

Supporting Information

for

Synthesis of diarylmethanes by means of Negishi cross-coupling enabled by cobalt-solvent coordination

Jakub Robaszkiewicz^{†‡}, Wojciech Chaładaj[§], Piotr Pawluć^{†‡}, Maciej Zaranek^{†*}

[†] Center for Advanced Technologies, Adam Mickiewicz University, Uniwersytetu Poznańskiego 10, 61-614 Poznań, Poland

[‡] Faculty of Chemistry, Adam Mickiewicz University, Uniwersytetu Poznańskiego 8, 61-614 Poznań, Poland

[§] Institute of Organic Chemistry, Polish Academy of Science, Kasprzaka 44/52, 01-224 Warszawa, Poland

*m.zaranek@amu.edu.pl

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1. General remarks

All reactions were carried out under argon atmosphere using standard Schlenk techniques and thoroughly dried glassware. Tetrahydrofuran was purified by distillation over sodium/benzophenone and stored under argon. *N,N*-dimethylacetamide (Merck/Sigma-Aldrich) was transferred to a Schlenk flask and degassed prior to use. Cobalt complexes were synthesized according to known literature procedures. Negishi reagents were prepared from the respective benzyl bromides in a direct reaction with zinc. Anhydrous cobalt(II) bromide and other reagents were purchased from Merck/Sigma-Aldrich and used as received. GC-MS analyses were performed using Agilent GC 8860 – MSD 5977B System. NMR spectra were collected using Bruker Avance Neo 300 MHz (^1H and ^{13}C) and Bruker Avance Neo 400 MHz (^{19}F) spectrometers with chemical shift scale referenced to residual solvent peaks assuming standardized values or, in case of ^{19}F , external reference and lock signal.

2. General procedure of Negishi cross-coupling

A calculated volume of solution of arylmethyl bromide in THF containing 4 mmol (2 eq. respectively to aryl halide) of this reagent was placed in a carefully dried Schlenk bomb flask with a PTFE valve plug. The introduced THF was evaporated *in vacuo* through the Schlenk line. Then, dimethylacetamide (0.4 ml), the corresponding organic halide (1 eq., 2 mmol) and cobalt bromide (21.8 mg, 5 mol%, 0.1 mmol) were added. After closing, the reaction mixture was stirred for 20 h at room temperature (for ArI), or at 80 °C (for ArBr). The mixture was quenched with concentrated aqueous NH_4Cl solution (10 ml) and ethyl acetate (10 ml) was added. The mixture was extracted with ethyl acetate (3 x 10 ml). The combined organic layers were washed with brine, dried over Na_2SO_4 , and concentrated *in vacuo*. Trace amounts of DMAc were removed by prolonged evacuation on the Schlenk line.

3. Optimization of Negishi cross-coupling reaction – additional tables

Table S1. DMA as an additive to reactions carried out in THF.

Entry	DMA loading [mol %] (equiv. rel. to Co)	Conversion of 4-iodotoluene [%]
1.	5 (1)	41
2.	10 (2)	47
3.	20 (4)	68
4.	30 (6)	85
5.	50 (19)	90
6.	100 (20)	93

Conditions: 4-iodotoluene 0.4 M in THF, [Negishi reagent]:[Ar-I]= 2:1, Cobalt bromide 5 mol %, temperature: 80 °C, inert gas.

Table S2. Using 3 mol% of cobalt bromide(II) as a precatalyst.

Table Entry	Time [hours]	Conversion of 4-iodotoluene [%]
1.	1	48
2.	2	57
3.	3	67
4.	6	80
5.	17	93

Conditions: 4-iodotoluene 5 M in DMA, [Negishi reagent]:[Ar-I]= 2:1, Cobalt bromide 3 mol %, room temperature, inert gas.

Table S3. Using 5 mol% of cobalt bromide(II) as a precatalyst.

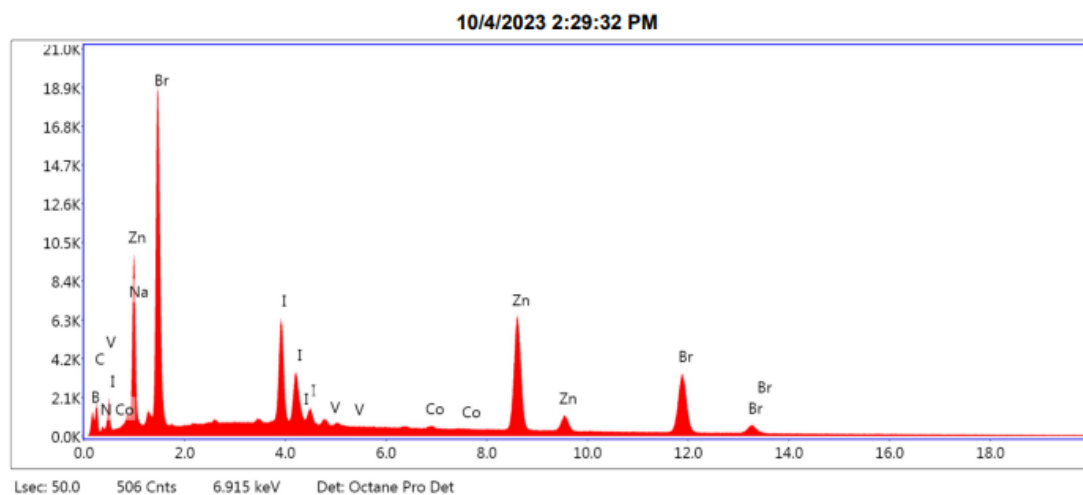
Entry	Time [hours]	Conversion of 4-iodotoluene [%]
1.	1	77
2.	2	88
3.	3	92
4.	6	96
5.	17	99

Conditions: 4-iodotoluene 5 M in DMA, [Negishi reagent]:[Ar-I]= 2:1, Cobalt bromide 5 mol %, room temperature, inert gas.

4. SEM-EDS analysis

Chart S1a. SEM-EDS analysis of the solid residue after a completed reaction run.

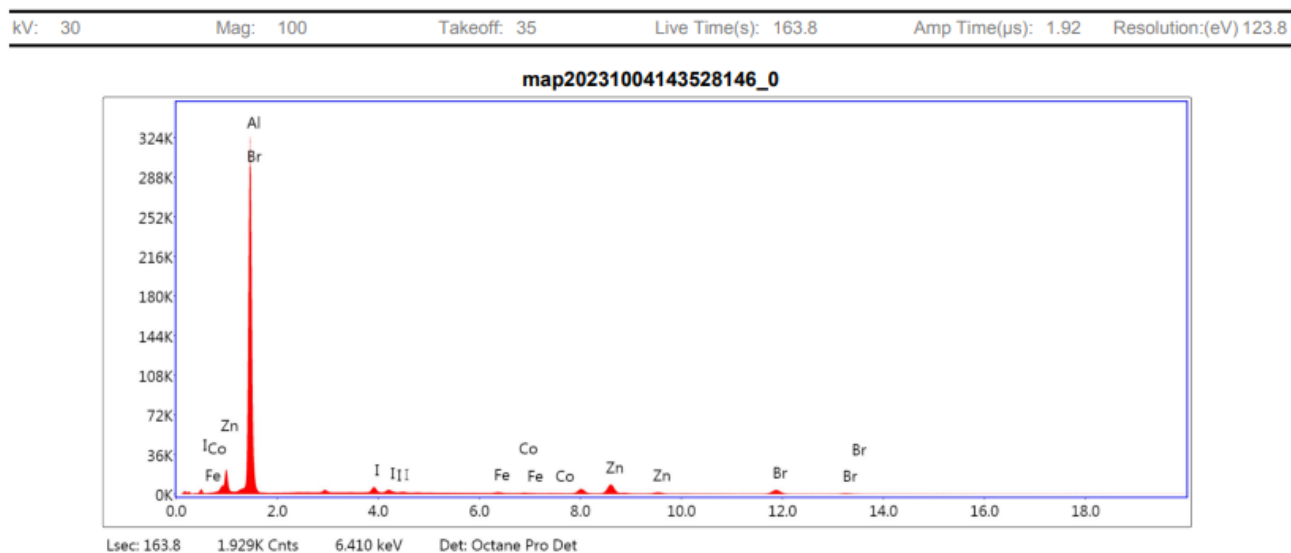
kV: 30 Mag: 200 Takeoff: 34.8 Live Time(s): 50 Amp Time(μs): 1.92 Resolution:(eV) 123.8



eZAF Smart Quant Results

Element	Weight %	Atomic %	Net Int.	Error %	Kratio	Z	R	A	F
B K	31.34	58.24	278.87	8.83	0.0935	1.0982	0.8896	0.2726	1.0000
C K	14.58	24.39	402.38	10.30	0.0189	1.1626	0.9031	0.1121	1.0000
V L	26.70	10.53	319.29	7.93	0.0872	0.8955	1.0568	0.3667	0.9979
I L	5.32	0.84	2590.15	3.67	0.0514	0.7766	1.2427	1.1777	1.0589
CoK	0.10	0.04	71.30	27.60	0.0010	0.8889	1.0608	0.9293	1.2131
ZnK	7.84	2.41	4030.48	2.64	0.0814	0.8786	1.0725	0.9722	1.2209
BrK	14.11	3.55	2487.20	2.78	0.1367	0.8174	1.0816	0.9914	1.2006

Chart S1b. SEM-EDS analysis of the solid residue after a completed reaction run (continuation).



eZAF Smart Quant Results

Element	Weight %	Atomic %	Net Int.	Error %	Kratio	Z	R	A	F
AlK	63.42	83.38	15371.31	5.89	0.3273	1.0650	0.9492	0.4836	1.0020
I L	6.26	1.75	697.10	2.52	0.0523	0.8106	1.2173	0.9858	1.0456
FeK	0.71	0.45	144.73	8.96	0.0072	0.9471	1.0369	0.9395	1.1318
CoK	0.30	0.18	56.28	13.75	0.0031	0.9279	1.0420	0.9572	1.1726
ZnK	12.39	6.72	1707.12	2.21	0.1306	0.9173	1.0552	0.9870	1.1646
BrK	16.92	7.51	805.13	2.77	0.1676	0.8541	1.0677	0.9925	1.1684

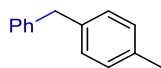
5. ICP-MS Analysis

Chart S2. SEM-EDS analysis of the solid residue after a completed reaction run.

Report Concentration Unit: ppb						
Analyte Intensities						
Analyte	Concentration	Intensity	Intensity Comment	Zr	0.000	0
H			Not Measured	Nb	0.137	6690
He			Not Measured	Mo	0.007	338
Li	1.813	60008		Ru	2.535	153361
Be	0.007	71		Rh	0.824	46301
B	18.305	188546		Pd	0.162	8851
C	32856.074	49284111		Ag	0.012	648
N	10332636.390	103326364		Cd	0.046	2313
O			Not Measured	In	0.007	518
F		0		Sn	0.000	0
Ne		0		Sb	0.195	6229
Na	884.093	49067170		Te	0.000	0
Mg	166.052	7306301		I	0.000	0
Al	137.531	7124104		Xe	0.000	0
Si	3095.455	95959117		Cs	0.030	2102
P	11.524	59928		Ba	0.000	0
S	0.000	0		La	0.002	162
Cl	834167.134	333666854		Ce	1.323	98528
Ar	0.000	0		Pr	0.002	182
K	497.744	9457139		Nd	0.003	210
Ca	1620.215	33214412		Sm	0.000	0
Sc	0.799	56179		Eu	0.000	0
Ti	94.860	5293183		Gd	0.000	0
V	315.598	17925942		Tb	0.001	34
Cr	43.586	2780798		Dy	0.004	196
Mn	0.506	34344		Ho	0.000	0
Fe	0.000	0		Er	0.000	0
Co	25423.718	1372880799		Tm	0.000	21
Ni	11.838	542197		Yb	0.000	0
Cu	0.000	0		Lu	0.000	0
Zn	173089.377	4656104250		Hf	0.006	246
Ga	0.000	0		Ta	0.000	17
Ge	0.000	0		W	0.018	556
As	257.300	1458890		Re	0.013	441
Se	33278.430	133113721		Os	0.000	0
Br	S	S		Ir	0.000	0
Kr	0.000	0		Pt	0.125	2579
Rb	0.000	0		Au	0.000	0
Sr	0.000	0		Hg	0.000	0
Y	0.034	2553		Tl	0.003	159
				Pb	0.000	0
				Bi	0.055	2207
				Th	0.000	9
				U	0.019	996
TotalQuant Equations						
Analyte	Equation					
Ca	740.74*mass 43					
Ti	13.44*mass 47					
Se	11.455*mass 82					
Fe	47.17*mass 57					

Note: presented are the relative concentrations by weight of elements and calculated Pd concentration in this case is $\cong 6 \times 10^{-7}$ mol per 1 mol of aryl halide, i.e., $\cong 0.6$ mol ppb.

6. Identification of Negishi cross-coupling products



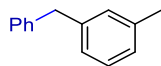
1-benzyl-4-methylbenzene (3a), Yield=96%, 348 mg

¹H NMR (300 MHz, CDCl₃) δ (ppm) 7.40 (m, 2H), 7.32 (m, 3H), 7.22 (s, 4H), 4.06 (s, 2H), 2.44 (s, 3H).

¹³C NMR (75 MHz, CDCl₃) δ (ppm) 141.51, 138.17, 135.60, 129.24, 128.96, 128.91, 128.51, 126.06, 41.62, 21.09.

MS : m/z (%) 167 (100), 182 (80), 152 (30), 91 (20), 77 (17), 104 (16), 51(10), 128 (8).

