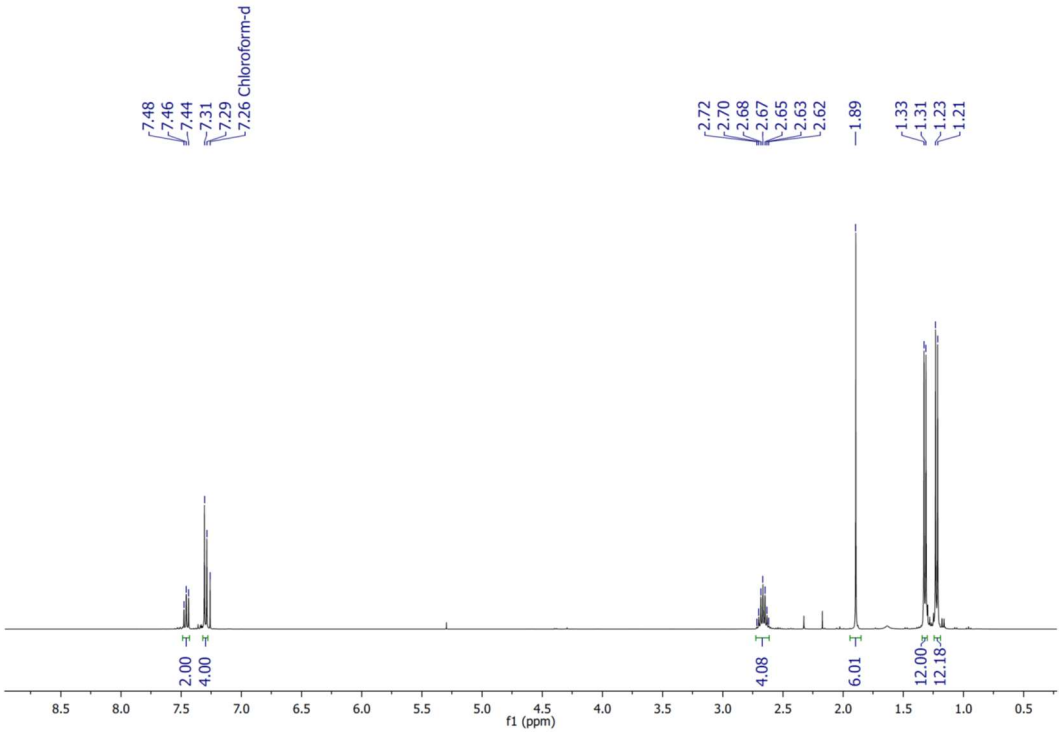


^{77}Se NMR


105.20
1000 950 900 850 800 750 700 650 600 550 500 450 400 350 300 250 200 150 100 50 0 -50 -100 -150 -200
f1 (ppm)

[S(IPr^{Me})]

^{1}H NMR



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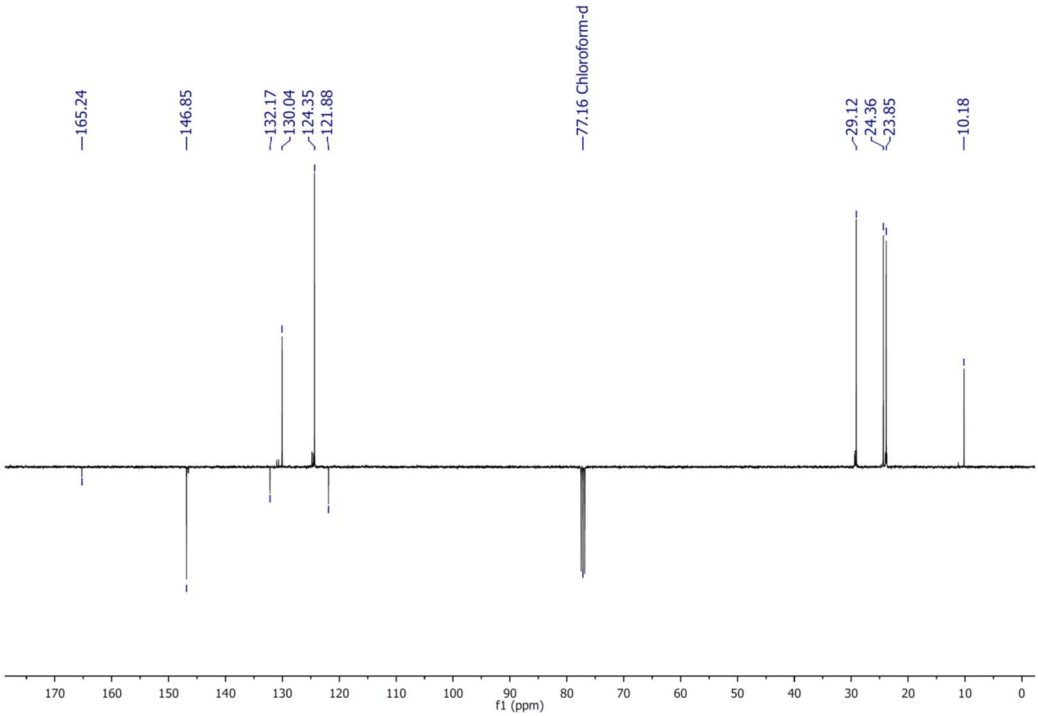
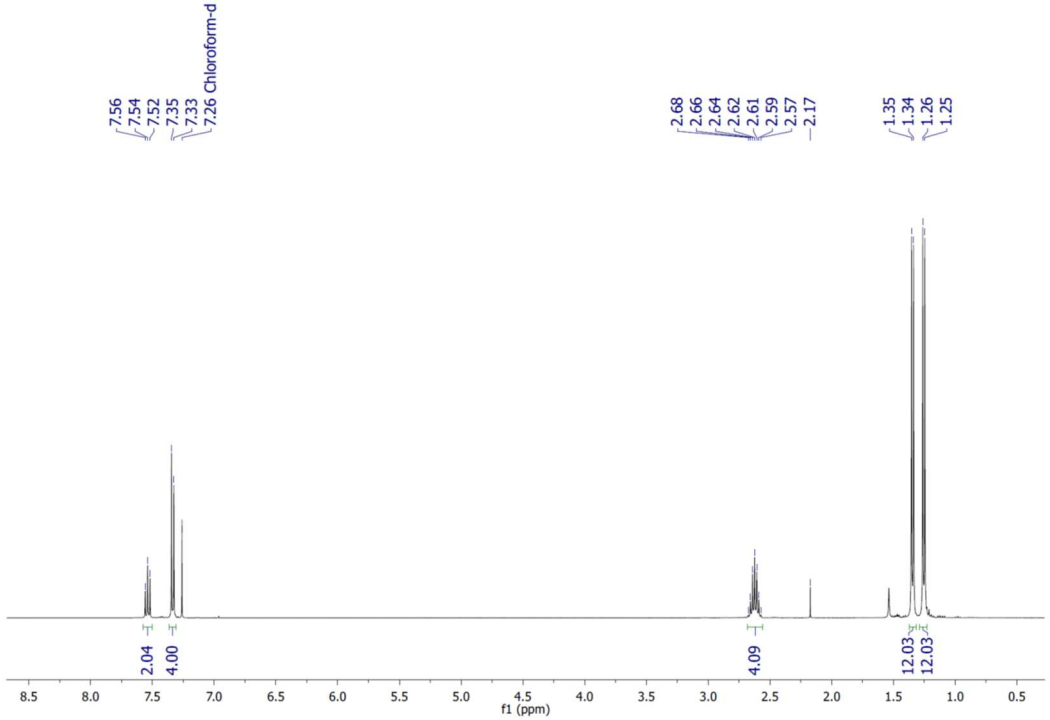


[Se(IPr^{Cl})]

^{1}H NMR



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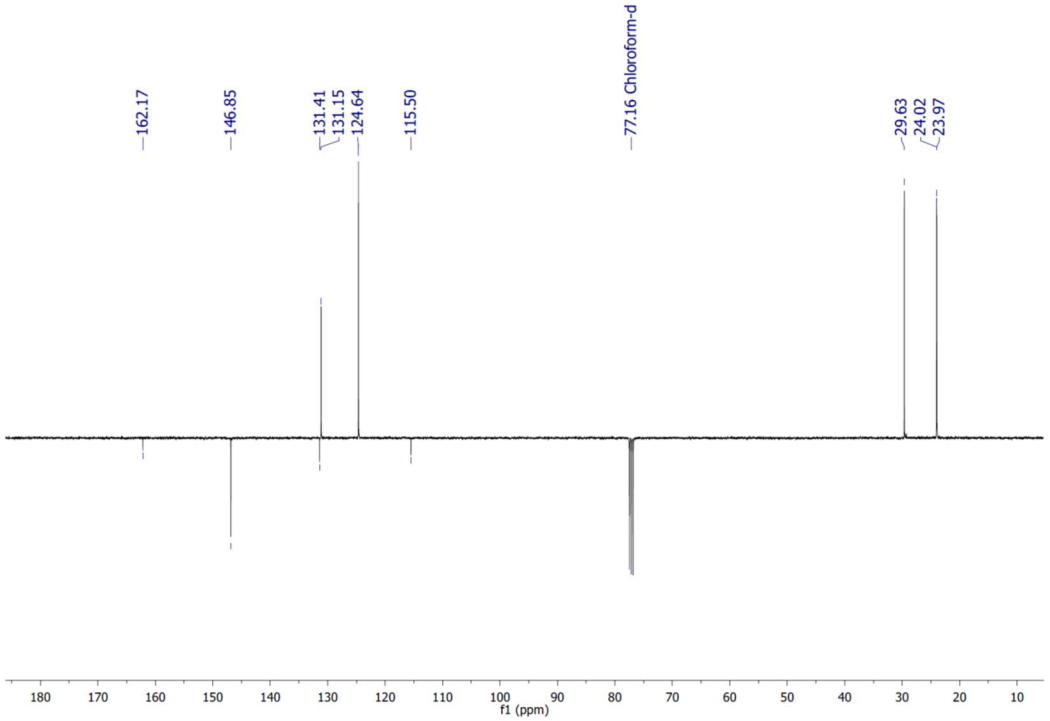
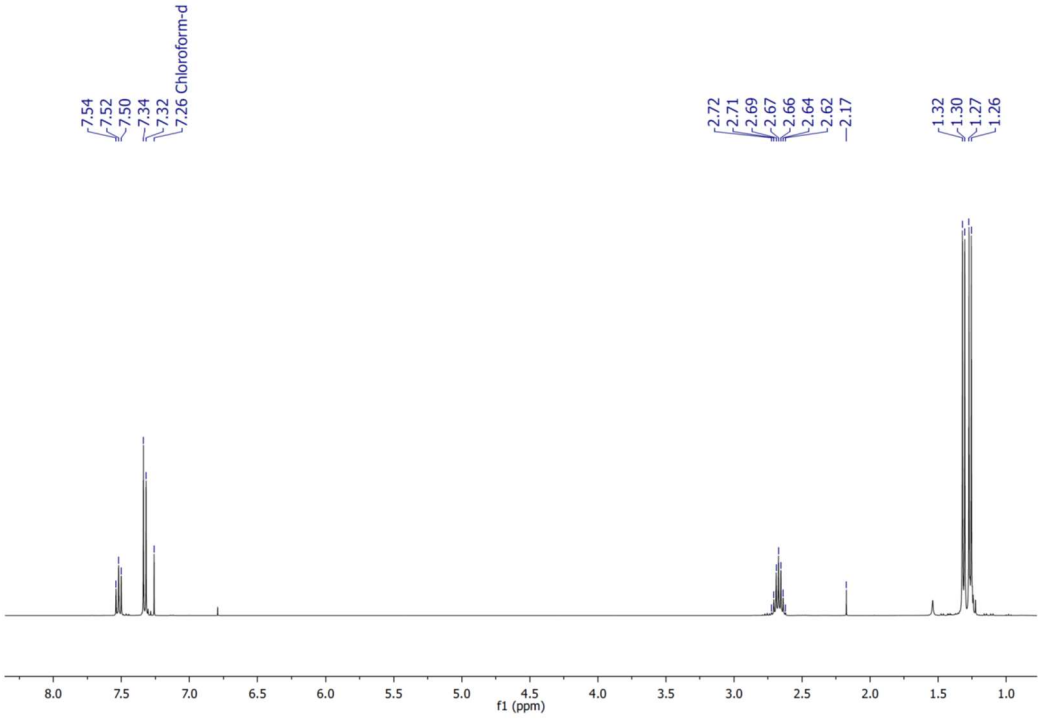


[S(IPr^{Cl})]