Data conforms to the literature.¹



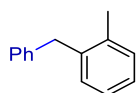
1-benzyl-3-methylbenzene (3b), Yield=84%, 306 mg

¹H NMR (300 MHz, CDCl₃) δ (ppm) 7.21 (m, 2H), 7.13 (m, 3H), 6.93 (m, 4H), 3.87 (s, 2H), 2.24 (s, 3H).

¹³C NMR (75 MHz, CDCl₃) δ (ppm) 141.87, 141.51, 138.17, 135.60, 129.24, 128.96, 128.91, 128.54, 128.51, 128.42, 126.06, 126.01, 41.62, 21.09.

MS : m/z (%) 167 (100), 182 (60), 91 (25), 152 (25), 77 (22), 104 (21), 65 (20), 51 (15).

Data conforms to the literature.¹



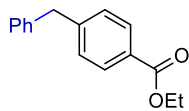
1-benzyl-2-methylbenzene (3c), Yield=74%, 270 mg

¹H NMR (300 MHz, CDCl₃) δ (ppm) 7.26 (m, 2H), 7.13 (m, 7H), 4.00 (s, 2H), 2.25 (s, 3H).

¹³C NMR (75 MHz, CDCl₃) δ (ppm) 140.44, 138.97, 136.68, 130.33, 130.00, 128.79, 128.50, 128.43, 128.38, 126.50, 126.03, 125.96, 39.50, 19.72.

MS : m/z (%) 167(100), 182 (80), 165 (40), 152 (25), 104 (23), 91 (20), 65 (18), 128 (18), 51 (15).

Data conforms to the literature.²



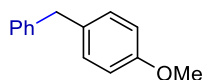
ethyl 4-benzylbenzoate (3d), Yield=87%, 417 mg

¹H NMR (300 MHz, CDCl₃) δ (ppm) 7.96 (d, 2H, J=8.3 Hz), 7.29 (m, 5H), 7.16 (d, J=8.3 Hz, 2H), 4.35 (q, J=7.12 Hz, 2H), 4.01 (s, 2H), 1.30 (t, J = 7.1 Hz, 3H).

¹³C NMR (75 MHz, CDCl₃) δ (ppm) 166.5, 146.3, 140.1, 129.7, 128.9, 128.8, 128.5, 128.4, 126.3, 60.7, 41.8, 14.3.

MS : m/z (%) 167 (100), 195 (80), 240 (45), 152 (42), 91 (35), 212 (25), 115 (20), 65 (18).

Data conforms to the literature.³



1-benzyl-4-methoxybenzene (3e), Yield=94%, 372 mg

¹H NMR (300 MHz, CDCl₃) δ (ppm) 7.16 (m, 2H), 7.07 (m, 3H), 6.98 (d, J=8.79 Hz, 2H), 6.71 (d, J=8.7 Hz, 2H), 3.80 (s, 2H), 3.63 (s, 3H).

¹³C NMR (75 MHz, CDCl₃) δ (ppm) 158.10, 141.70, 133.37, 129.98, 128.93, 128.54, 126.09, 114.01, 55.31, 41.15.

MS : m/z (%) 198 (100), 167 (60), 121 (50), 153 (40), 91 (36), 77 (34), 183 (25), 128 (20), 51 (18).

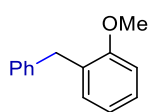
Data conforms to the literature.¹

Gram-scale synthesis:

¹H NMR (300 MHz, CDCl₃) δ (ppm) 7.17(m, 2H), 7.08(m, 3H), 7.00(d, J=8.82 Hz, 2H), 6.72(d, J=8.7 Hz, 2H), 3.82(s, 2H), 3.66(s, 3H).

¹³C NMR (75 MHz, CDCl₃) δ (ppm) 158.06, 141.67, 133.33, 129.95, 128.90, 128.52, 126.06, 113.96, 55.30, 41.12.

MS : m/z (%) 198 (100), 167 (60), 121 (50), 153 (40), 91 (36), 77 (34), 183 (25), 128 (20), 51 (18).



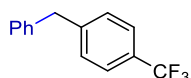
1-benzyl-2-methoxybenzene (3f), Yield=88%, 349 mg

¹H NMR (300 MHz, CDCl₃) δ (ppm) 7.12 (m, 6H), 6.96 (d, 1, J=7.3 Hz, 1H), 6.76 (t, J=9.0 Hz, 2H), 3.88 (s, 2H), 3.68 (s, 3H).

¹³C NMR (75 MHz, CDCl₃) δ (ppm) 157.3, 141.0, 130.3, 129.6, 128.9, 128.2, 127.4, 125.7, 120.4, 110.4, 55.3, 35.8.

MS : m/z (%) 198 (100), 165 (80), 91 (45), 183 (44), 152 (35), 77 (25), 115 (24), 128 (22), 139 (20).

Data conforms to the literature.⁴



1-benzyl-4-(trifluoromethyl)benzene (3g), Yield=74%, 349 mg

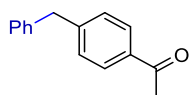
¹H NMR (300 MHz, CDCl₃) δ (ppm) 7.45 (d, J = 8.0 Hz, 2H), 7.21 (m, 4H), 7.15 (m, 1H), 7.08 (m 2H), 3.94 (s, 2H).

¹³C NMR (75 MHz, CDCl₃) δ (ppm) 145.25 (d, ¹J_{CF}=5.13 Hz), 141.83, 140.01, 129.22, 128.97, 128.70, 128.49, 128.37, 128.30, 126.51, 126.15, 125.95, 125.45 (q, ²J_{CF}=15.06 Hz), 125.40, 122.55, 41.75.

¹⁹F NMR (376 MHz, CDCl₃): δ (ppm) -63.00.

MS : m/z (%) 167 (100), 165 (49), 236 (43), 166 (20), 91 (19), 152 (16), 168 (15), 51 (11), 69 (10), 63 (9).

Data conforms to the literature.¹



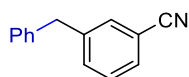
1-(4-benzylphenyl)ethan-1-one (3h), Yield=86%, 361 mg

¹H NMR (300 MHz, CDCl₃) δ (ppm) 7.80 (d, J = 8.4 Hz, 2H), 7.21 (m, 4H), 7.12 (m, 1H), 7.10 (m, 2H), 3.95 (s, 2H), 2.48 (s, 3H).

¹³C NMR (75 MHz, CDCl₃) δ (ppm) 197.84, 146.87, 140.12, 135.34, 130.69, 129.14, 128.96, 128.67, 126.44, 41.93, 26.59.

MS : m/z (%) 195 (100), 165 (46), 210 (43), 91 (30), 65 (25), 115 (22), 139 (15).

Data conforms to the literature.¹



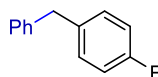
3-benzylbenzonitrile (3i), Yield=84%, 324 mg

¹H NMR (300 MHz, CDCl₃) δ (ppm) 7.50 (m, 2H), 7.45 (m, 1H), 7.42 (m, 1H), 7.34 (m, 2H), 7.28 (m, 1H), 7.19 (m, 2H), 4.03 (s, 2H).

¹³C NMR (75 MHz, CDCl₃) δ (ppm) 142.6, 139.4, 133.4, 132.4, 129.9, 129.2, 128.9, 128.8, 126.7, 118.9, 112.5, 41.4.

MS : m/z (%) 193 (100), 165 (40), 91 (35), 191 (25), 63 (20), 178 (18), 51 (15).

Data conforms to the literature.¹



1-benzyl-4-fluorobenzene (3j), Yield=90%, 335 mg

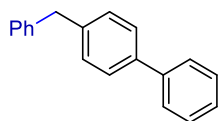
¹H NMR (300 MHz, CDCl₃) δ (ppm) 7.32 (m, 2H), 7.24 (m, 1H), 7.17 (m, 4H), 6.99 (m, 2H), 3.97 (s, 2H).

¹³C NMR (75 MHz, CDCl₃) δ (ppm) 161.44 (d, ¹J_{CF}=243.8 Hz), 140.99, 136.79 (d, ⁴J_{CF}=3.4 Hz), 130.30 (d, ³J_{CF}=7.8 Hz), 128.85, 128.55, 126.22, 115.20 (d, ²J_{CF}=21.2 Hz), 41.10.

¹⁹F NMR (376 MHz, CDCl₃): δ (ppm) -117.41.

MS : m/z (%) 186(100), 165 (60), 109 (30), 171 (24), 91 (22), 83 (20), 133 (15), 51 (15).

Data conforms to the literature.¹



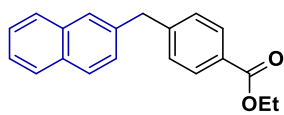
4-benzyl-1,1'-biphenyl (3k), Yield=75%, 366 mg

¹H NMR (300 MHz, CDCl₃) δ (ppm) 7.48 (m, 2H), 7.42 (m, 2H), 7.3 (t, J=7.68 Hz, 2H), 7.23 (m, 3H), 7.14 (m, 5H), 3.94 (s, 2H).

¹³C NMR (75 MHz, CDCl₃) δ (ppm) 141.95, 141.05, 140.29, 139.09, 129.36, 129.01, 128.76, 128.56, 127.25, 127.11, 127.05, 126.19, 41.64.

MS : m/z (%) 244(100), 165 (60), 152 (35), 91 (34), 115 (28), 229 (25), 215 (20), 77 (18), 51 (15).

Data conforms to the literature.⁵



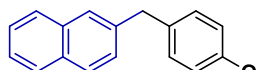
ethyl 4-(naphthalen-2-ylmethyl)benzoate (3l), Yield=64%, 333 mg

¹H NMR (300 MHz, CDCl₃) δ (ppm) 7.8 (m, 2H), 7.71(3H), 7.52 (s, 1H), 7.35 (m, 2H), 7.20 (m, 3H), 4.26 (q, J=7.11 Hz, 2H), 4.19 (s, 2H), 1.28 (t, J=7.11 Hz, 3H).

¹³C NMR (75 MHz, CDCl₃) δ (ppm) 166.64, 137.68, 133.62, 132.20, 129.85, 129.05, 128.57, 128.30, 127.74, 127.68, 127.58, 127.46, 127.27, 126.16, 125.58, 60.88, 42.09, 14.37.

MS : m/z (%) 290 (100), 217 (82), 202 (45), 245 (42), 141 (22), 115 (16), 189 (14), 261 (12), 101 (8).

Data conforms to the literature.⁶



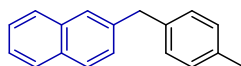
2-(4-methoxybenzyl)naphthalene (3m), Yield=75%, 372 mg

¹H NMR (300 MHz, CDCl₃) δ (ppm) 7.66 (m, 3H), 7.60 (s, 1H), 7.40 (m, 2H), 7.22 (d, J=7.6 Hz, 1H), 7.04 (d, J=8.73 Hz, 2H), 6.73 (d, J=8.7 Hz, 2H), 3.98 (s, 2H), 3.67 (s, 3H).

¹³C NMR (75 MHz, CDCl₃) δ (ppm) 158.10, 139.14, 133.69, 133.16, 132.13, 130.03, 128.10, 127.65, 127.61, 126.97, 126.01, 125.36, 125.22, 113.99, 55.30, 41.27.

MS : m/z (%) 248 (100), 217 (55), 202 (49), 121 (24), 141 (22), 233 (18), 101 (16), 77 (14), 189 (12), 178 (11).

Data conforms to the literature.⁷



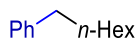
2-(4-methylbenzyl)naphthalene (3n), Yield=86%, 399mg

¹H NMR (300 MHz, CDCl₃) δ (ppm) 7.66 (m, 3H), 7.52 (s, 1H), 7.31 (m, 2H), 7.20 (dd, J = 8.46, 1.68 Hz, 1H), 7.01 (m, 4H), 3.99 (s, 2H), 2.22 (s, 3H).

¹³C NMR (75 MHz, CDCl₃) δ (ppm) 138.98, 138.01, 135.71, 133.70, 132.15, 129.27, 128.99, 128.12, 127.71, 127.70, 127.63, 127.08, 126.01, 125.37, 41.76, 21.11.

MS : m/z (%) 232 (100), 217 (86), 115 (60), 202 (36), 141 (33), 77 (28), 91(27), 63 (22), 51 (20), 127 (20).

Data conforms to the literature.⁸



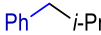
heptylbenzene (3o), Yield=58%, 204 mg

¹H NMR (300 MHz, CDCl₃) δ (ppm) 7.18 (t, J=8.2 Hz, 2H), 7.10 (d, J=7.2 Hz, 3H), 2.51 (t, J = 7.53 Hz, 2H), 1.54 (t, J=7.5 Hz, 2H), 1.21 (m, 8H), 0.81 (t, J=7.1 Hz, 3H).

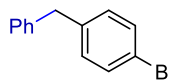
¹³C NMR (75 MHz, CDCl₃) δ (ppm) 143.00, 128.45, 128.26, 125.59, 36.07, 31.90, 31.60, 29.38, 29.26, 22.74, 14.15.

MS : m/z (%) 91 (100), 65(27), 182 (25), 51 (10), 104 (8), 77 (6), 165 (4).

Data conforms to the literature.⁹

 **isobutylbenzene (3p)**, not isolated

MS : m/z (%) 91 (100), 134 (40), 65 (20), 115 (10), 51 (6), 89 (6), 103 (4).



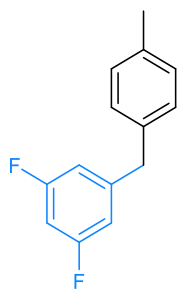
1-benzyl-4-bromobenzene, (3q), Yield=81%, 403 mg

¹H NMR (300 MHz, CDCl₃) δ (ppm) 7.32 (m, 2H), 7.21 (m, 2H), 7.14 (m, 1H), 7.08 (m, 2H), 6.97 (m, 2H), 3.85 (s, 2H).