^{1}H NMR



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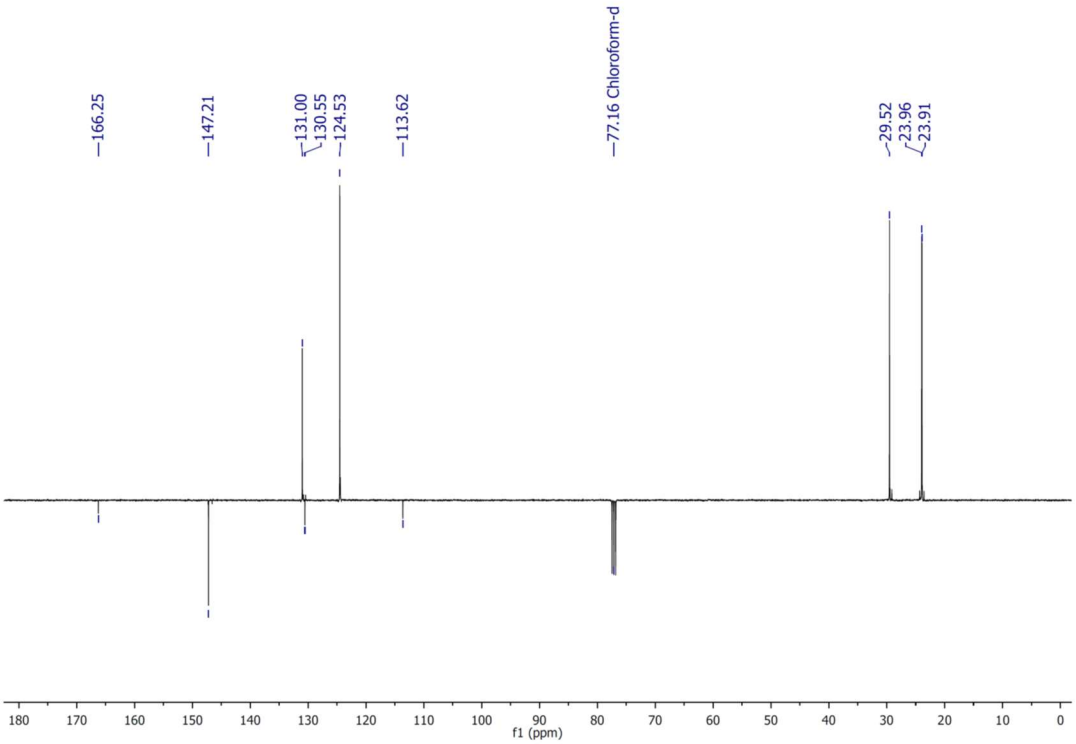
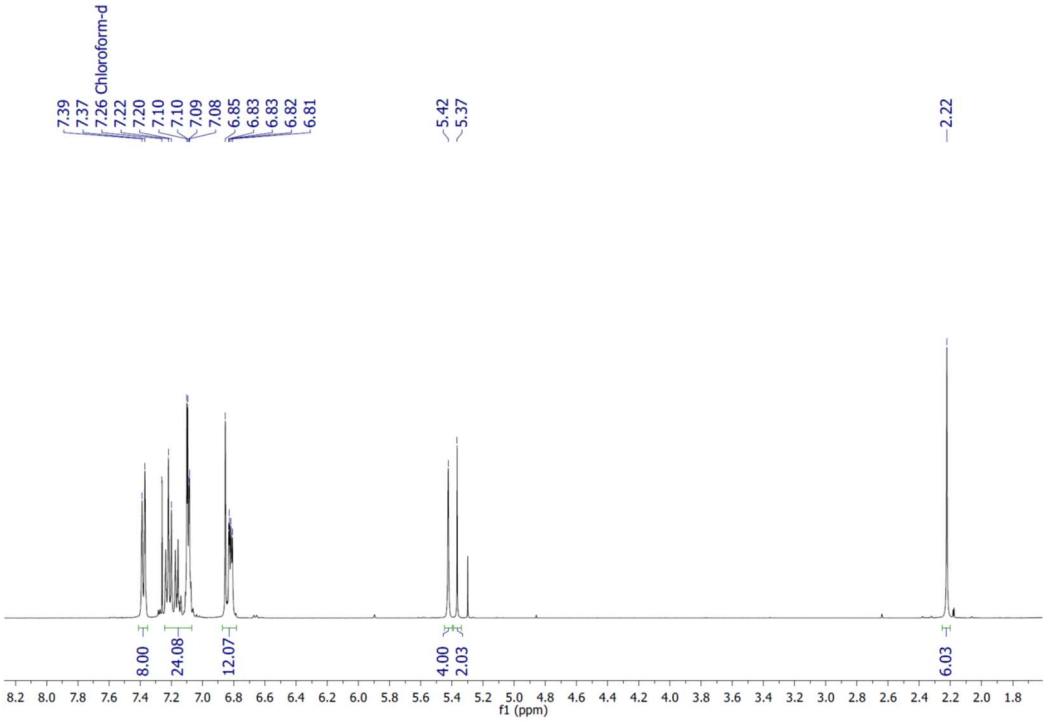
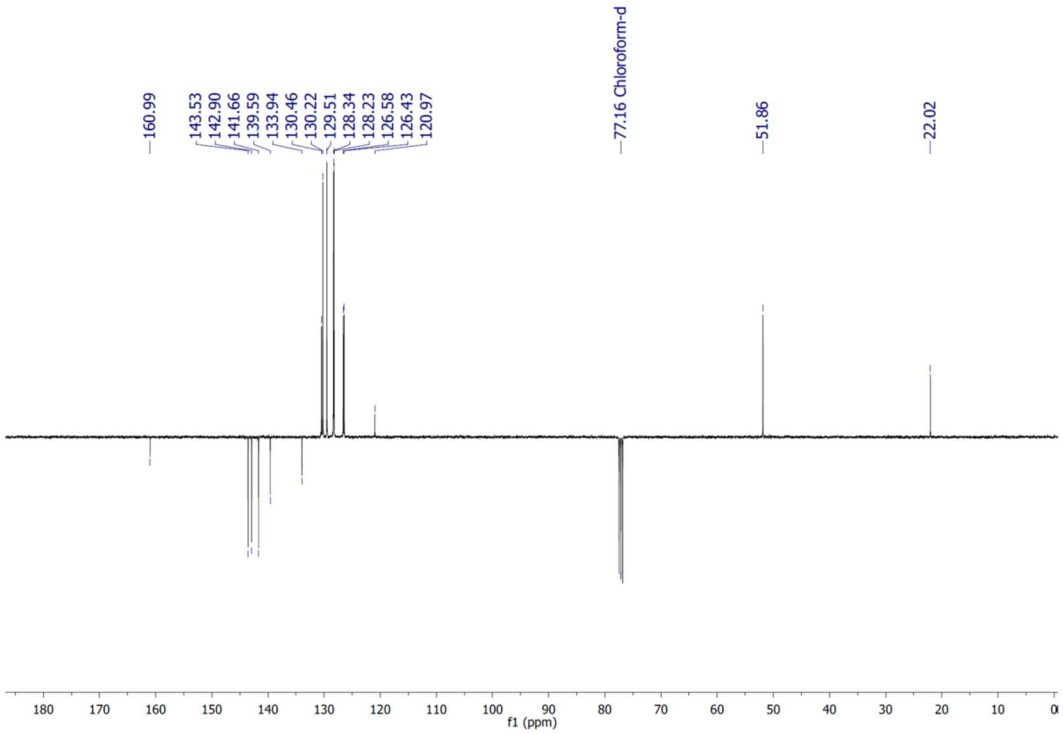


[Se(IPr*)]

^{1}H NMR

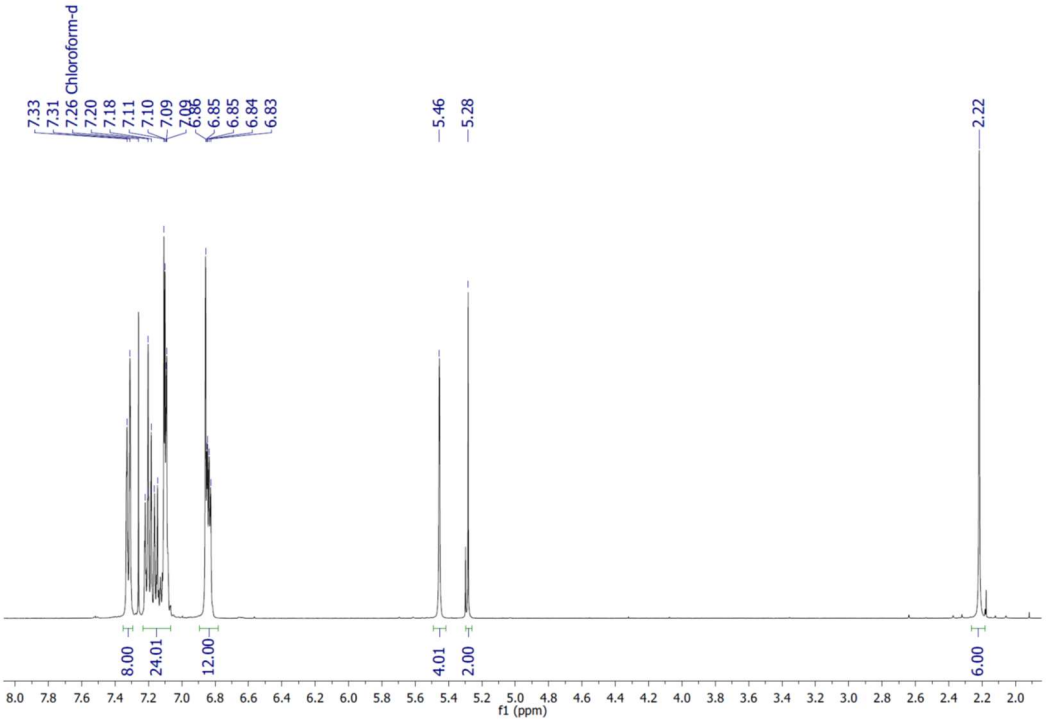


^{13}C{^{1}H} DEPT Q NMR

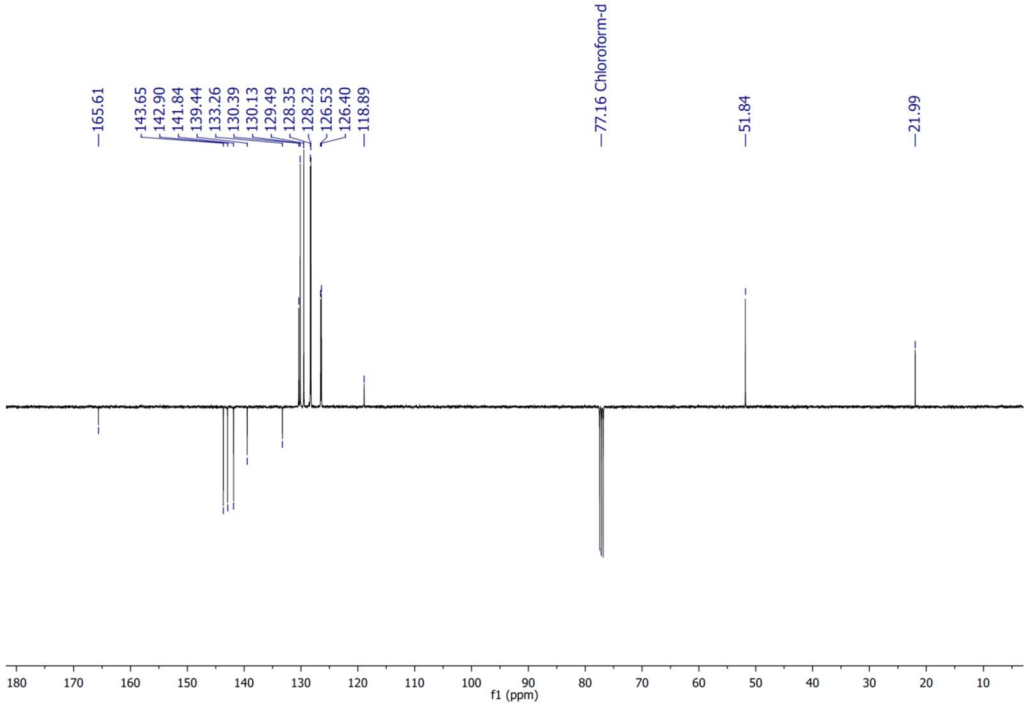


[S(IPr*)]

^{1}H NMR

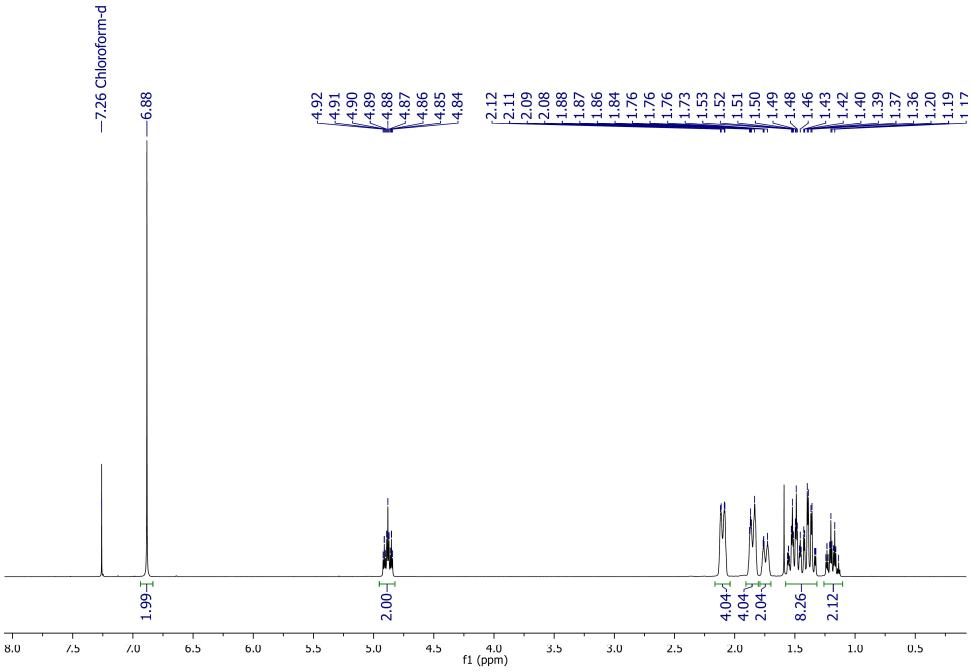


^{13}C{^{1}H} DEPT Q NMR



[Se(ICy)]