¹³C NMR (75 MHz, CDCl₃) δ (ppm) 140.47, 140.13, 131.54, 130.69, 128.89, 128.60, 126.33, 119.97, 41.33.

MS : m/z (%) 91 (100), 165 (91), 167 (67), 195 (51), 104 (44), 152 (36), 89 (34), 51 (31), 240 (30).

Data conforms to the literature.¹⁰



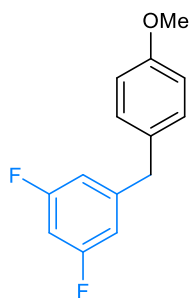
1,3-difluoro-5-(4-methylbenzyl)benzene, (3r), X=I: Yield=87%, 189 mg; X=Br: Yield=64%, 140 mg

¹H NMR (300 MHz, CDCl₃) δ (ppm) 7.10(m, 4H), 6.65(m, 3H), 3.91(s, 2H), 2.34(s, 3H).

¹³C NMR (75 MHz, CDCl₃) δ (ppm) 163.06 (dd, ¹J_{CF}=248.0 Hz, ³J_{CF}=12.9 Hz), 145.42 (t, ³J_{CF}=8.8 Hz), 136.40, 136.23, 129.41, 128.83, 111.59 (dd, ²J_{CF}=16.8 Hz, ⁴J_{CF}=7.6 Hz), 101.50 (t, ²J_{CF}=25.4 Hz), 41.21, 21.04.

¹⁹F NMR (376 MHz, CDCl₃): δ (ppm) -109.03, -109.88.

MS : m/z (%) 203 (100), 218 (86), 183 (43), 201 (36), 202 (21), 91 (19), 105 (16).



1,3-difluoro-5-(4-methoxybenzyl)benzene, (3s), Yield=90%, 210 mg

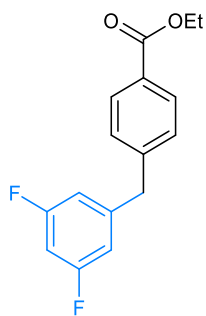
¹H NMR (300 MHz, CDCl₃) δ (ppm) 7.09(m, 2H), 6.86(m, 2H), 6.66(m, 3H), 3.89(s, 2H), 3.80(s, 3H).

¹³C NMR (75 MHz, CDCl₃) δ (ppm) 163.06 (dd, ¹J_{CF}=248.0 Hz, ³J_{CF}=12.9 Hz), 158.37, 145.63 (t, ³J_{CF}=8.8 Hz), 131.51, 129.95, 114.12, 111.52 (dd, ²J_{CF}=16.8 Hz, ⁴J_{CF}=7.6 Hz), 101.48 (t, ²J_{CF}=25.4 Hz), 55.27, 40.52.

¹⁹F NMR (376 MHz, CDCl₃): δ (ppm) -110.45.

MS : m/z (%) 234 (100), 121 (64), 233 (31), 170 (24), 77 (24), 201 (23), 63 (23), 203 (22).

HRMS (APCI): found: 247.0941, calc. for C₁₅H₁₃OF₂: 247.0934, diff. 2.8 ppm.



ethyl 4-(3,5-difluorobenzyl)benzoate, (3t), X=I: Yield=73%, 202 mg; X=Br: Yield=71%, 195 mg

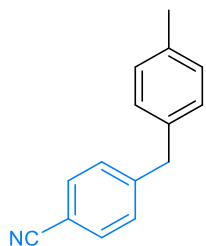
¹H NMR (300 MHz, CDCl₃) δ (ppm) 7.92(m, 2H), 7.16(m, 2H), 6.60(m, 3H), 4.30(q, J=7.11 Hz, 2H), 3.92(s, 2H), 1.31(t, J=7.14 Hz, 3H).

¹³C NMR (75 MHz, CDCl₃) δ (ppm) 166.40, 163.12 (dd, ¹J_{CF}=248.6 Hz, ³J_{CF}=12.8 Hz), 144.53, 130.02, 128.93, 111.71 (dd, ²J_{CF}=17.7 Hz, ⁴J_{CF}=7.6 Hz), 101.94(t, ²J_{CF}=25.3 Hz), 60.96, 41.50, 14.35.

¹⁹F NMR (376 MHz, CDCl₃): δ (ppm) -109,94.

MS : m/z (%) 231 (100), 183 (53), 201 (39), 203 (37), 276 (31), 248 (22), 232 (19), 127 (12).

HRMS (APCI): found: 277.1045, calc. for C₁₅H₁₃O₂F₂: 277.1040, diff. 1.8 ppm.



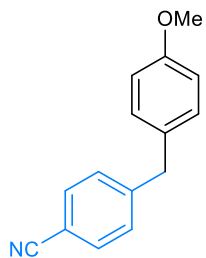
4-(4-methylbenzyl)benzonitrile, (3u), Yield=78%, 162 mg

¹H NMR (300 MHz, CDCl₃) δ (ppm) 7.48(d, J=8.52 Hz, 2H), 7.20(d, J=8.67 Hz, 2H), 7.04(d, J=8.22, 2H), 6.96(d, J=7.92 Hz, 2H), 3.92(s, 2H), 2.25(s, 3H).

¹³C NMR (75 MHz, CDCl₃) δ (ppm) 147.08, 136.29, 132.29, 129.59, 129.46, 128.85, 126.82, 119.05, 109.95, 41.58, 21.03.

MS : m/z (%) 192 (100), 91 (63), 63 (50), 89 (47), 190 (43), 65 (43), 165 (31), 191 (29).

Data conforms to the literature.¹¹



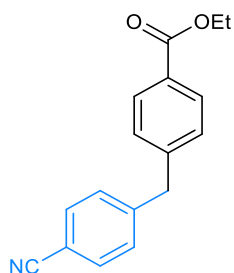
4-(4-methoxybenzyl)benzonitrile, (3v), Yield=77%, 171 mg

¹H NMR (300 MHz, CDCl₃) δ (ppm) 7.54(m, 2H), 7.24(m, 2H), 7.06(m, 2H), 6.83(m, 2H), 3.95(s, 2H), 3.77(s, 3H).

¹³C NMR (75 MHz, CDCl₃) δ (ppm) 158.38, 147.27, 132.29, 131.41, 129.97, 129.53, 127.74, 114.18, 109.93, 55.30, 41.11.

MS : m/z (%) 223 (100), 121 (65), 77 (35), 222 (32), 208 (29), 180 (28), 51 (25), 190 (23).

Data conforms to the literature.¹²



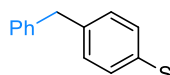
ethyl 4-(4-cyanobenzyl)benzoate, (3w), X=I: Yield=68%, 180 mg ; X=Br: Yield=56%, 148 mg

¹H NMR (300 MHz, CDCl₃) δ (ppm) 7.92(m, 2H), 7.51(m, 2H), 7.17(m, 4H), 4.30(q, J=7.1 Hz, 2H), 4.01(s, 2H), 1.31(t, J=7.1 Hz, 3H).

¹³C NMR (75 MHz, CDCl₃) δ (ppm) 166.15, 145.90, 144.39, 132.45, 132.30, 130.07, 129.67, 129.04, 128.96, 110.21, 60.79, 41.76, 14.26.

MS : m/z (%) 220 (100), 190 (43), 165 (39), 191 (29), 220 (23), 264 (22), 237 (22).

Data conforms to the literature.¹³



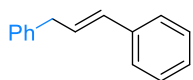
(4-benzylphenyl)(methyl)sulfane, (3y), Yield=79%, 169 mg

¹H NMR (300 MHz, CDCl₃) δ (ppm) 7.18 (m, 2H), 7.09 (m, 5H), 7.01 (m, 2H), 3.84 (s, 2H), 2.35 (s, 3H).

¹³C NMR (75 MHz, CDCl₃) δ (ppm) 141.04, 138.26, 135.81, 129.52, 128.93, 128.55, 127.18, 126.19, 41.43, 16.26.

MS : m/z (%) 167 (100), 214 (83), 165 (79), 166 (35), 152 (30), 91 (24), 137 (18).

Data conforms to the literature.¹⁴



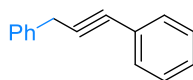
(E)-prop-1-ene-1,3-diyl dibenzene, (3x), Yield=87%, 169 mg

¹H NMR (300 MHz, CDCl₃) δ (ppm) 7.16(m, 5H), 7.06(m, 5H), 6.23(m, 2H), 3.42(d, J=6.27 Hz, 2H).

¹³C NMR (75 MHz, CDCl₃) δ (ppm) 139.53, 136.83, 130.43, 128.59, 128.04, 127.86, 126.47, 125.55, 125.49, 38.72.

MS : m/z (%) 115 (100), 91 (60), 194 (46), 77(42), 51 (40), 65 (38), 179 (36), 103 (34).

Data conforms to the literature.¹⁵



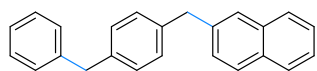
prop-1-yne-1,3-diyl dibenzene, (3z), Yield=67%, 128 mg

¹H NMR (300 MHz, CDCl₃) δ (ppm) 7.44(m, 4H), 7.30(m, 6H), 3.84(s, 2H).

¹³C NMR (75 MHz, CDCl₃) δ (ppm) 136.78, 131.66, 128.57, 128.25, 127.98, 127.84, 126.66, 123.70, 87.53, 82.68, 25.77.

MS: m/z (%) 192 (100), 91 (67), 115 (52), 77 (45), 89 (41), 63 (28), 103 (26), 65 (23).

Data conforms to the literature.¹⁶



2-(4-benzylbenzyl)naphthalene, (3aa), Yield=78%, 240 mg

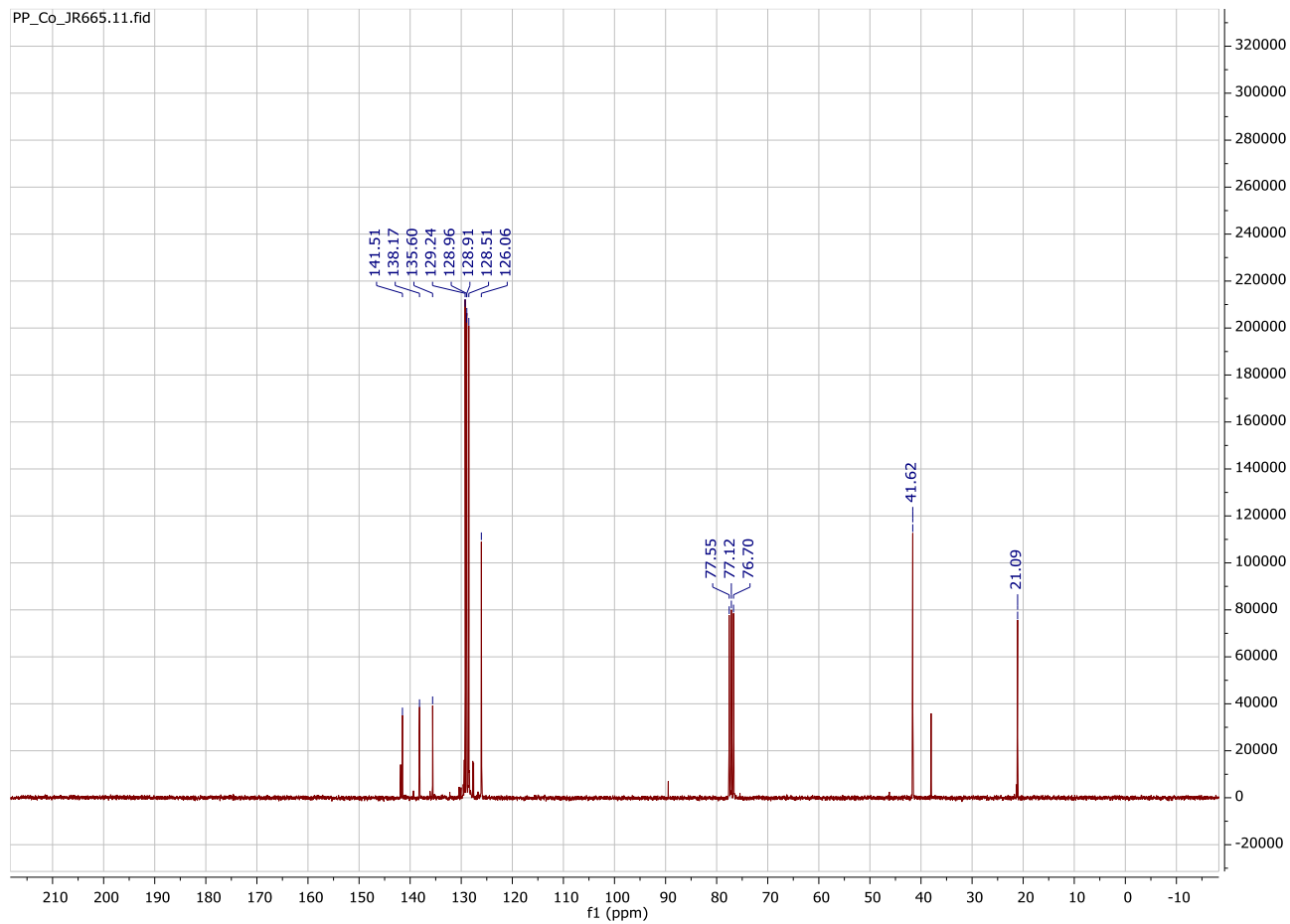
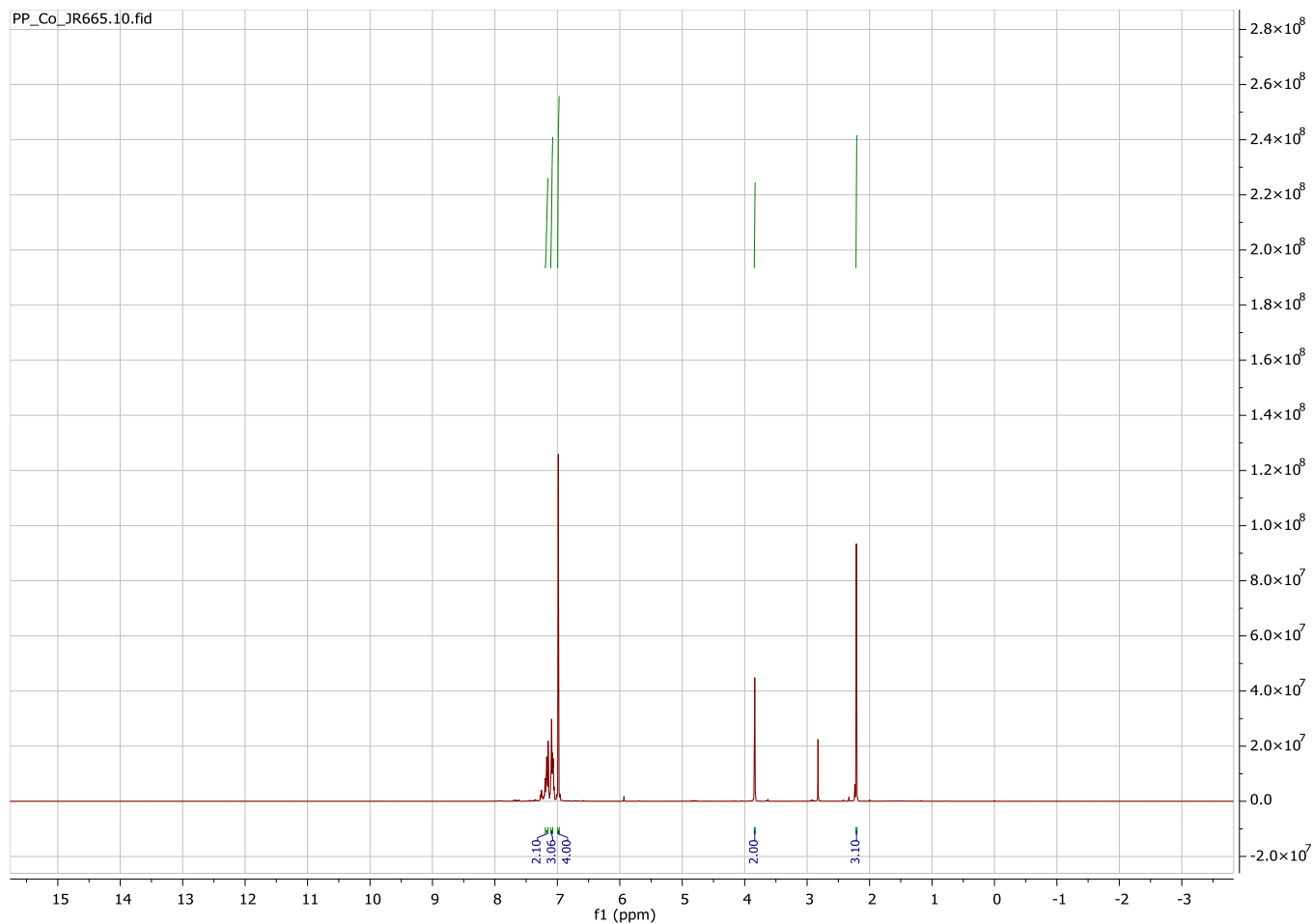
¹H NMR (300 MHz, CDCl₃) δ (ppm) 7.67(m, 4H), 7.35(m, 5H), 7.10(m, 12H), 4.00(s, 2H), 3.85(s, 2H).

¹³C NMR (75 MHz, CDCl₃) 138.77, 138.75, 132.12, 129.34, 129.13, 129.09, 129.02, 128.97, 128.57, 128.50, 128.11, 127.70, 127.67, 127.60, 127.11, 126.09, 126.01, 125.37, 41.77, 41.60.

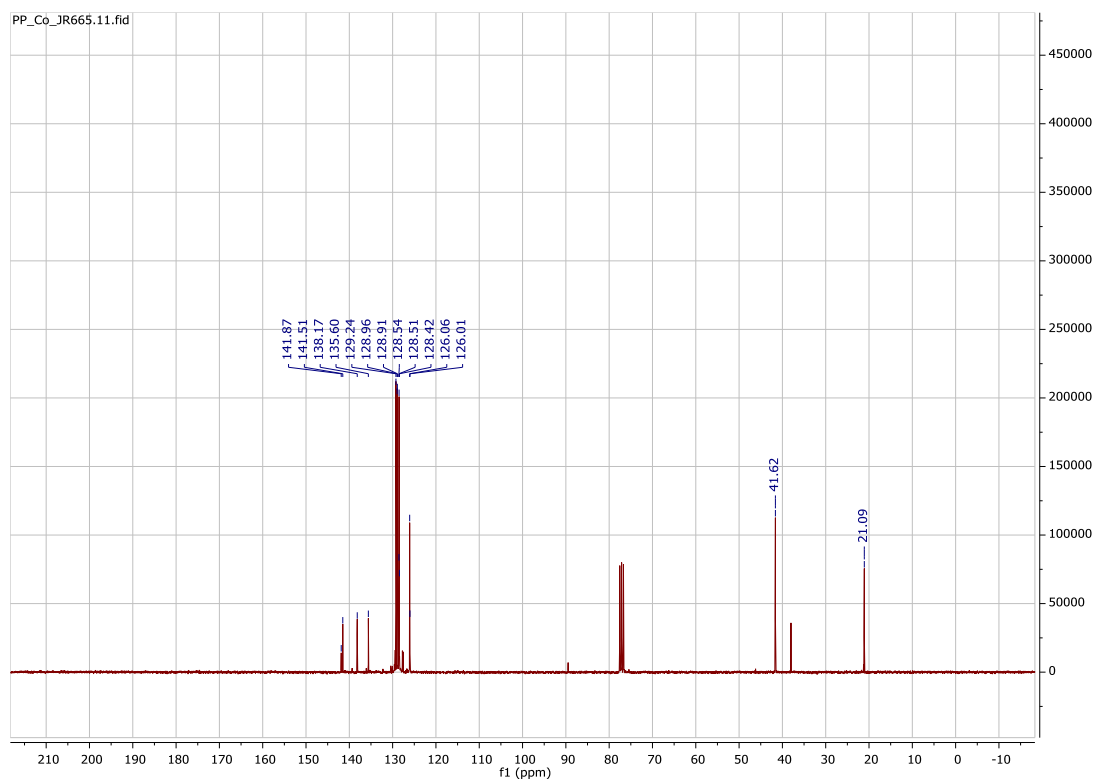
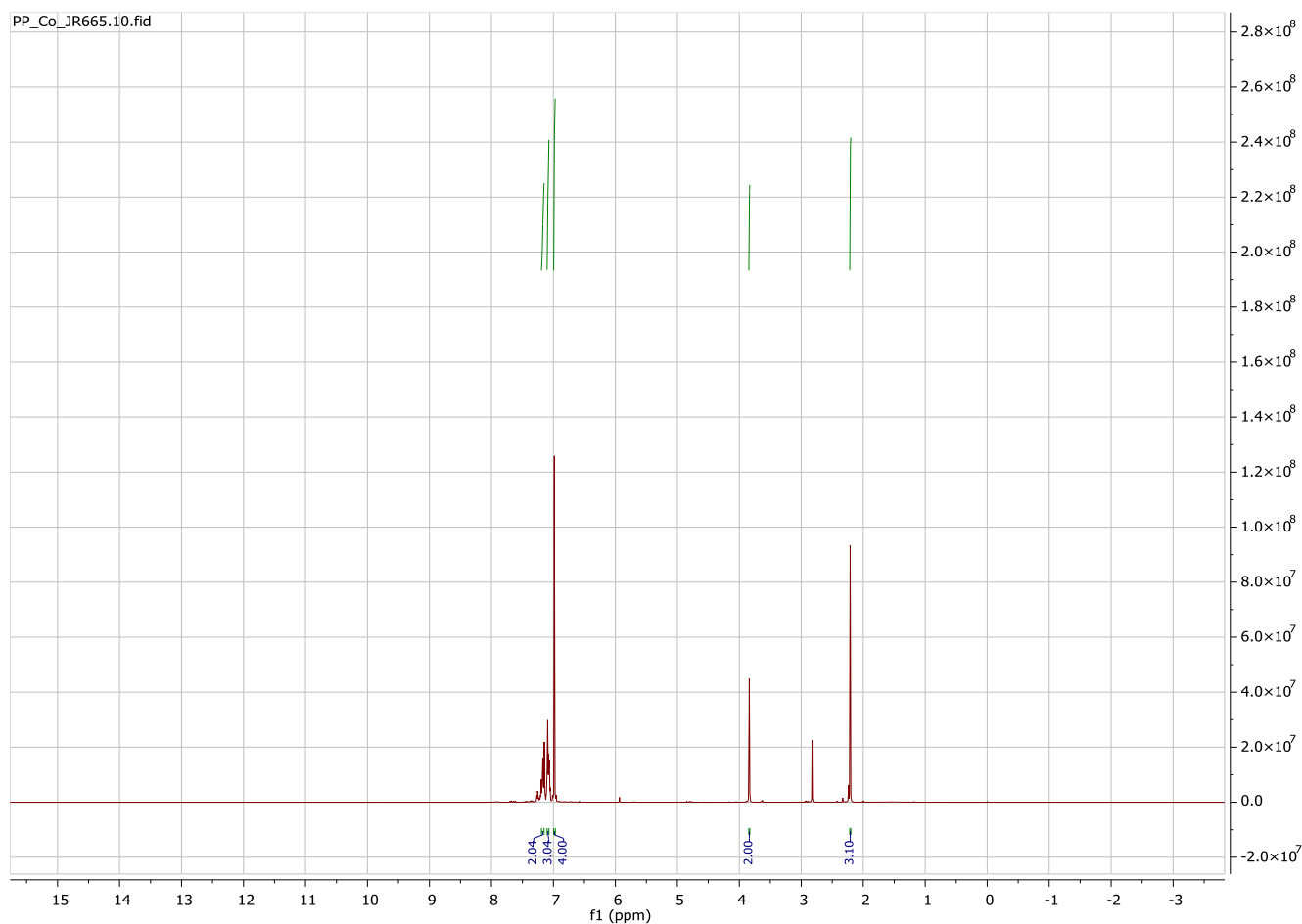
MS : m/z (%) 90 (100), 139 (78), 162 (74), 139 (70), 113 (68), 126 (56), 76 (42), 212 (34).

HRMS (APCI): found: 308.1564 , calc. for C₂₄H₂₀: 308.1565 , diff. 0.3 ppm.