^{1}H NMR



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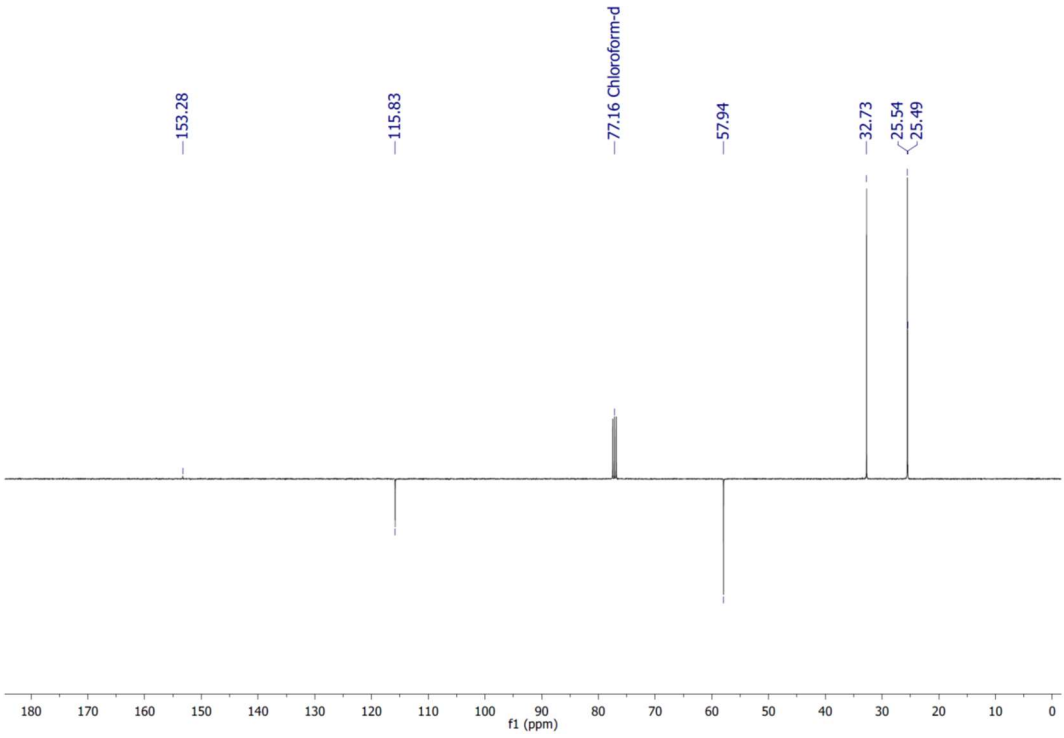
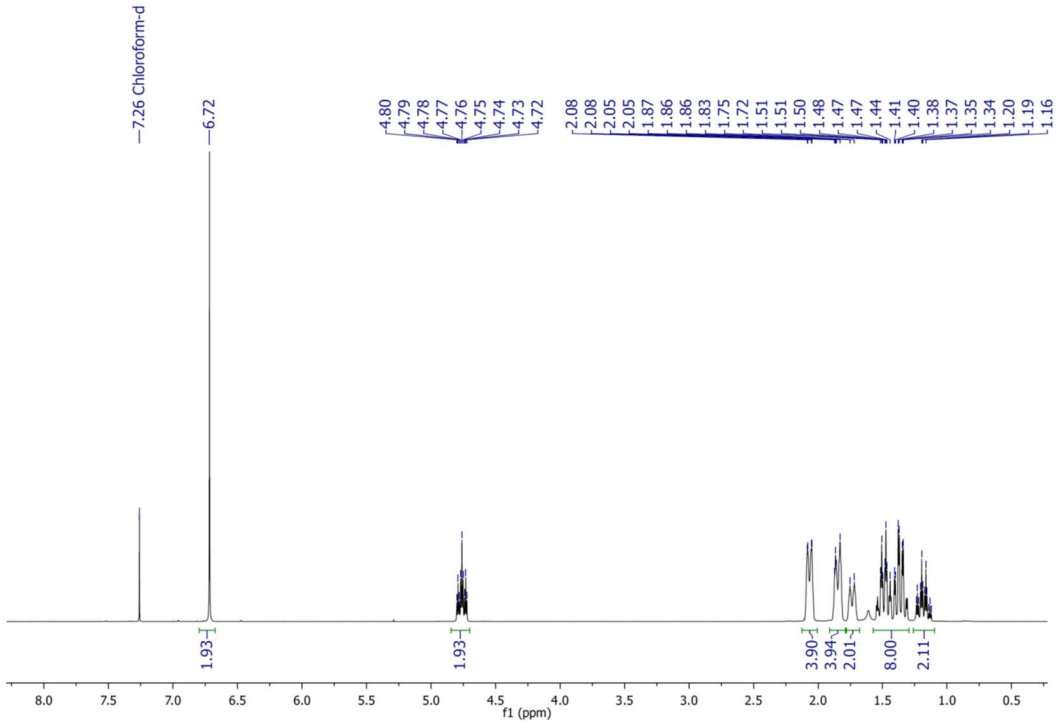


[S(ICy)]

^{1}H NMR



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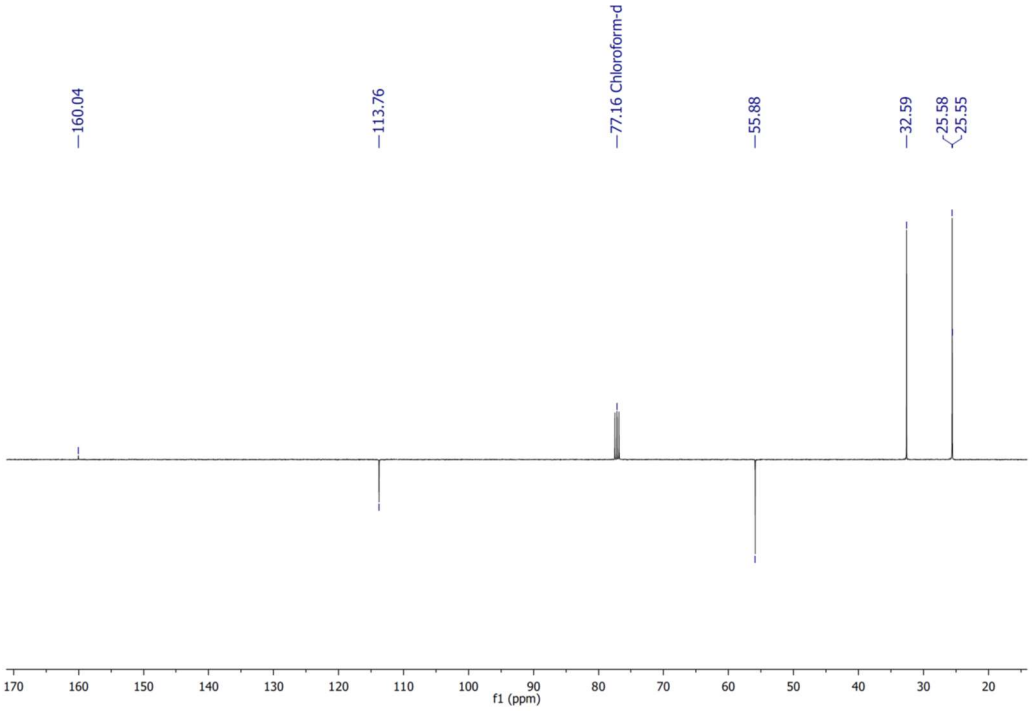

[Se(IAd)]

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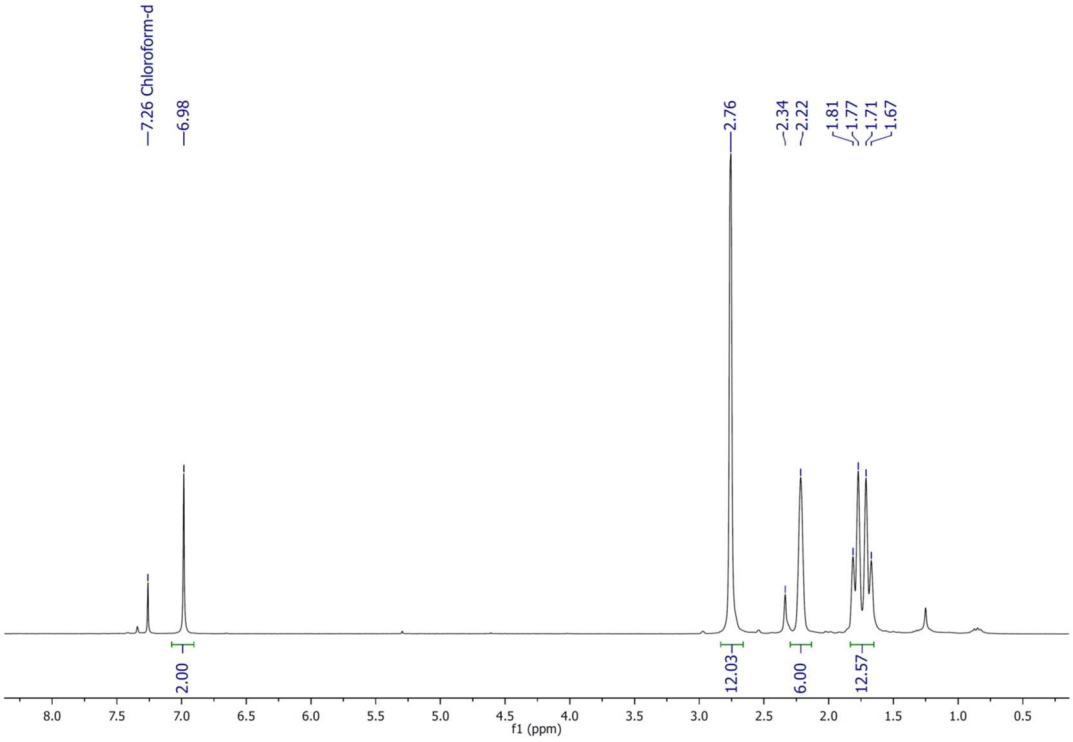

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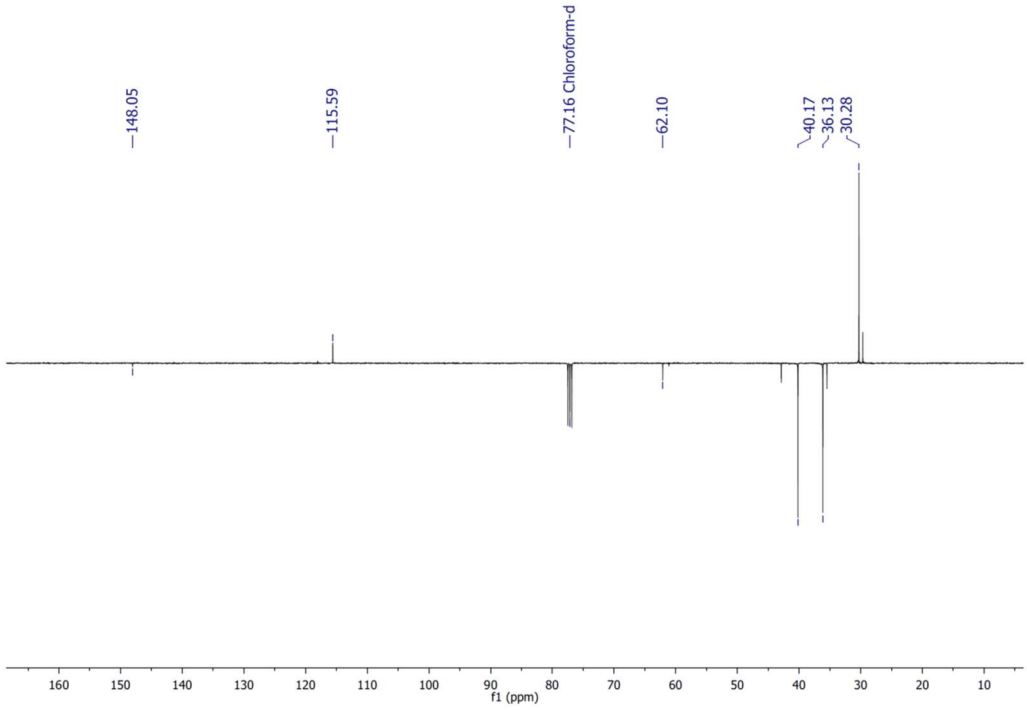
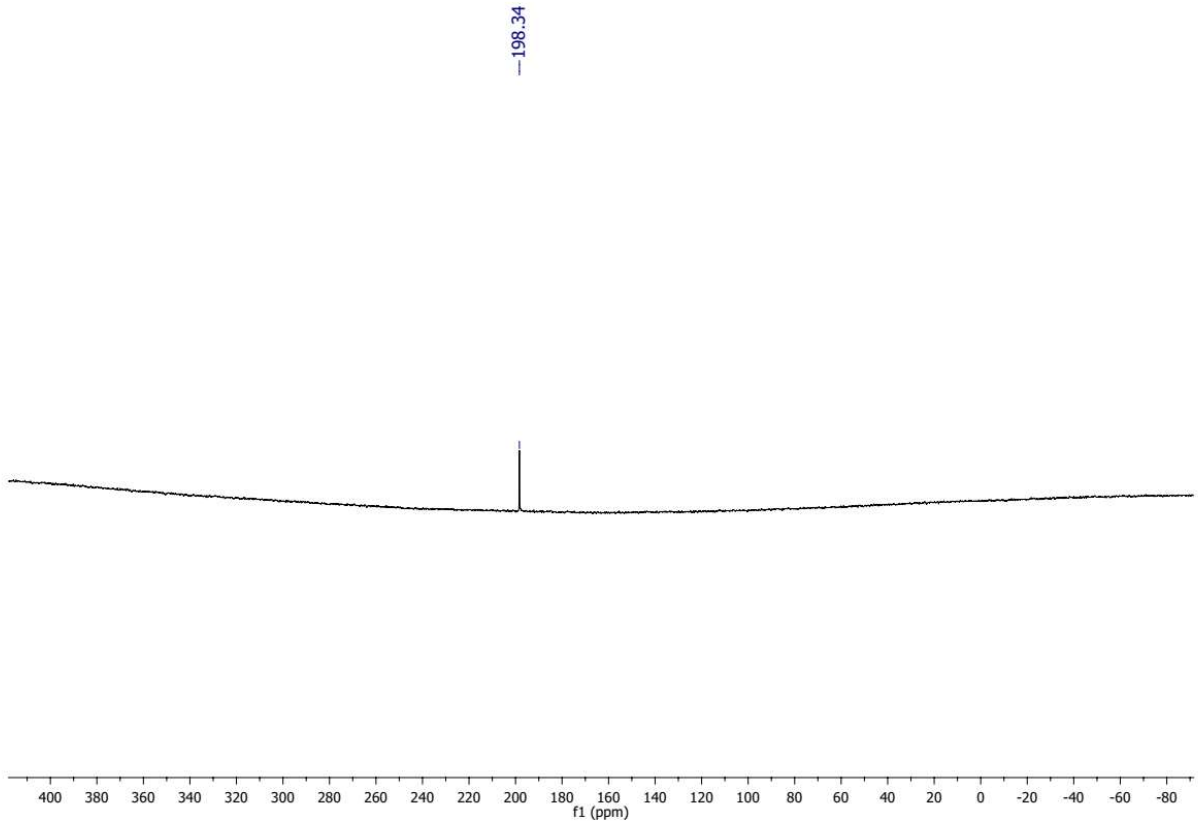
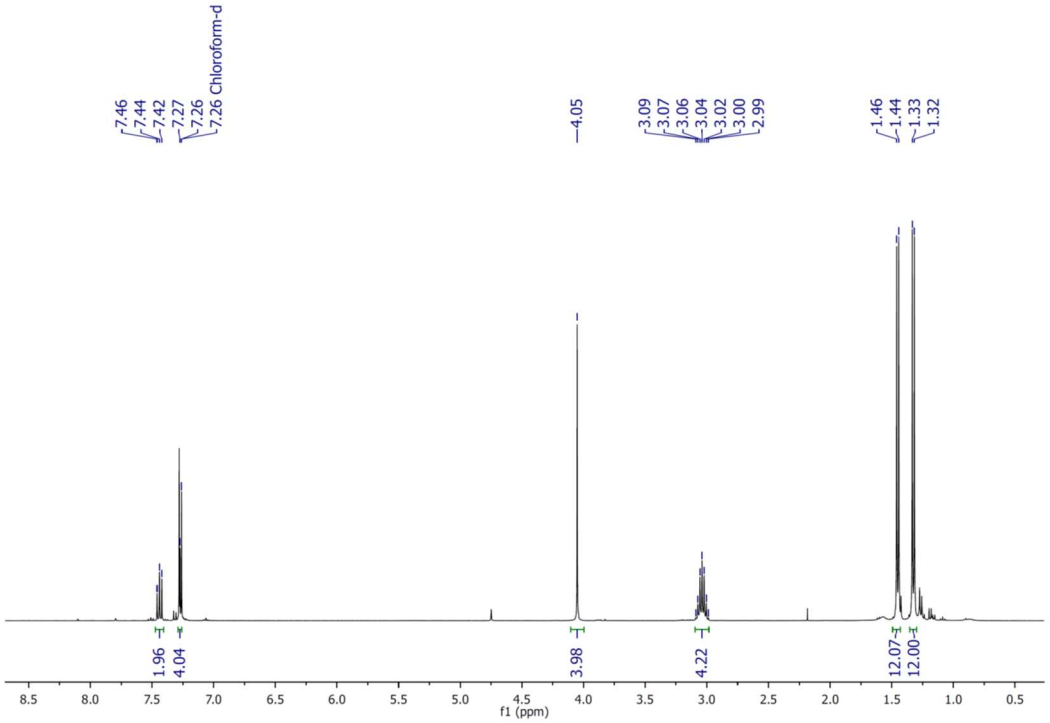