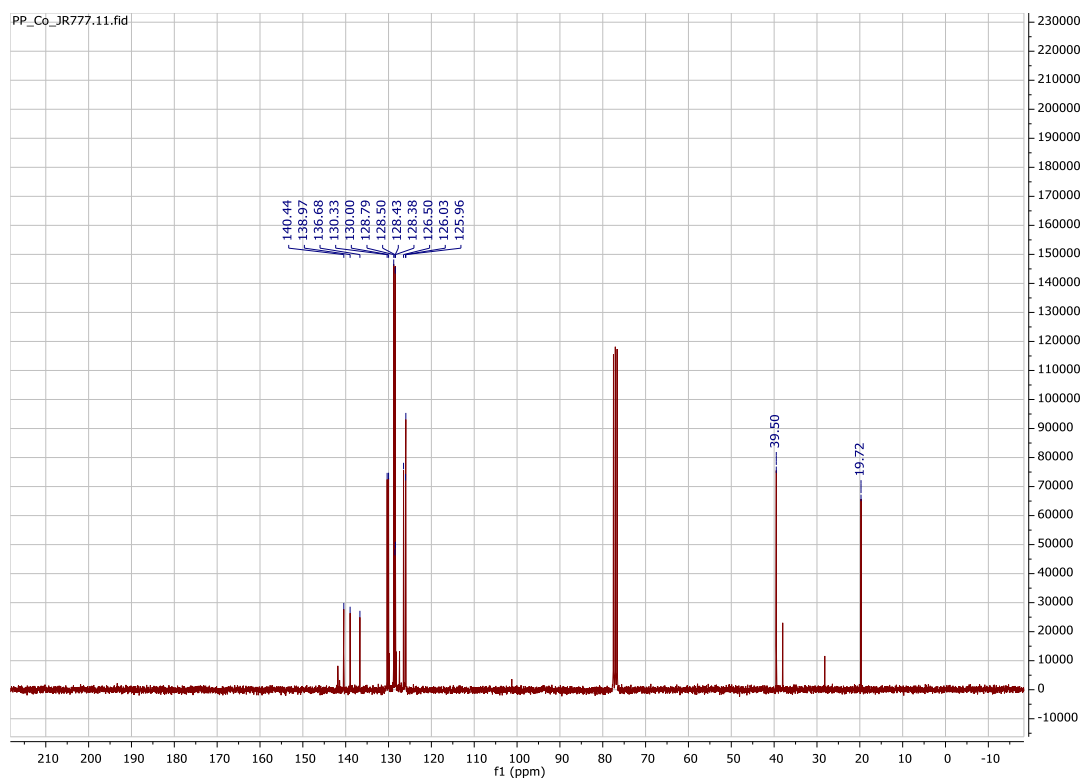
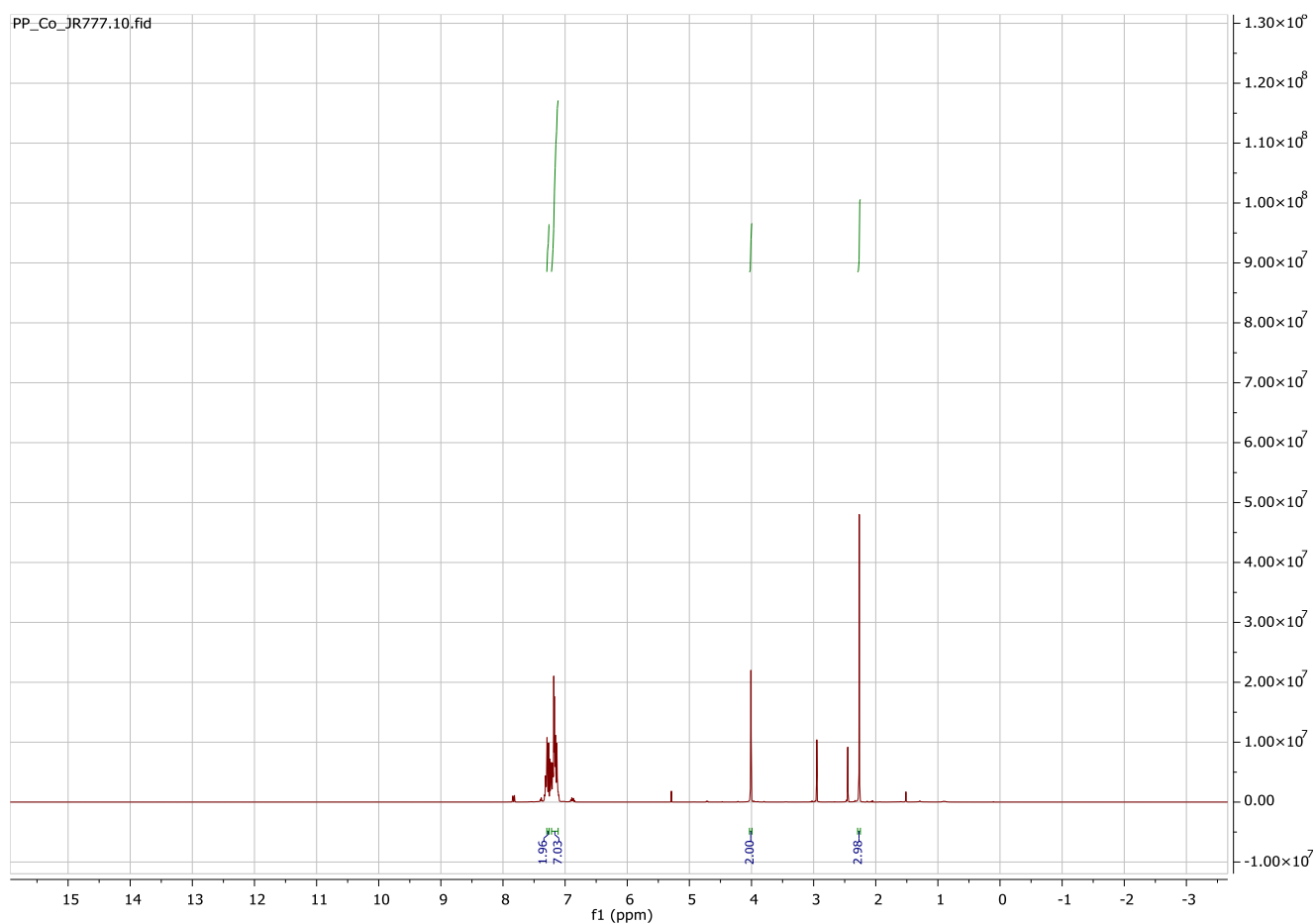
3a



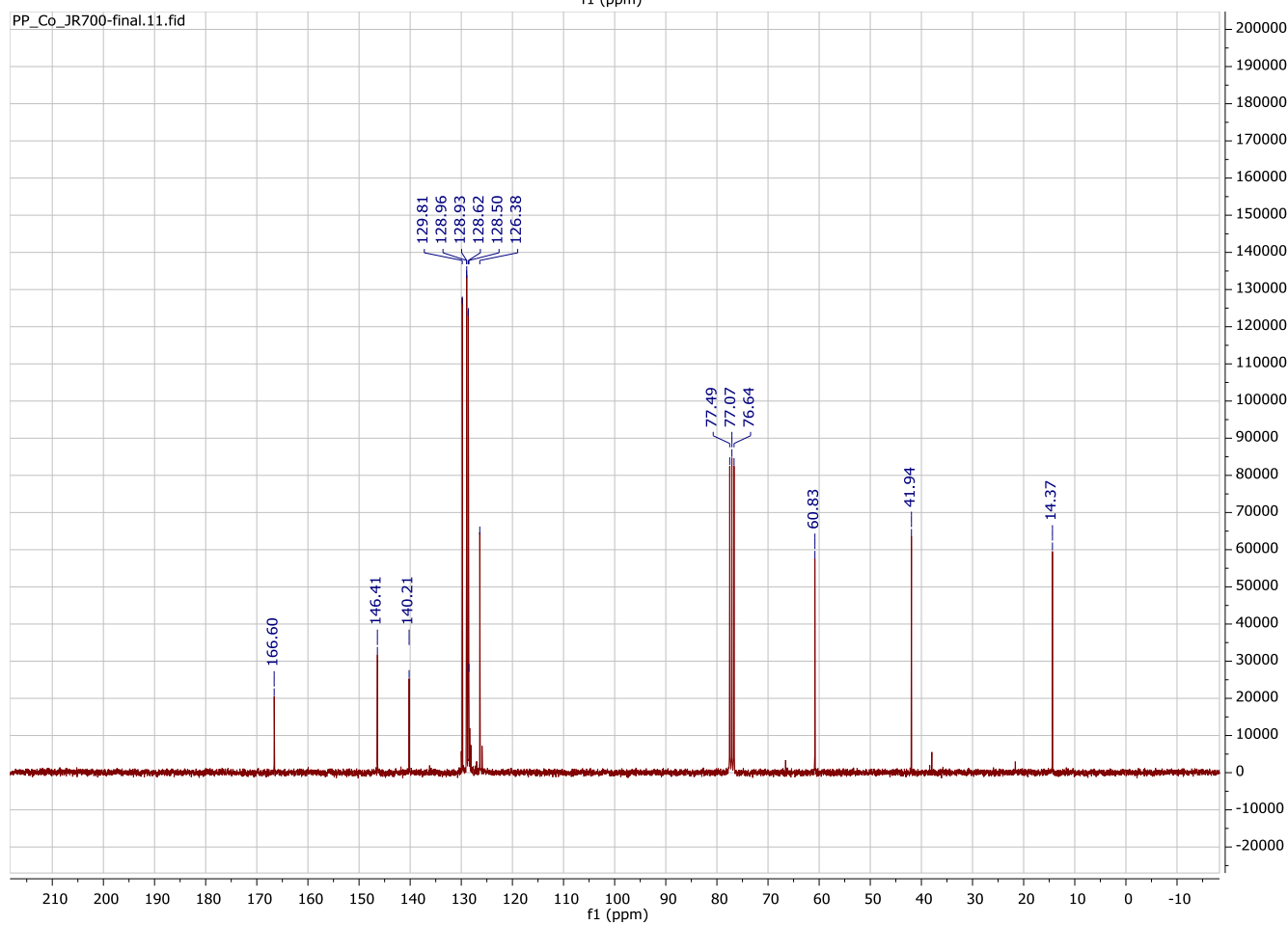
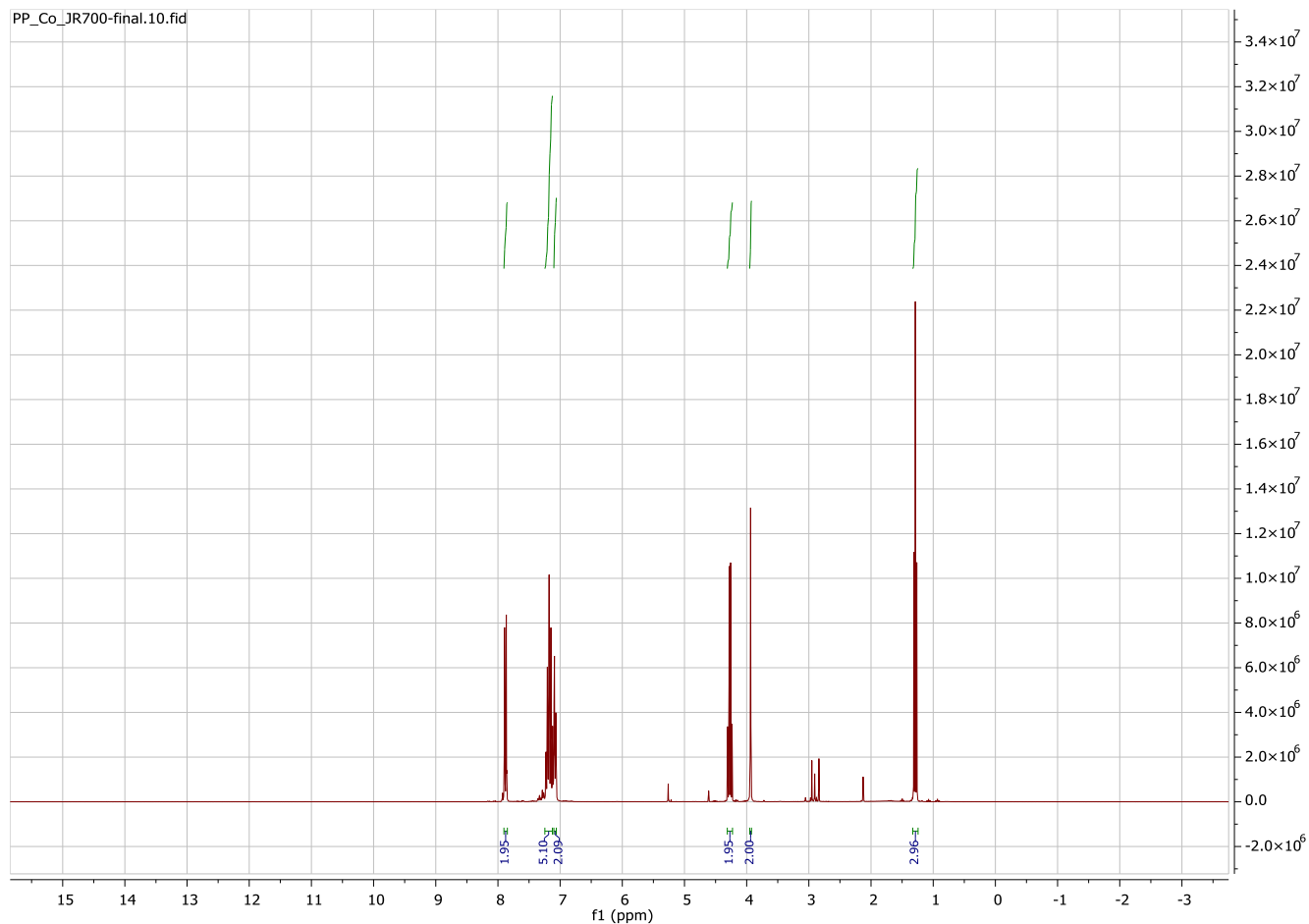
3b