^{77}Se NMR


198.34
400 380 360 340 320 300 280 260 240 220 200 180 160 140 120 100 80 60 40 20 0 -20 -40 -60 -80
f1 (ppm)

[Te(SIPr)]

^{1}H NMR



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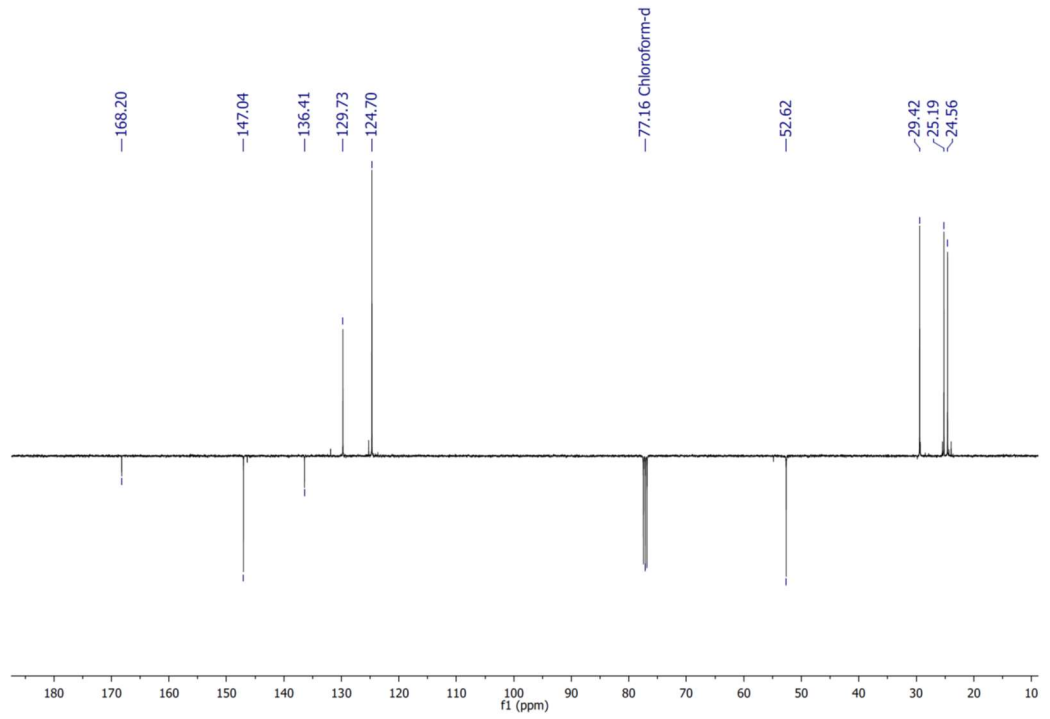
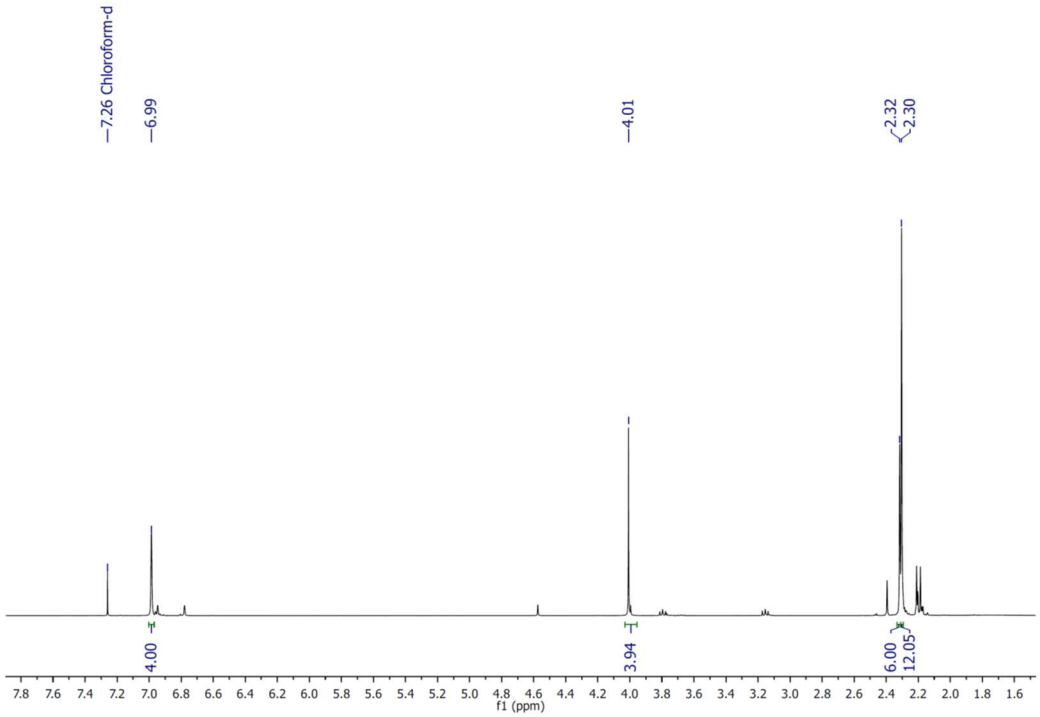


[Te(SIMes)]

^{1}H NMR



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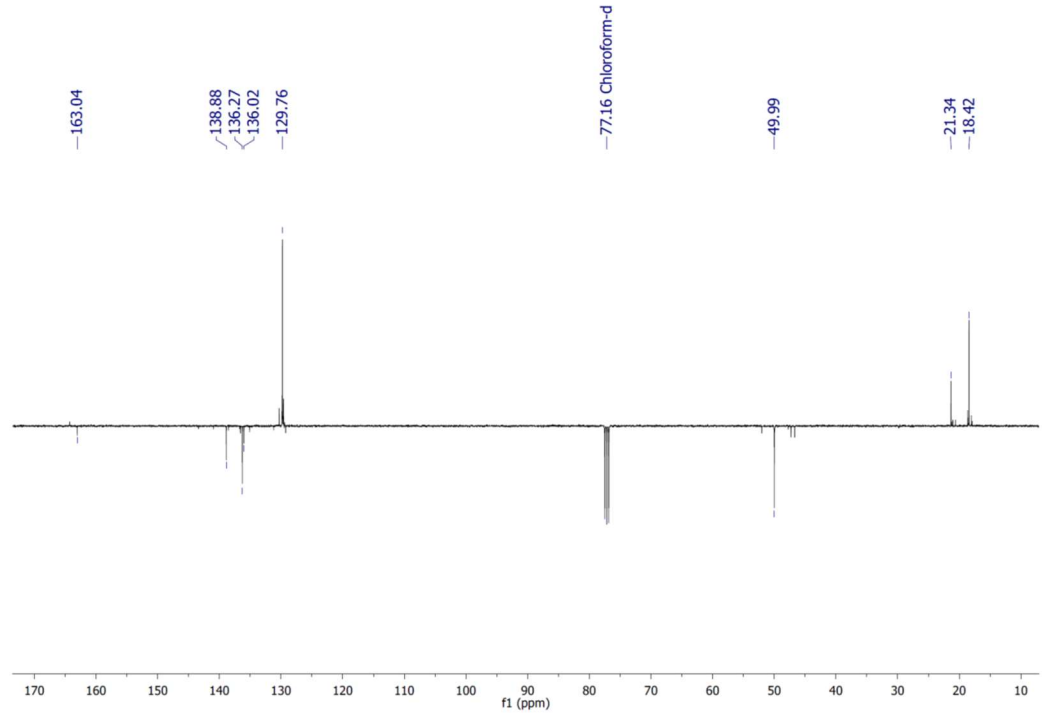
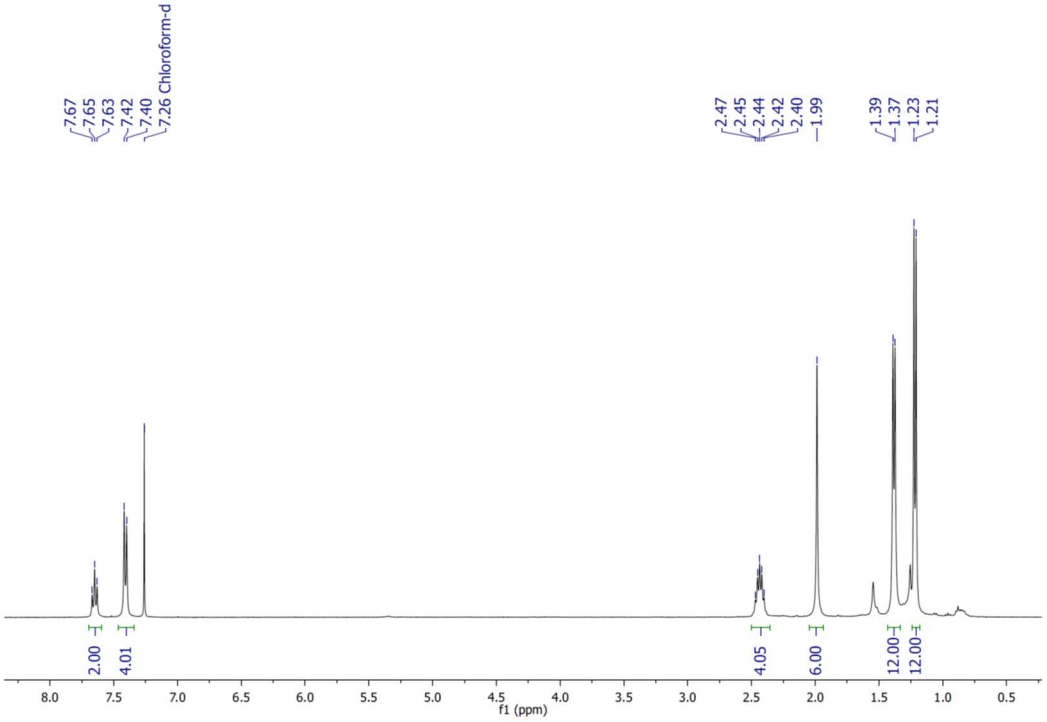


NMR spectra of Copper complexes

[CuCl{Se(IPr^{Me})}]