3c

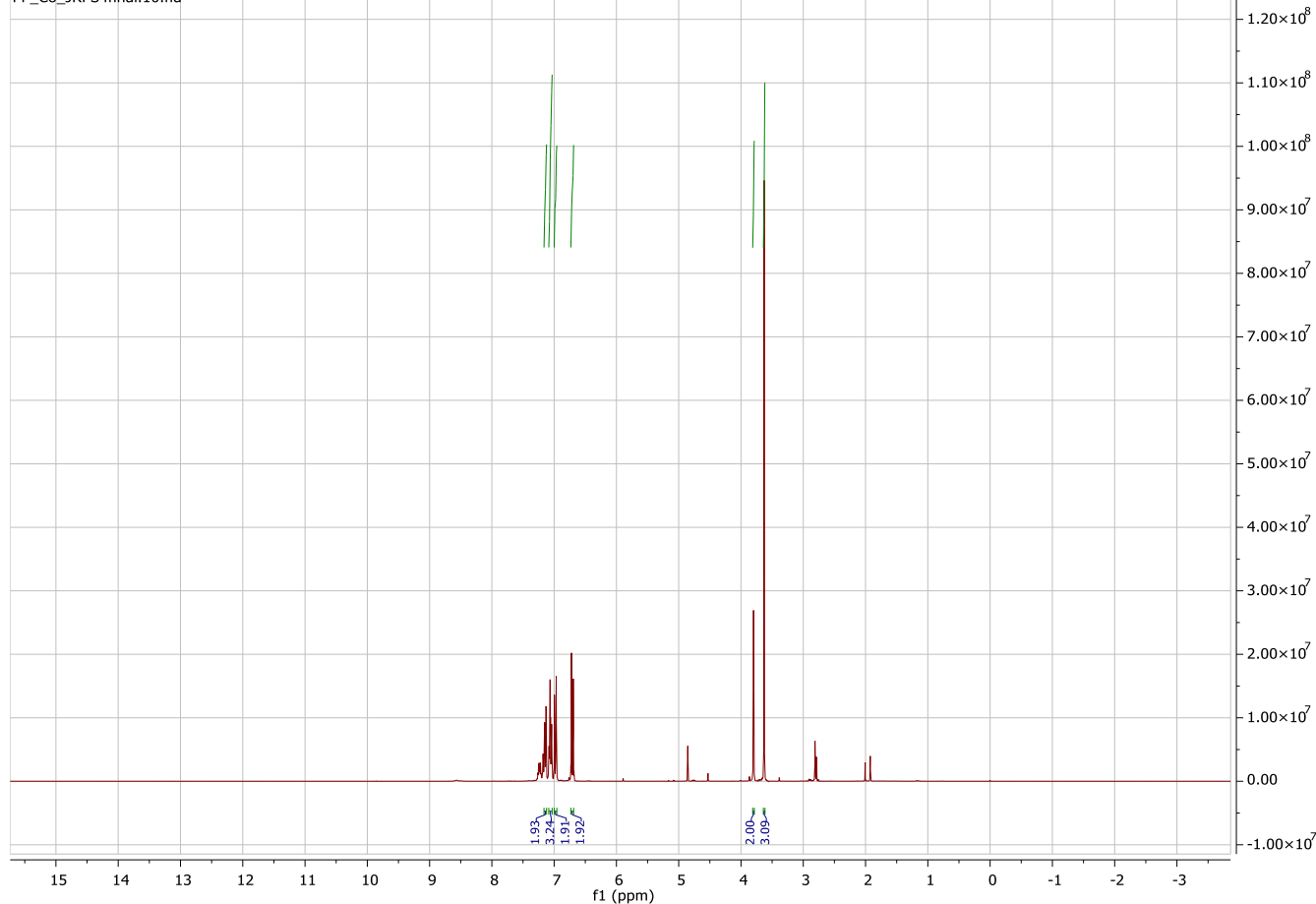


3d

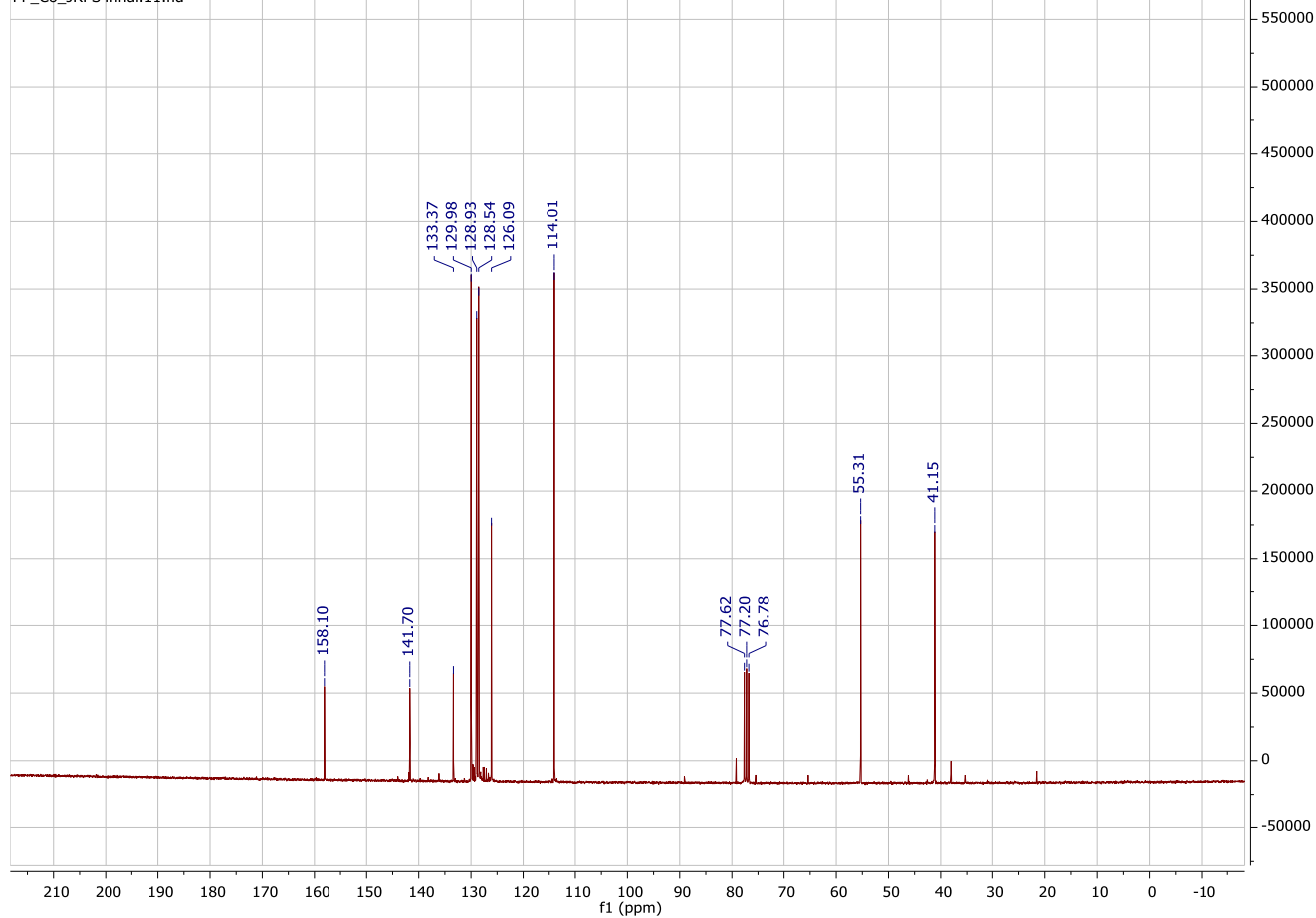


3e

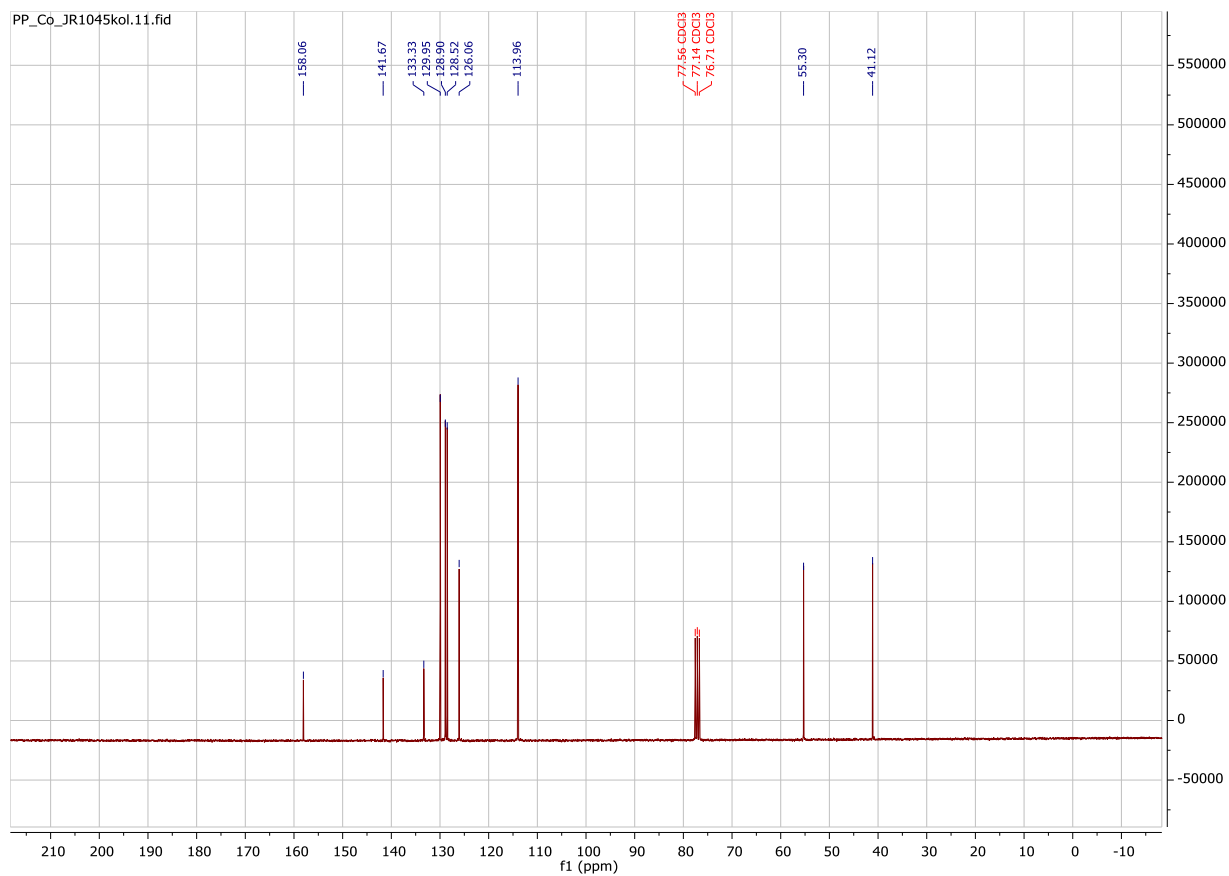
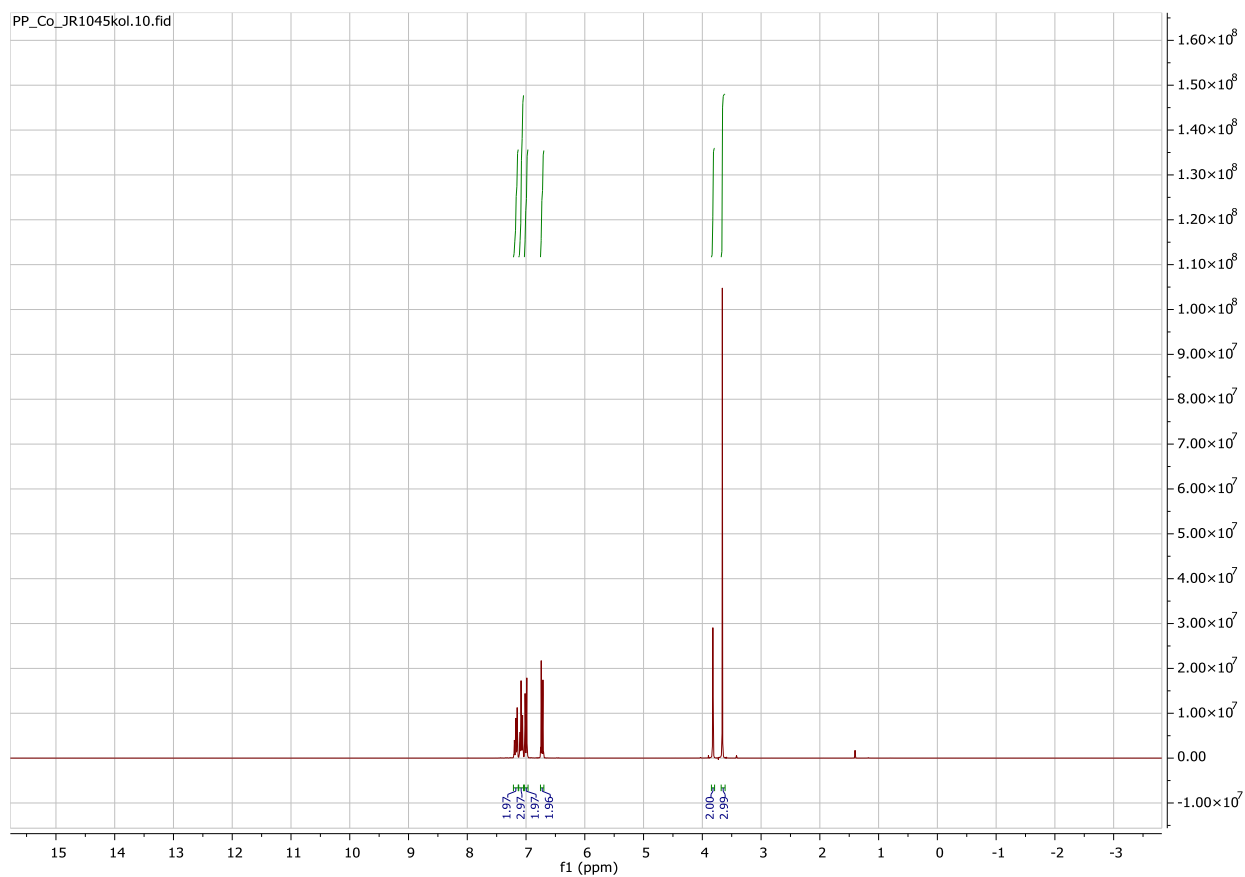
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