^{1}H NMR



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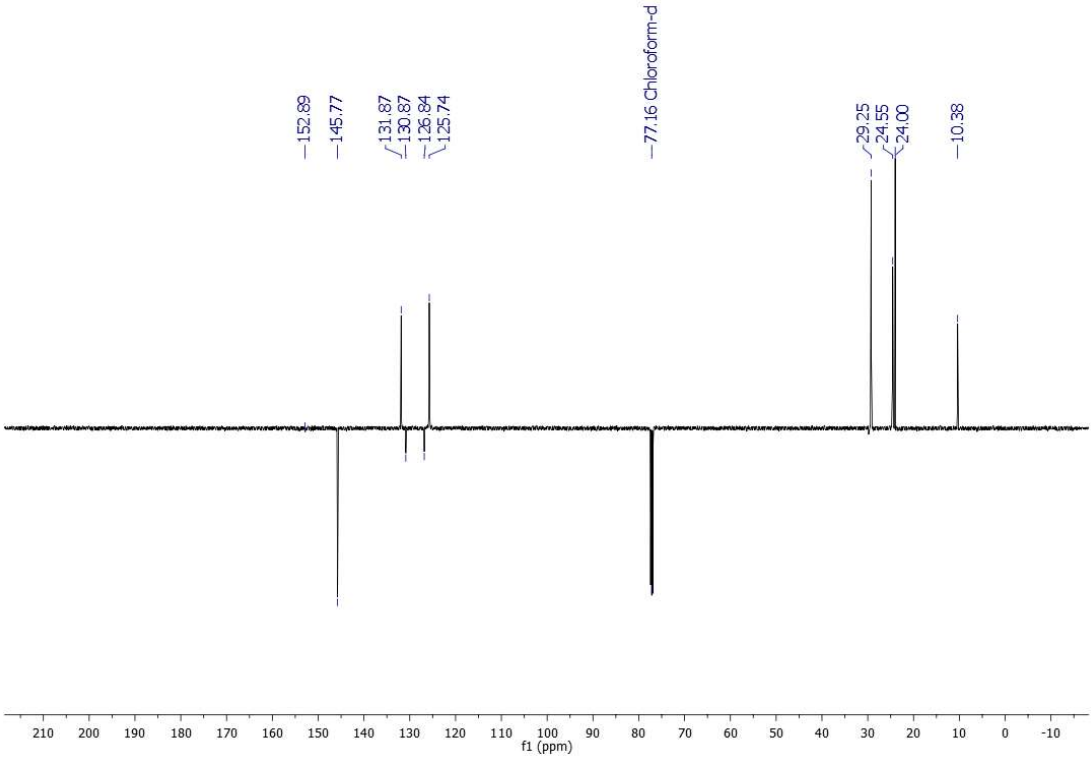
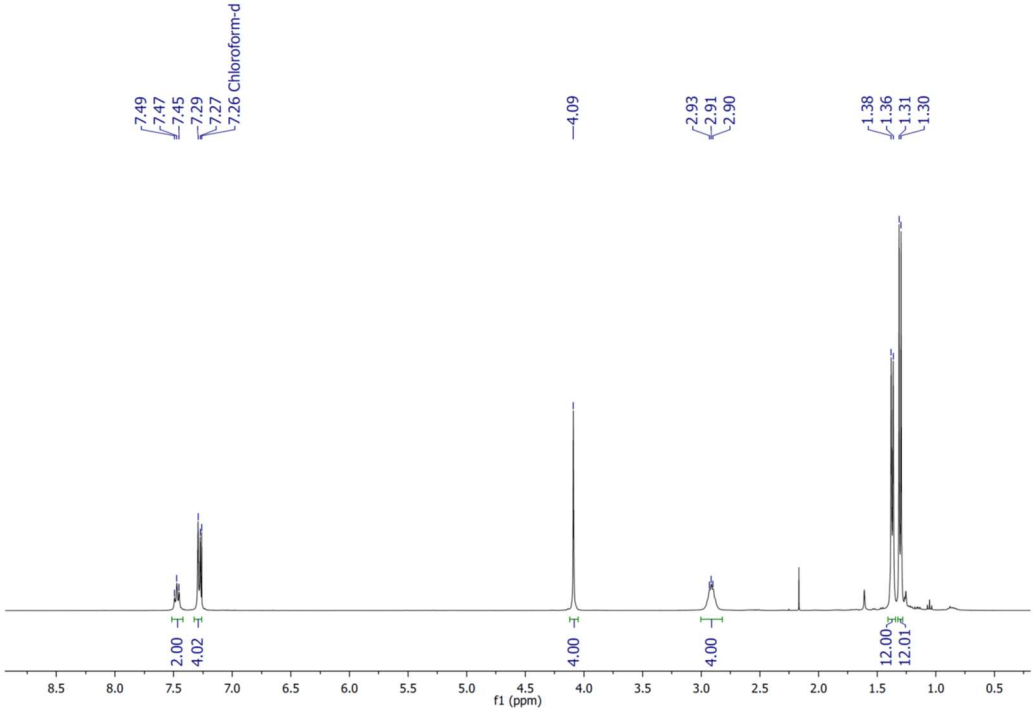


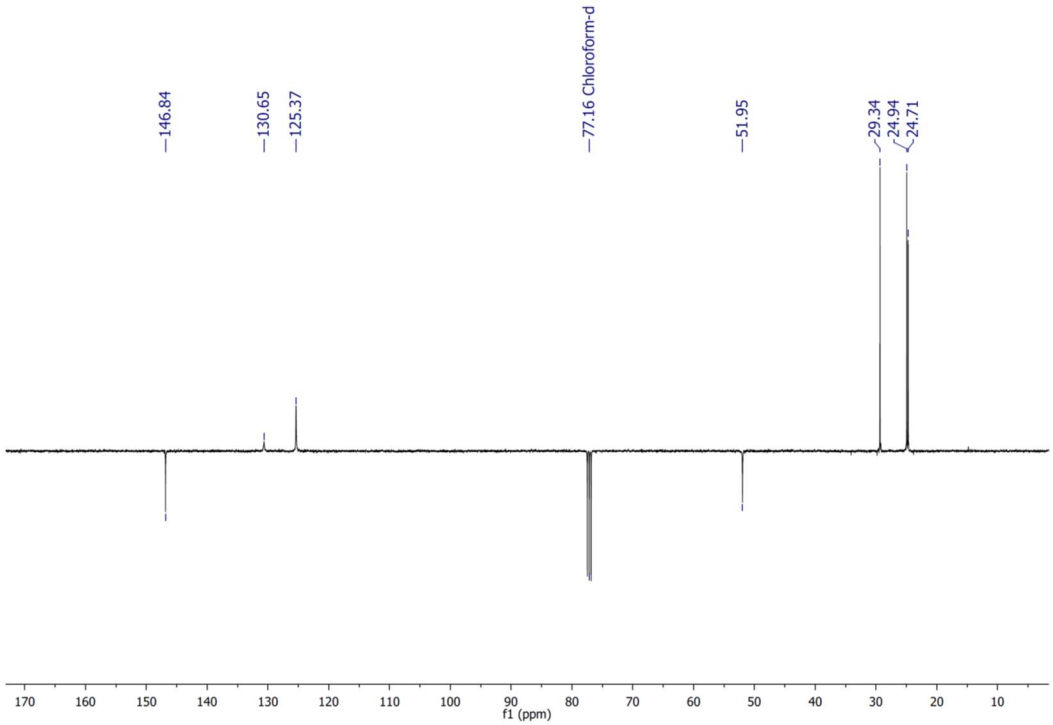
NMR spectra of Silver complexes

[Ag{Se(SIPr)}$_2$][AgCl$_2$]

^{1}H NMR

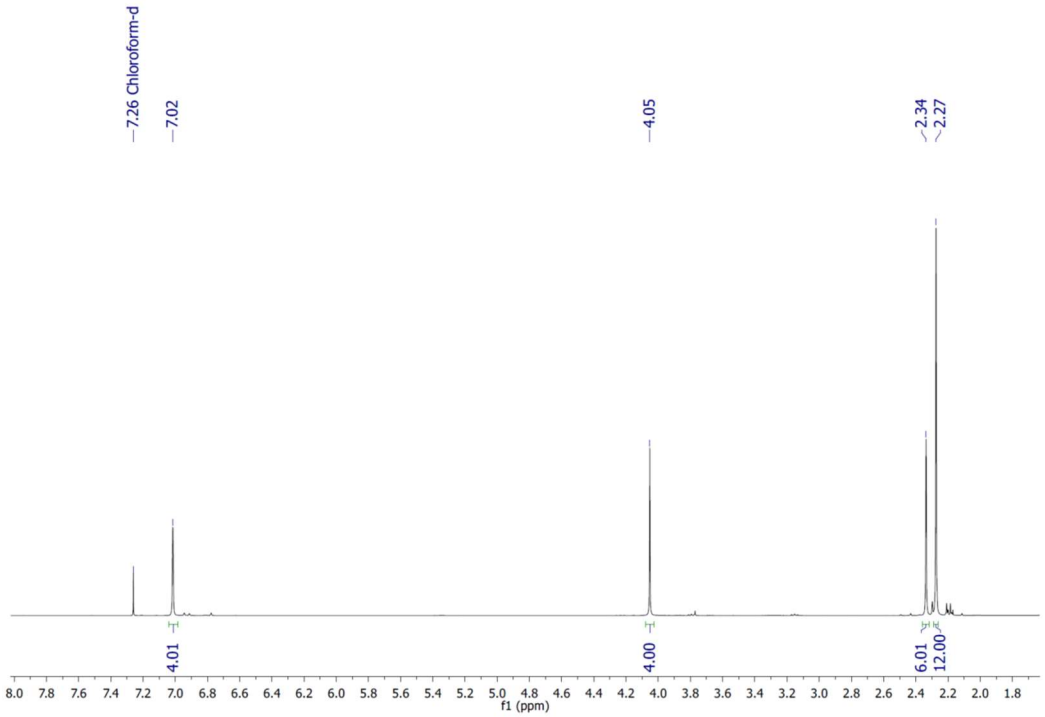


^{13}C{^{1}H} DEPT Q NMR

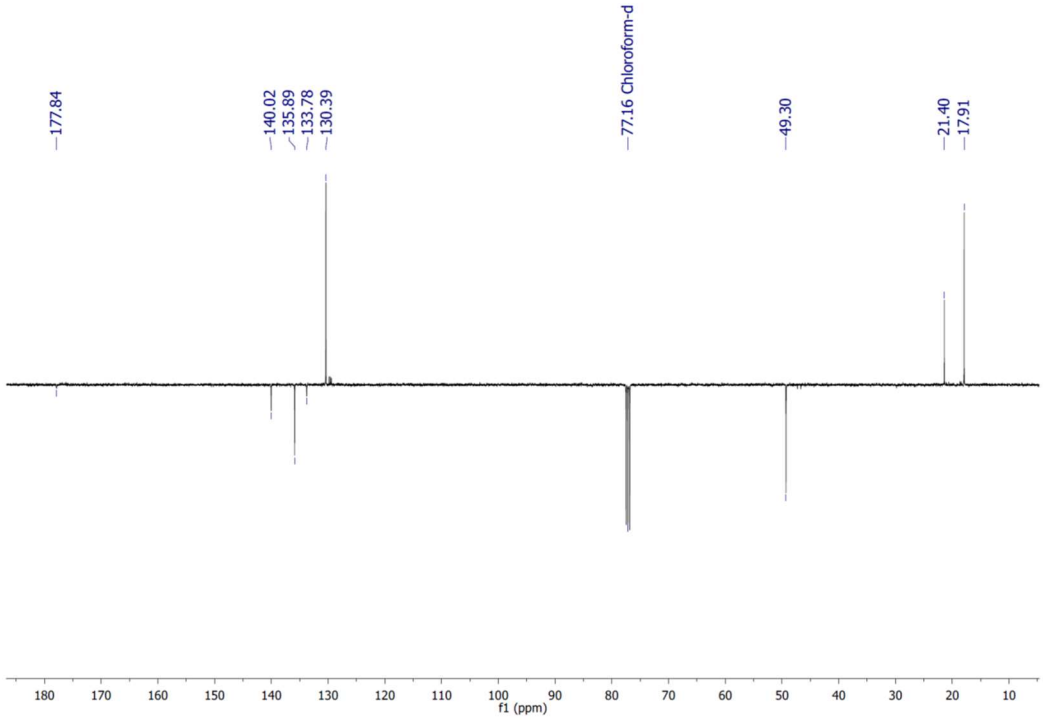


[AgCl{μ-Se(SIMes)}]$_2$

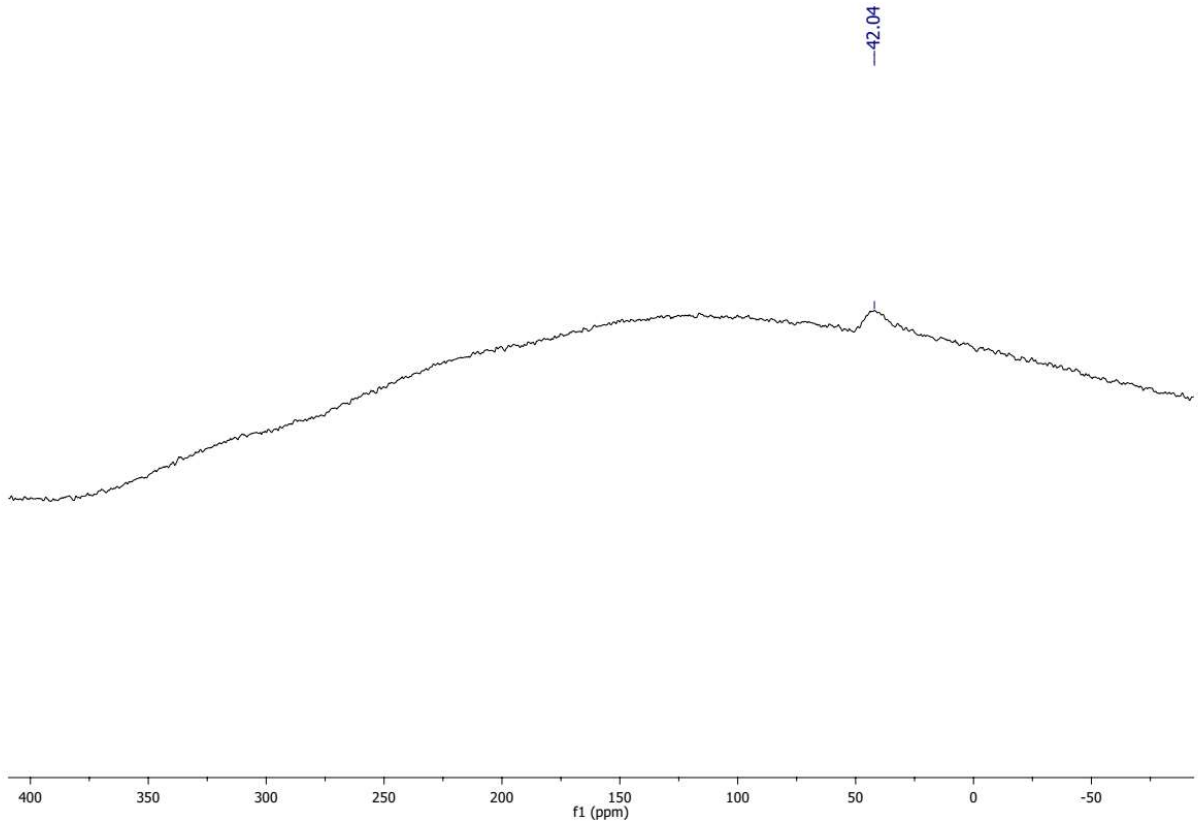
^{1}H NMR



^{13}C{^{1}H} DEPT Q NMR

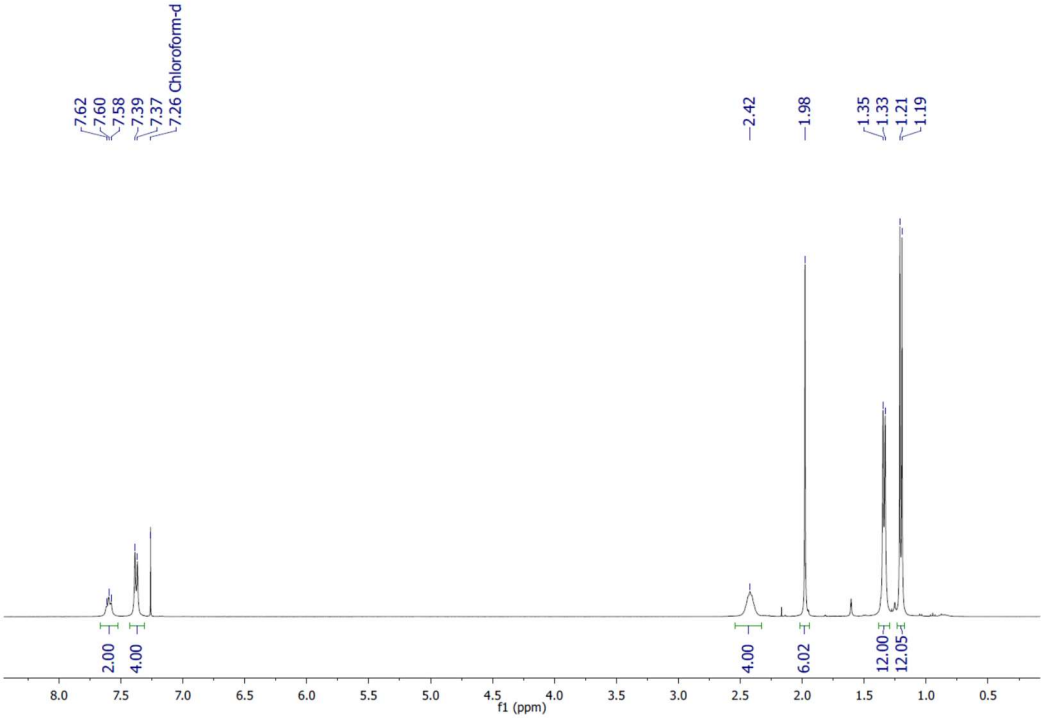


^{77}Se NMR

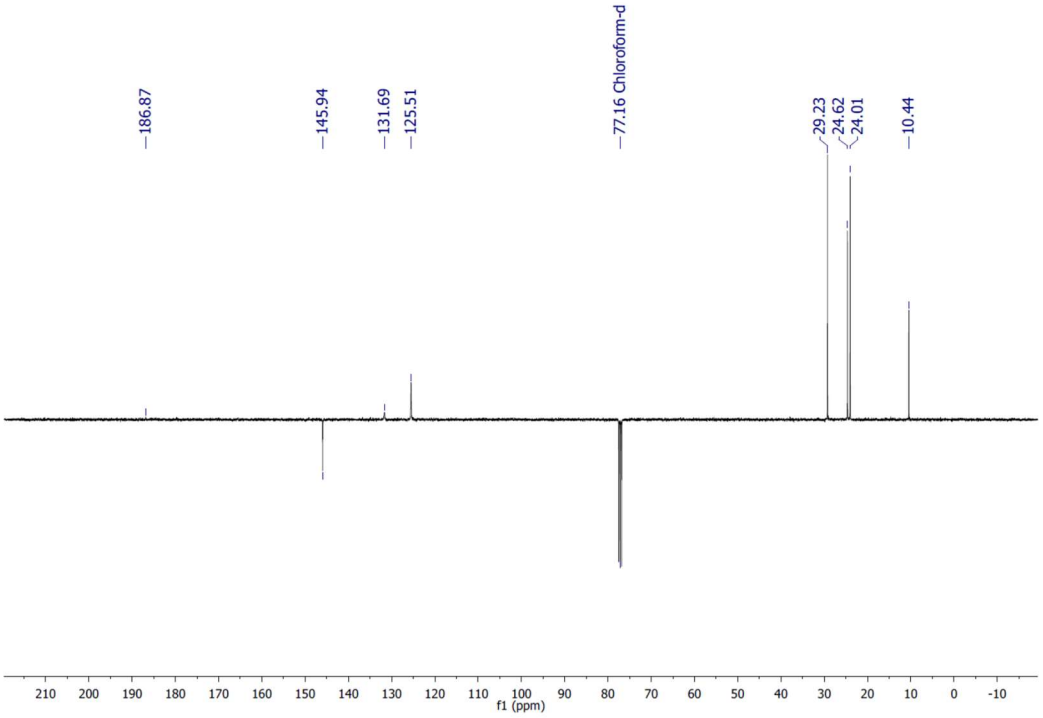


[AgCl{Se(IPr^{Me})}]

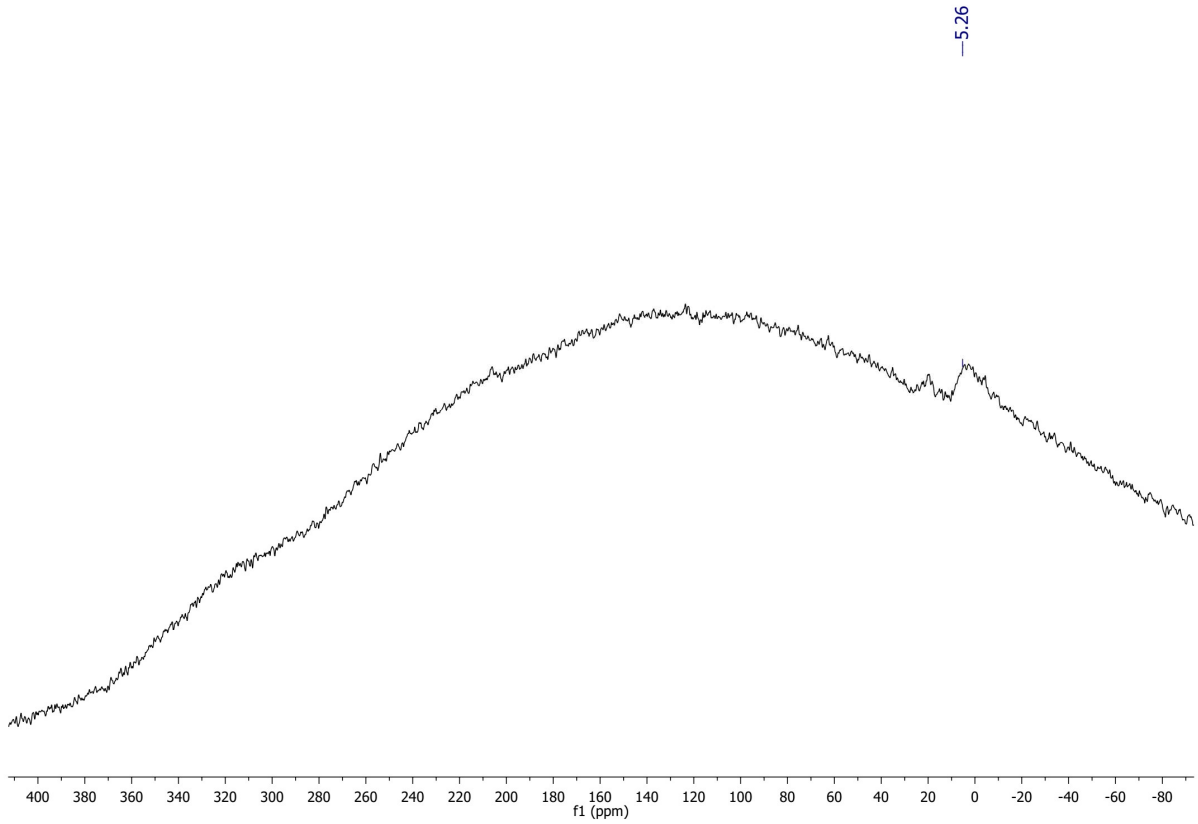
^{1}H NMR



^{13}C{^{1}H} DEPT Q NMR



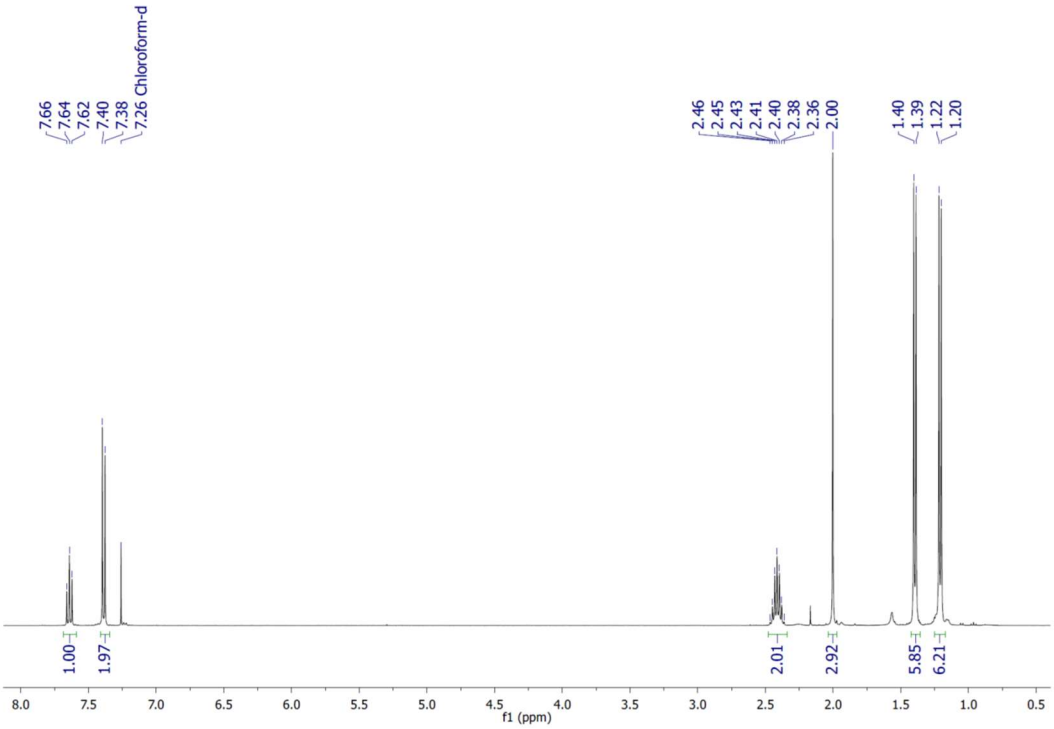
^{77}Se NMR


5.26
400 380 360 340 320 300 280 260 240 220 200 180 160 140 120 100 80 60 40 20 0 -20 -40 -60 -80
f1 (ppm)

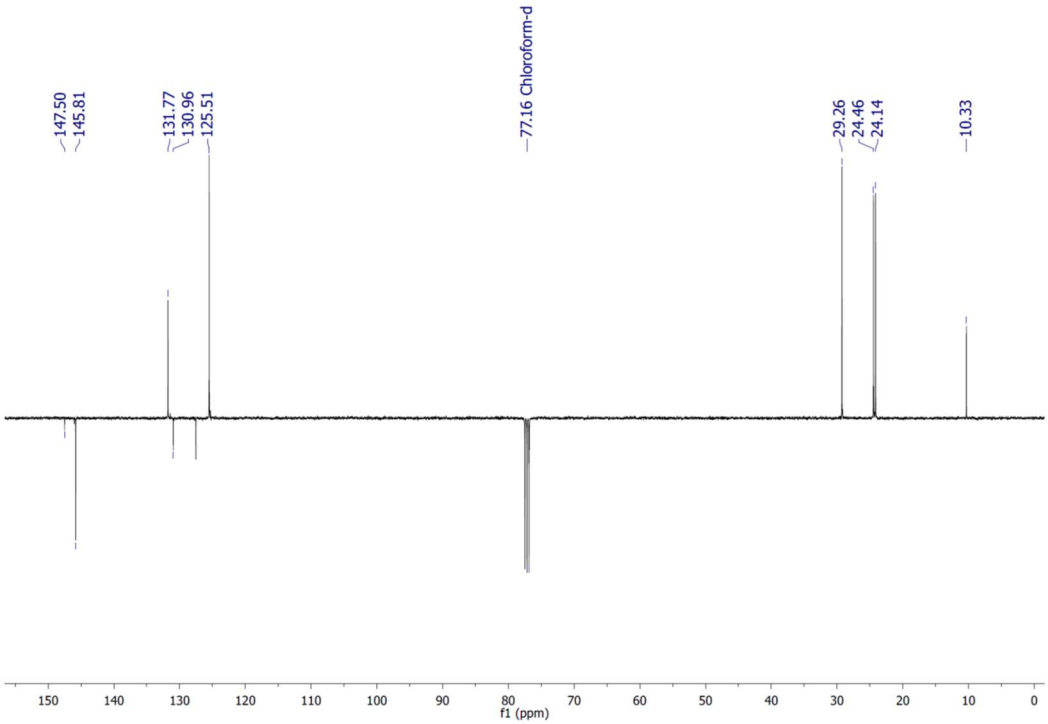
NMR spectra of Gold complexes

[AuCl{Se(IPr^{Me})}]