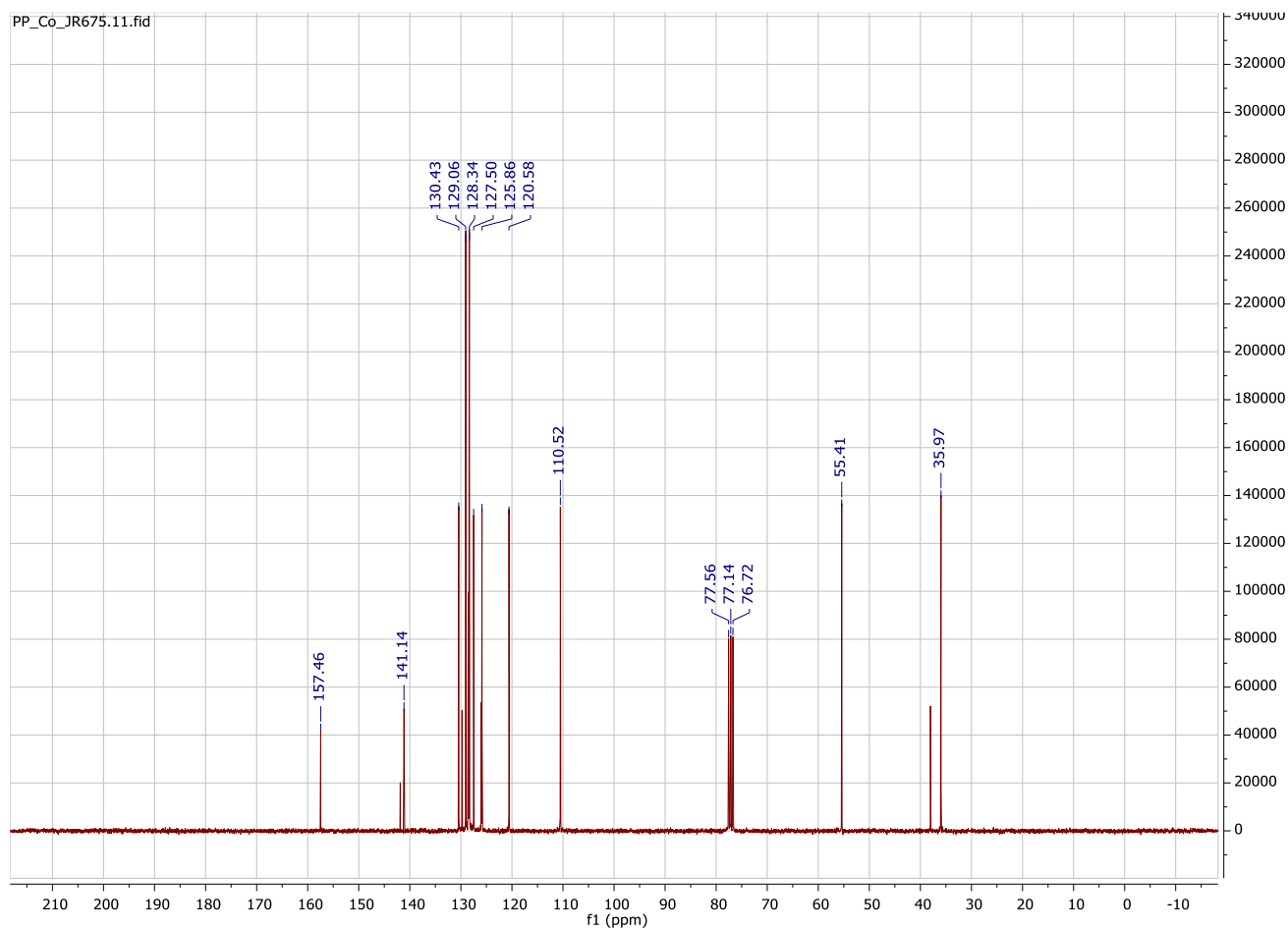
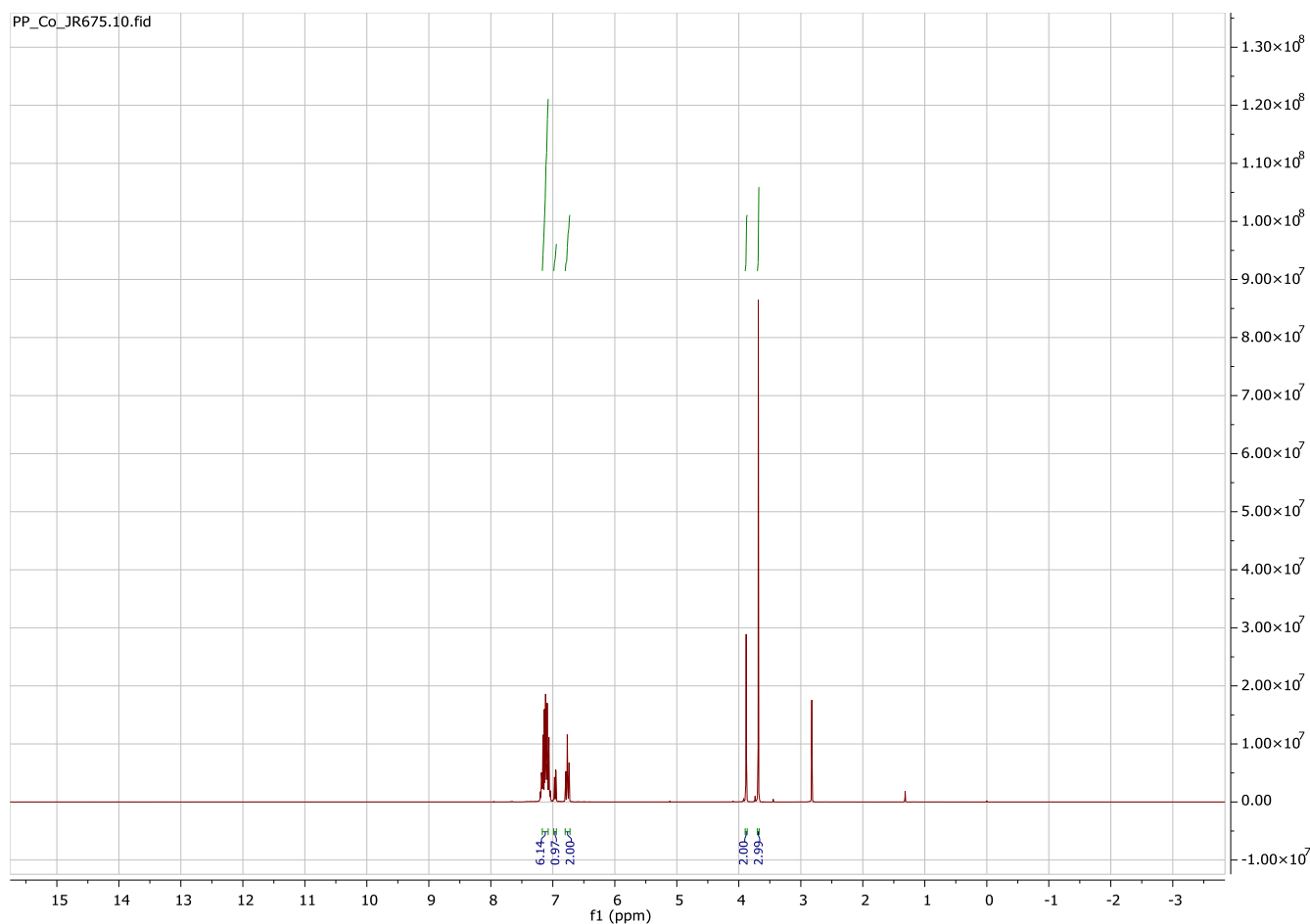
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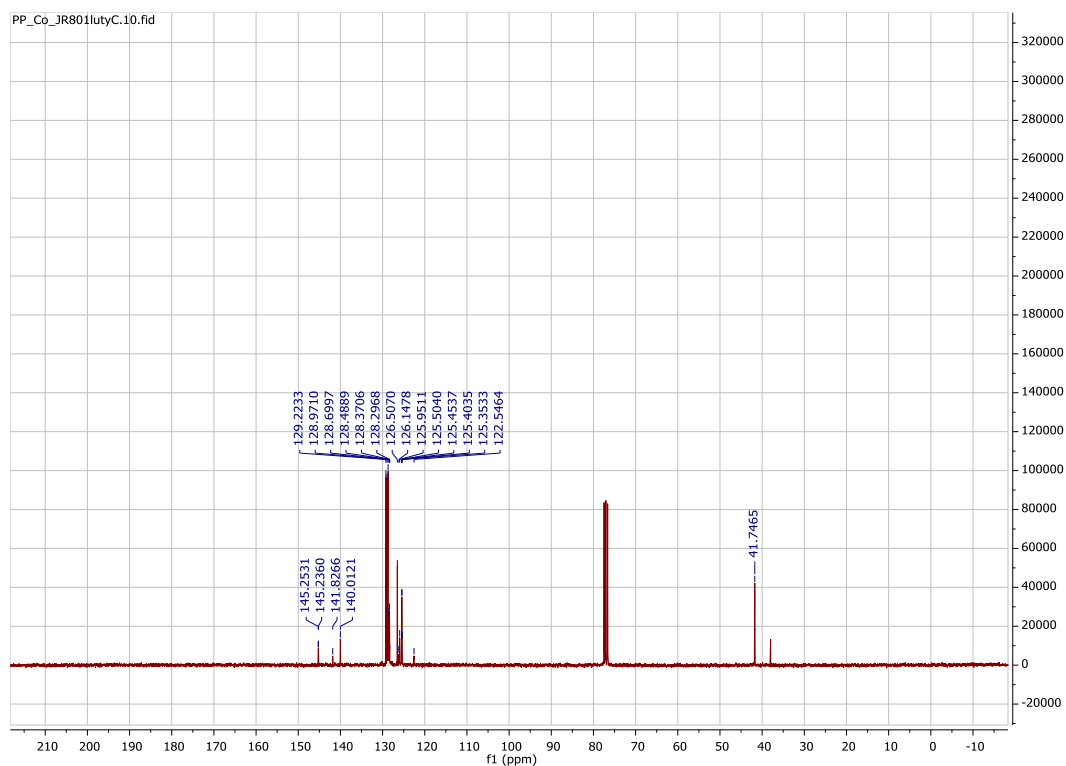
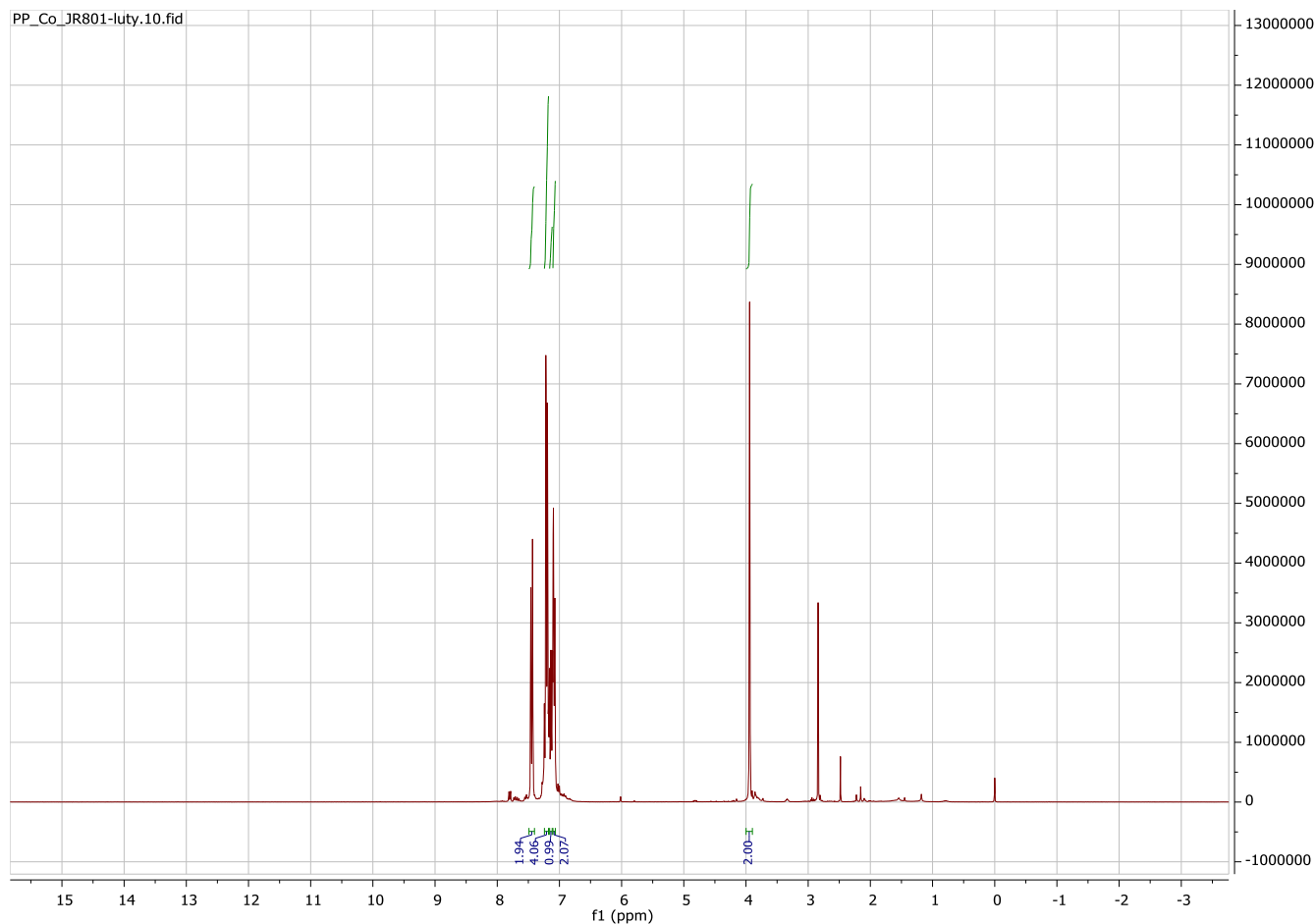
3e GRAM-SCALE