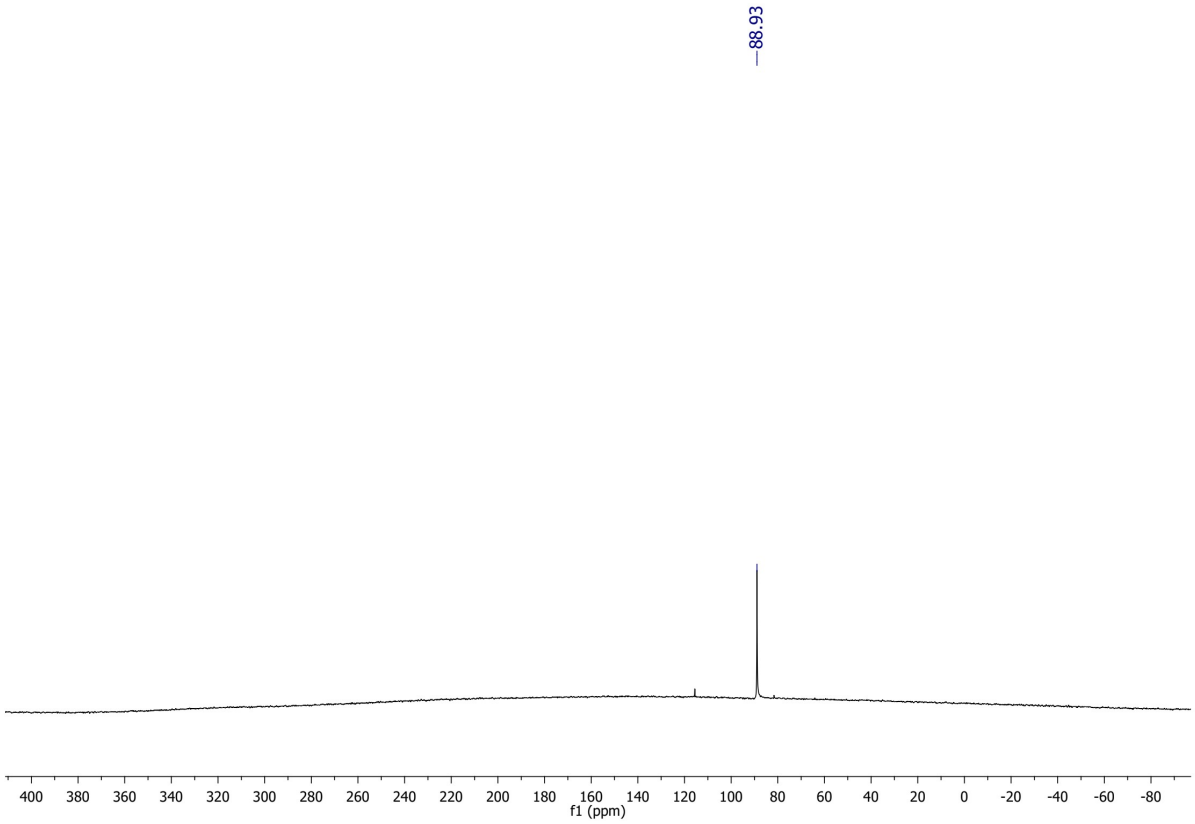
^{1}H NMR



^{13}C{^{1}H} DEPT Q NMR

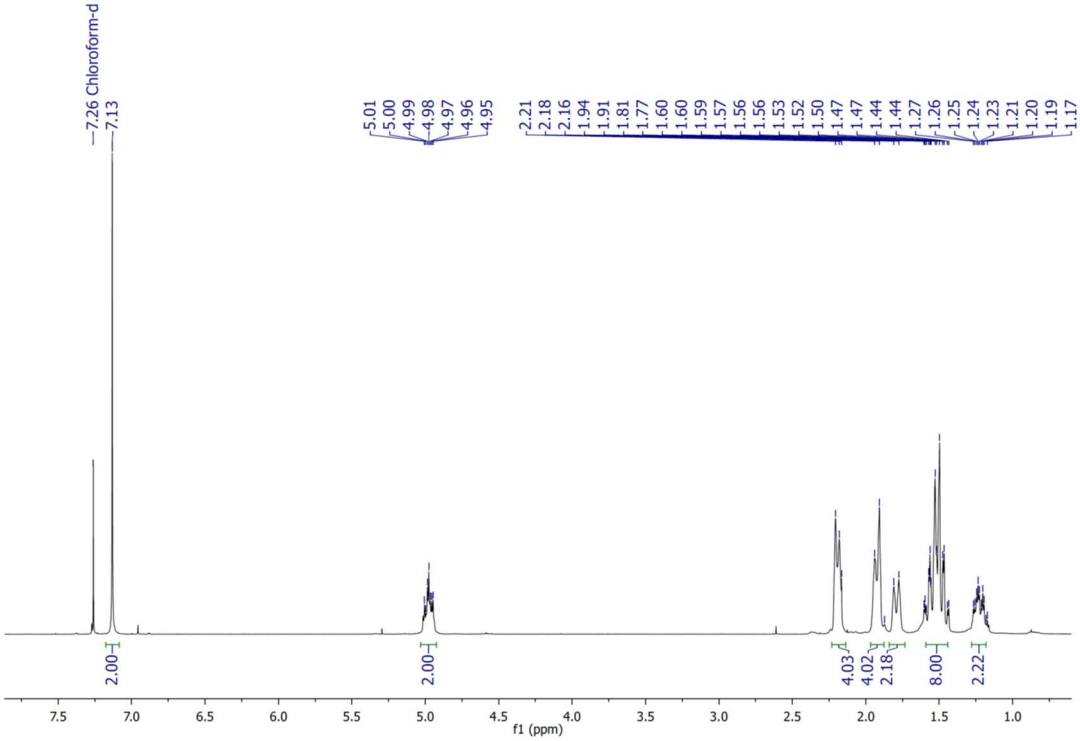


^{77}Se NMR

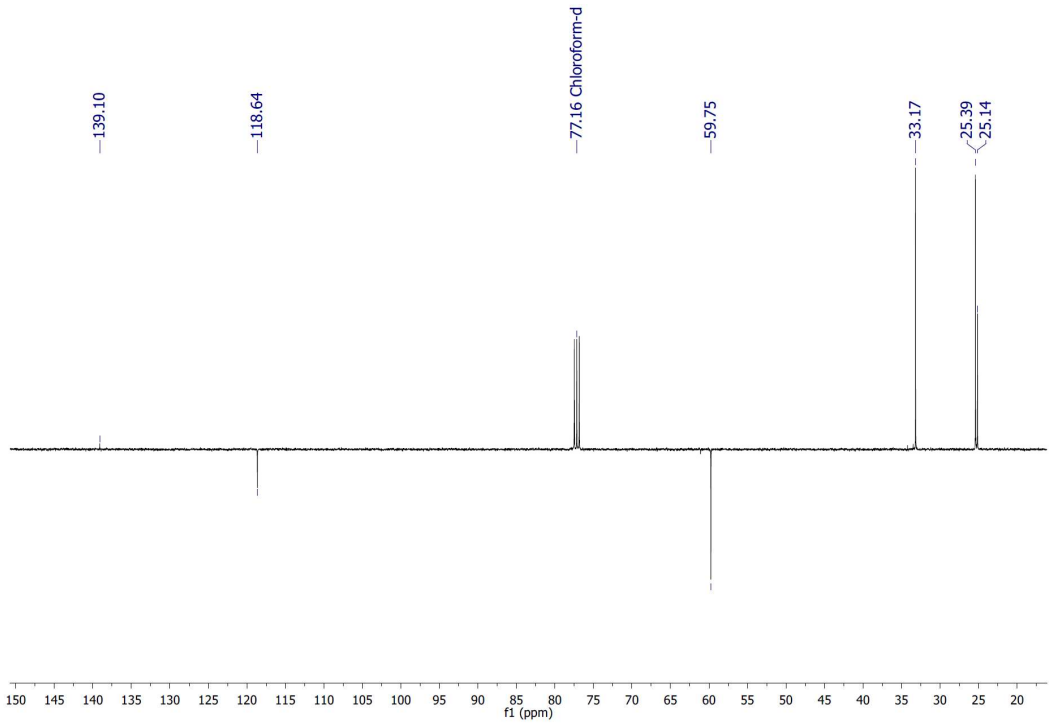

88.93
400 380 360 340 320 300 280 260 240 220 200 180 160 140 120 100 80 60 40 20 0 -20 -40 -60 -80
f1 (ppm)

[AuCl{Se(ICy)}]

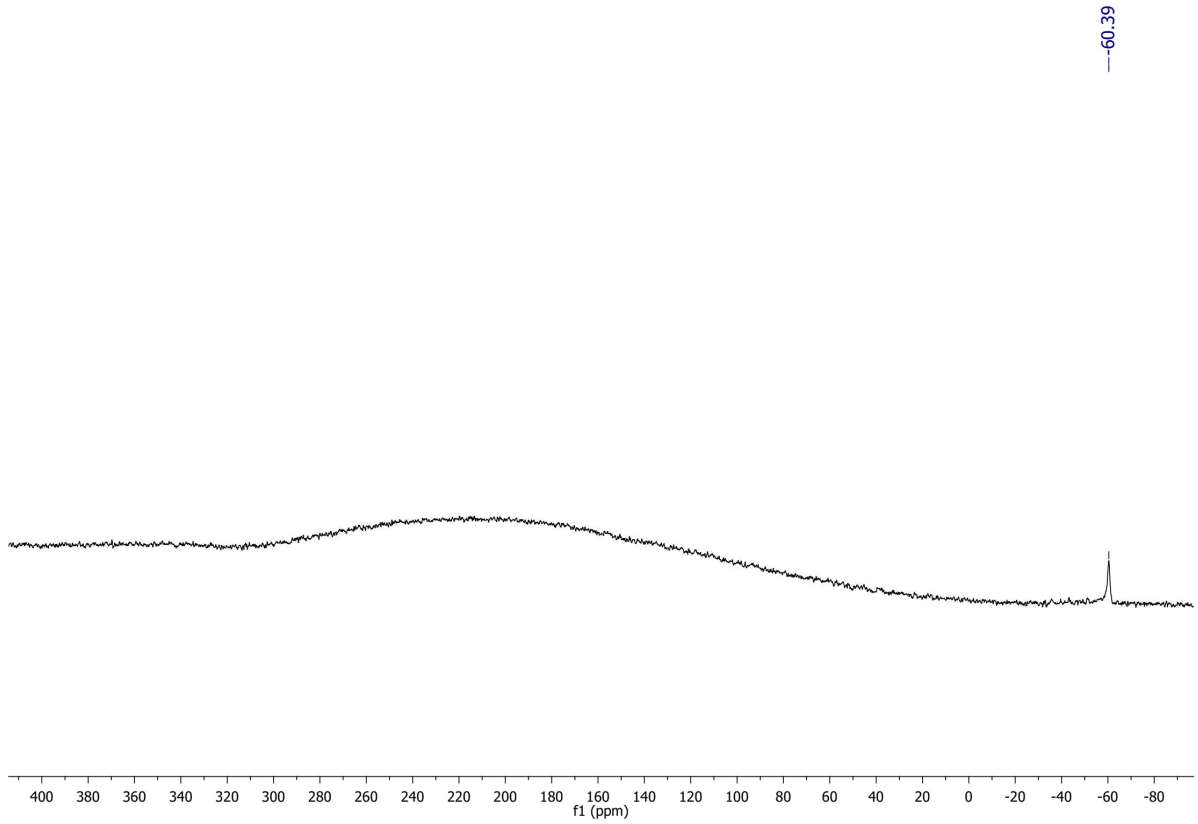
^{1}H NMR



^{13}C{^{1}H} DEPT Q NMR

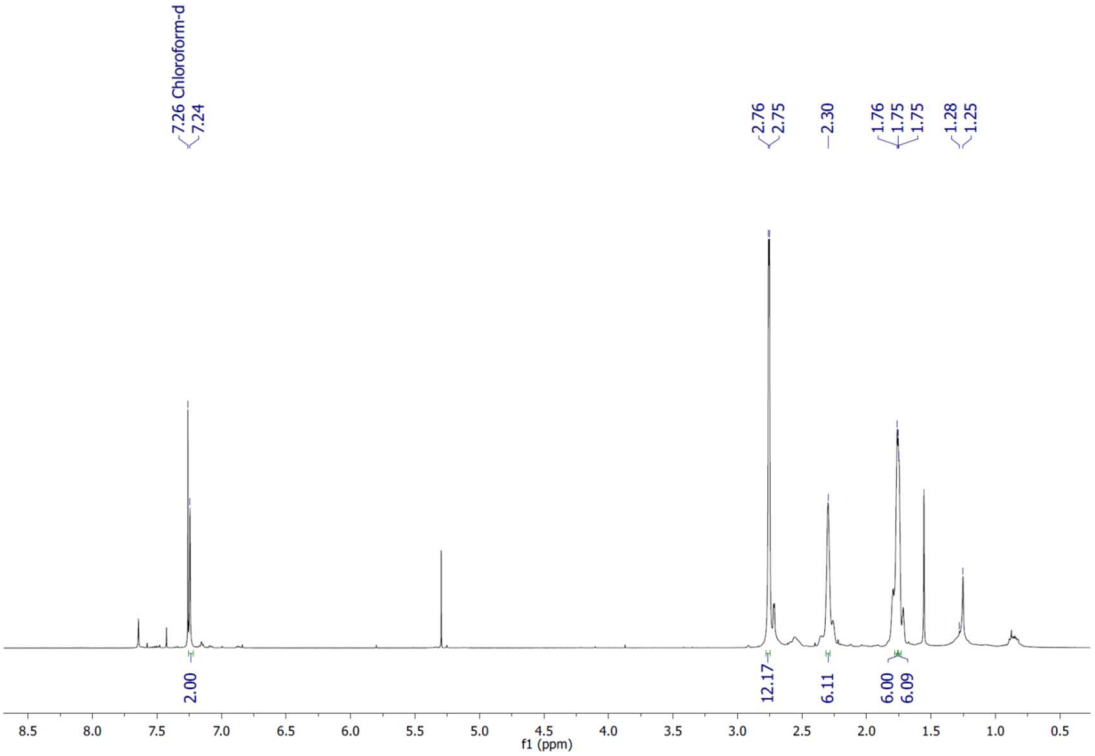


^{77}Se NMR

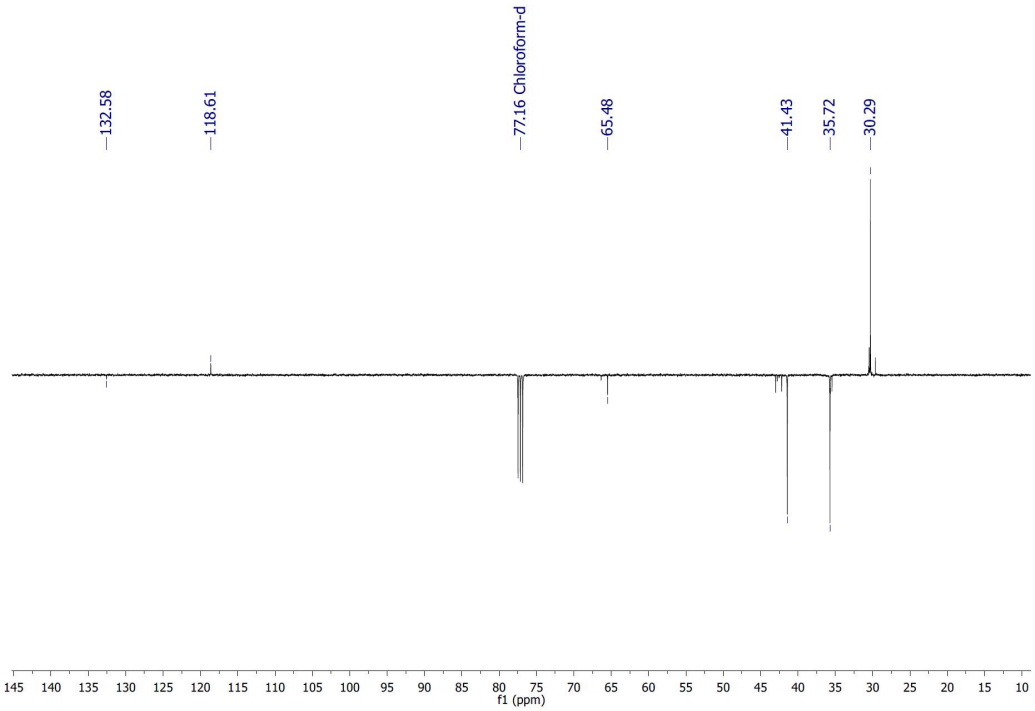

-60.39
400 380 360 340 320 300 280 260 240 220 200 180 160 140 120 100 80 60 40 20 0 -20 -40 -60 -80
f1 (ppm)

[Au{Se(IAd)}$_2$][AuCl$_2$]

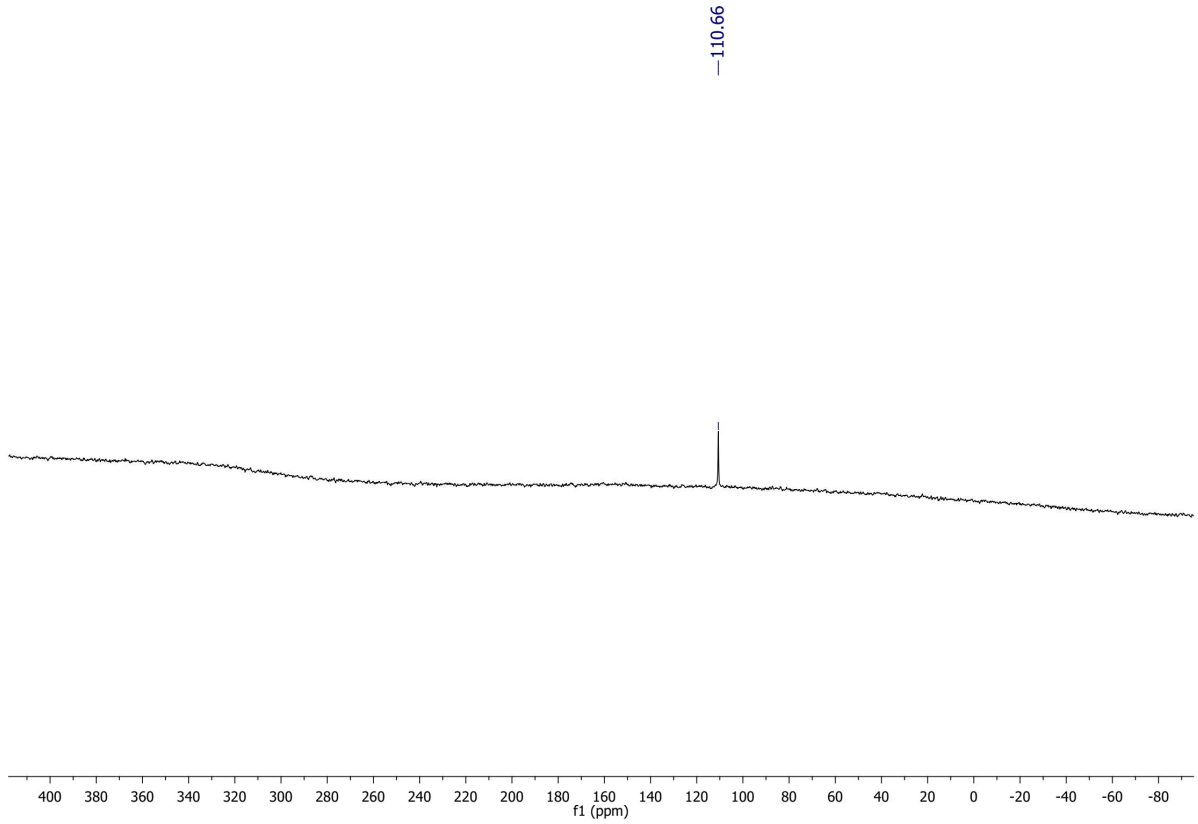
^{1}H NMR



^{13}C{^{1}H} DEPT Q NMR

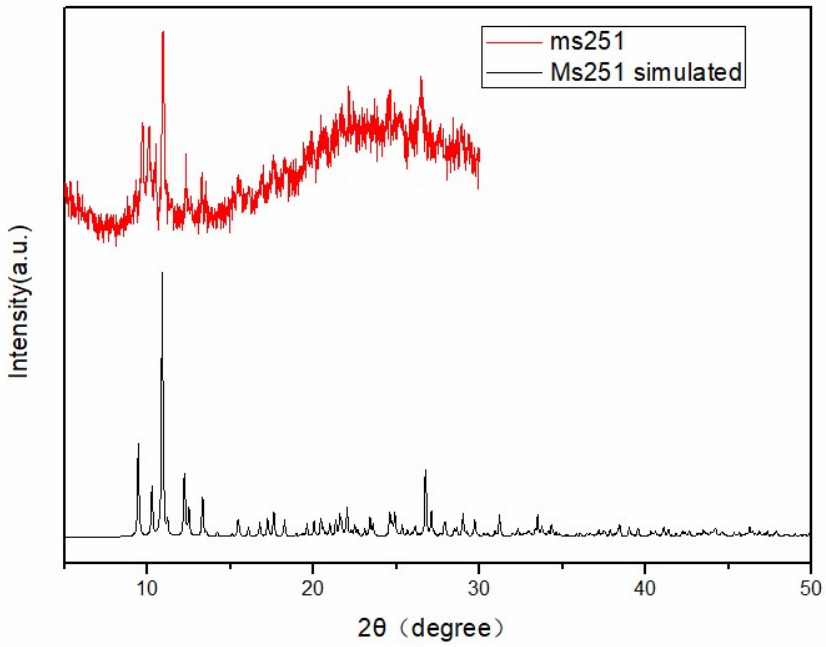


^{77}Se NMR

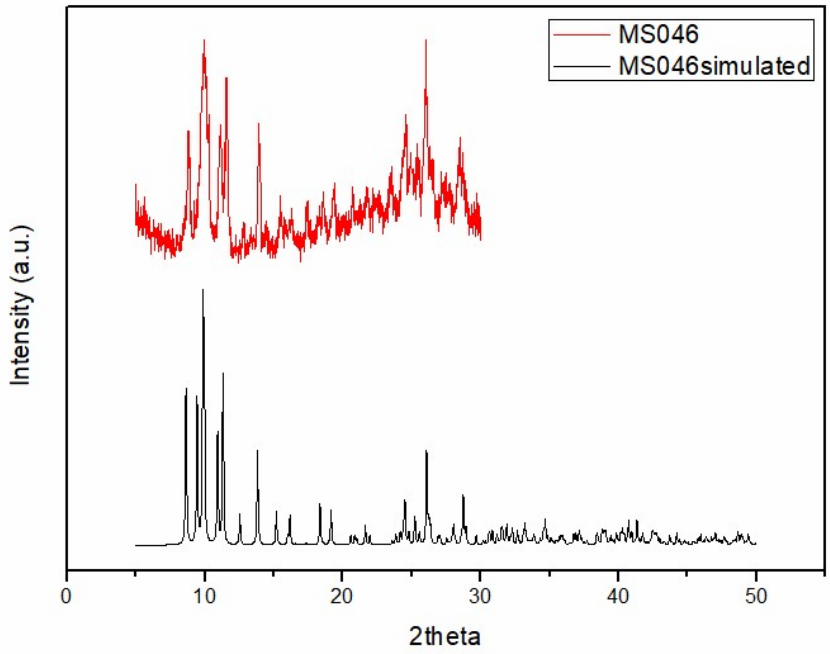

110.66
400 380 360 340 320 300 280 260 240 220 200 180 160 140 120 100 80 60 40 20 0 -20 -40 -60 -80
f1 (ppm)

Powder XRD measurement

[CuCl{Se(IPr^{Me})}]



[AgCl{Se(SIMes)}]



Crystallography data

	[Se(IPr^{Me})]	**[S(IPr^{Me})]**	**[S(ICy)]**	**Cu(IPr^{Me}Se)Cl**
CCDC no	1997590	1997588	1997589	1997592
Empirical formula	$C_{29}H_{40}N_2Se$	$C_{29}H_{40}N_2S$	$C_{15}H_{24}N_2S$	$C_{29}H_{40}ClCuN_2Se$
Formula weight (g mol-1)	495.59	448.69	264.42	594.59
T (K)	100.0(1)	100.0(1)	100.0(1)	100.0(1)
λ (Å)	1.54184	1.54184	1.54184	0.71073
Crystal system	monoclinic	monoclinic	monoclinic	triclinic
Space group	P21/n	P21/n	P21/n	P-1
a (Å)	12.0893	12.1573	13.9143	8.5955
b (Å)	16.9648	16.6275	9.1573	9.2596
c (Å)	13.0385	13.0547	12.6229	19.3041
α (°)	90	90	90	101.611
β (°)	100.14	100.079	114.545	94.598
γ (°)	90	90	90	107.181
V (Å3)	2632.3	2598.22	1463.04	1421.74
Z	4	4	4	2
ρcalc (g cm-3)	1.25	1.147	1.201	1.389
μ (mm-1)	2.048	1.224	1.826	2.162
F (000)	1048	976	576	616
Crystal dimensions (mm3)	0.118 x 0.08 x 0.045	0.124 x 0.069 x 0.03	0.115 x 0.111 x 0.06	0.54 x 0.138 x 0.065
2θ max (°)	151.812	150.742	147.844	59.48
Reflections collected	19740	25046	14137	31861
Independent reflections	5122	5294	2919	7297
Parameters refined	299	299	163	317
Final R indexes [I0>2σ(I0)]	R1= 0.0522 ωR2= 0.1252	R1= 0.0359 ωR2= 0.0900	R1= 0.0438 ωR2= 0.0904	R1= 0.0388 ωR2= 0.0758
R indexes (all data)	R1= 0.0753 ωR2= 0.1384	R1= 0.0443 ωR2= 0.0957	R1= 0.0711 ωR2= 0.1026	R1= 0.0589 ωR2= 0.0849
Goodness-of-fit on F2	1.053	1.033	1.065	1.036

	[Cu{Se(SIPr)}2][CuCl2]	**[AgCl{μ-Se(SIMes)}]$_2$**	**[Ag{Se(SIPr)}2][AgCl2]**
CCDC no	1997591	1997598	1997597
Empirical formula	$C_{56}H_{80}Cl_6Cu_2N_4Se_2$	$C_{42}H_{52}Ag_2Cl_2N_4Se_2$	$C_{56}H_{80}Ag_2Cl_6N_4Se_2$
Formula weight (g mol-1)	1306.96	1057.44	1395.60

T (K)	100.0(1)	100.0(1)	100.0(1)
λ (Å)	1.54184	0.71073	0.71073
Crystal system	monoclinic	triclinic	monoclinic
Space group	P21	P-1	P21
a (Å)	10.4151	9.7146	10.482
b (Å)	25.5169	11.1573	25.692
c (Å)	12.1509	11.6057	12.101
α (°)	90	62.337	90
β (°)	110.7710	74.688	110.519
γ (°)	90	66.627	90
V (Å3)	3019.35	1017.76	3052.51
Z	2	1	2
ρcalc (g cm-3)	1.438	1.725	1.518
μ (mm-1)	4.978	2.917	2.135
F (000)	1344	528	1416
Crystal dimensions (mm3)	0.13 x 0.104 x 0.067	0.199 x 0.148 x 0.101	0.158 x 0.124 x 0.09
2θ max (°)	147.752	59.374	59.502
Reflections collected	29.410	22497	36467
Independent reflections	11394	5176	14022
Parameters refined	648	241	648
Final R indexes [I0>2σ(I0)]	R1= 0.0348 ωR2= 0.0873	R1= 0.0263 ωR2= 0.0571	R1= 0.0264 ωR2= 0.0557
R indexes (all data)	R1= 0.0376 ωR2= 0.0897	R1= 0.0318 ωR2= 0.0601	R1= 0.0299 ωR2= 0.0572
Goodness-of-fit on F2	1.042	1.04	1.021

	[AuCl{Se(IPr^{Me})}]	**[AuCl{Se(IPr^{Cl})}]**	**[AuCl{Se(ICy)}]**	**[Au{Se(IAd)}$_2$][AuCl$_2$]**
CCDC no	1997593	1997594	1997595	1997596
Empirical formula	$C_{30}H_{42}AuCl_3N_2Se$	$C_{27}H_{34}AuCl_3N_2Se$	$C_{15}H_{24}AuClN_2Se$	$C_{46}H_{64}Au_2Cl_2N_4Se_2$
Formula weight (g mol-1)	812.94	768.84	543.74	1295.77
T (K)	100.0(1)	100.0(1)	100.0(1)	100.0(1)
λ (Å)	0.71073	0.71073	0.71073	1.54184
Crystal system	triclinic	monoclinic	monoclinic	orthorhombic
Space group	P-1	P21/n	I2/a	$P2_12_12_1$
a (Å)	9.9301	10.3338	13.5976	71.6904
b (Å)	10.5160	21.5875	14.8217	20.9451
c (Å)	17.0134	13.5109	19.8001	28.7144
α (°)	79.757	90	90	90
β (°)	73.610	89.972	107.901	90

γ (°)	74.505	90	90	90
V (Å3)	1632.36	3014.02	3797.32	4311.65
Z	2	4	8	4
ρcalc (g cm-3)	1.654	1.694	1.902	1.996
μ (mm-1)	5.888	6.372	9.799	15.971
F (000)	800	1496	2064	2512
Crystal dimensions (mm3)	0.16 x 0.14 x 0.117	0.214 x 0.138 x 0.082	0.313 x 0.055 x 0.027	0.197 x 0.083 x 0.046
2θ max (°)	59.424	59.29	59.456	147.884
Reflections collected	36446	18664	21743	52642
Independent reflections	8332	6976	4868	8640
Parameters refined	354	315	181	505
Final R indexes [I0>2σ(I0)]	R1= 0.0270 ωR2= 0.0548	R1= 0.0273 ωR2= 0.0515	R1= 0.0173 ωR2= 0.0351	R1= 0.0396 ωR2= 0.0918
R indexes (all data)	R1= 0.0324 ωR2= 0.0574	R1= 0.0357 ωR2= 0.0547	R1= 0.0205 ωR2= 0.0361	R1= 0.0472 ωR2= 0.0965
Goodness-of-fit on F2	1.025	1.034	1.032	1.032