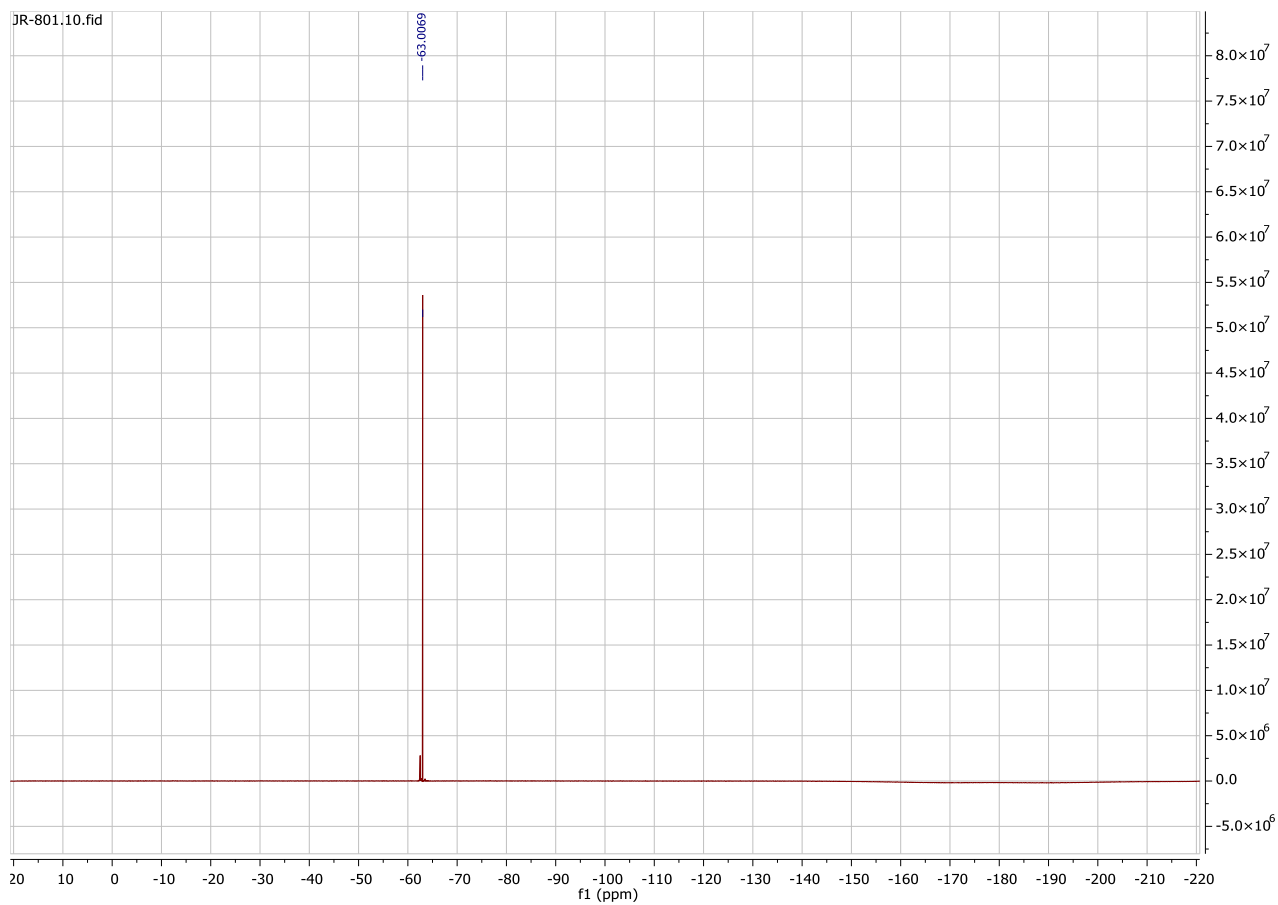


3f

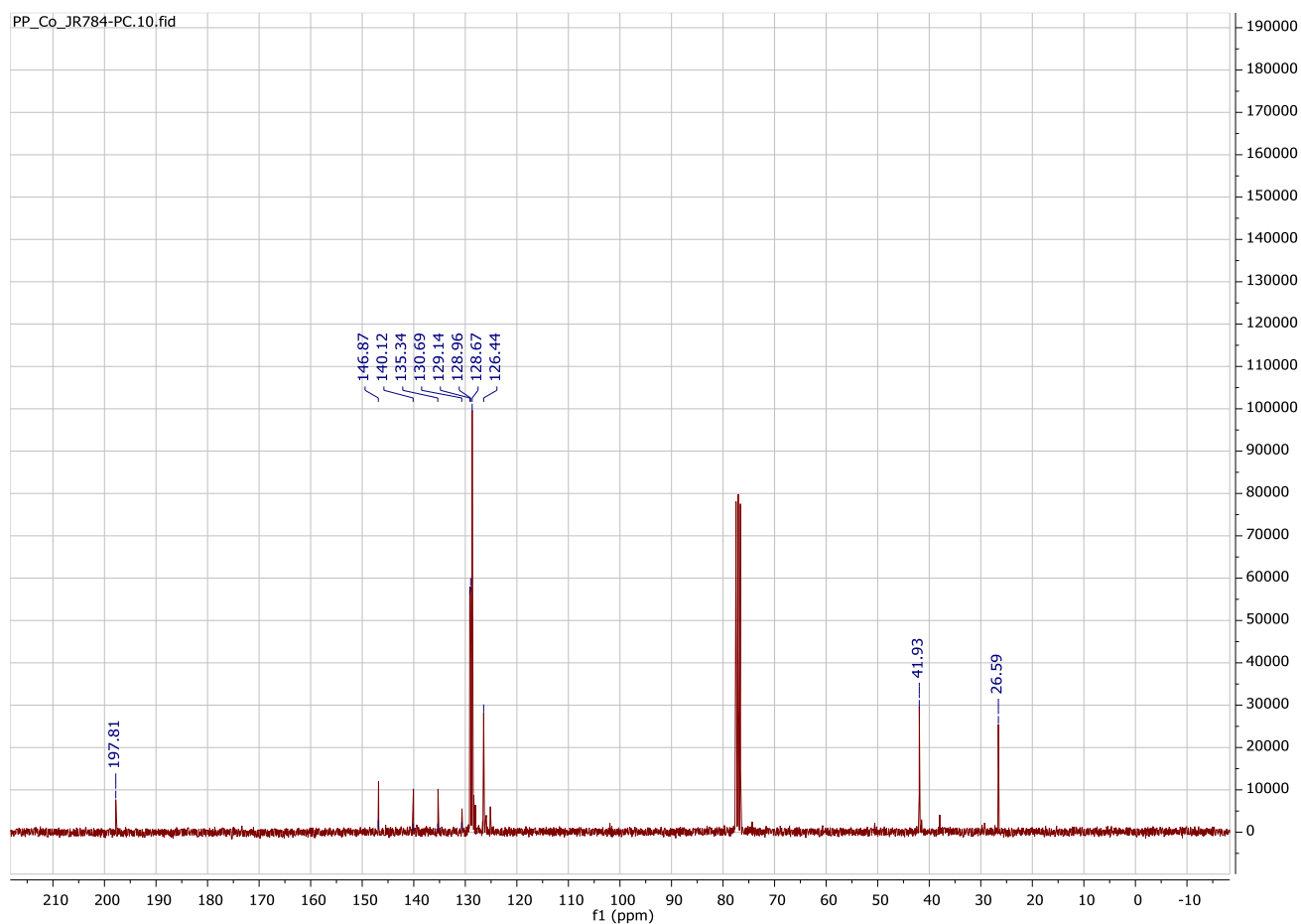
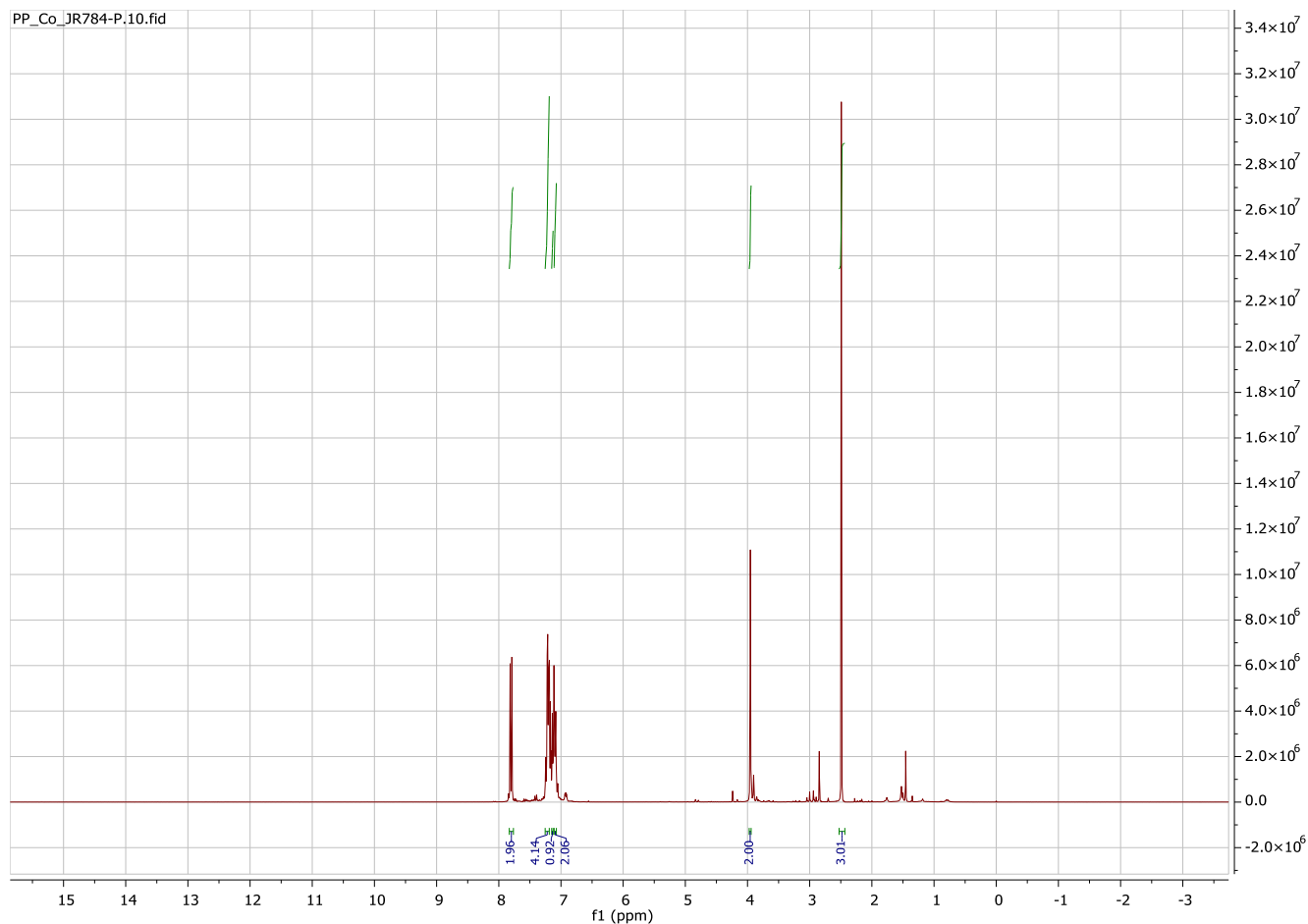


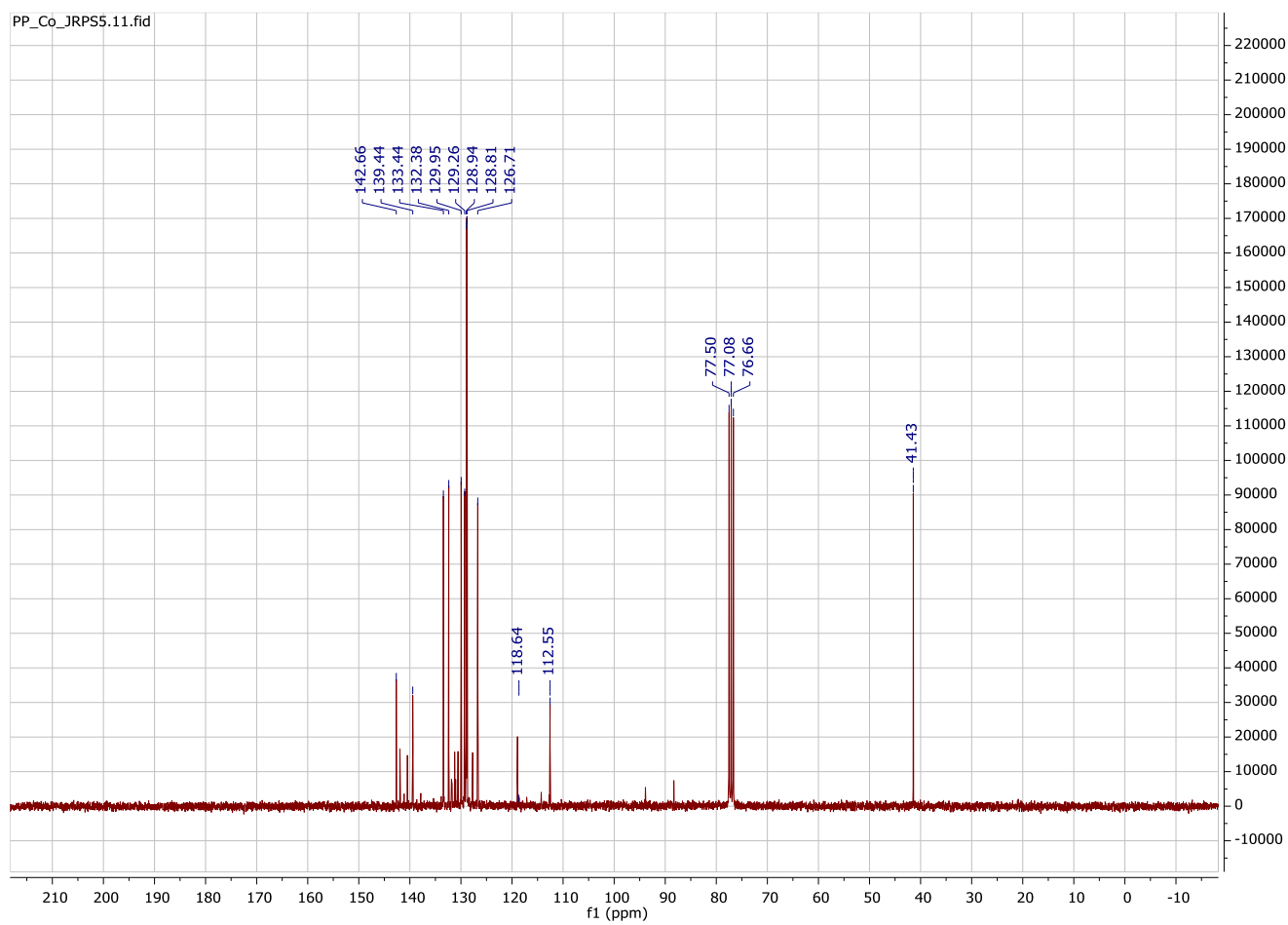
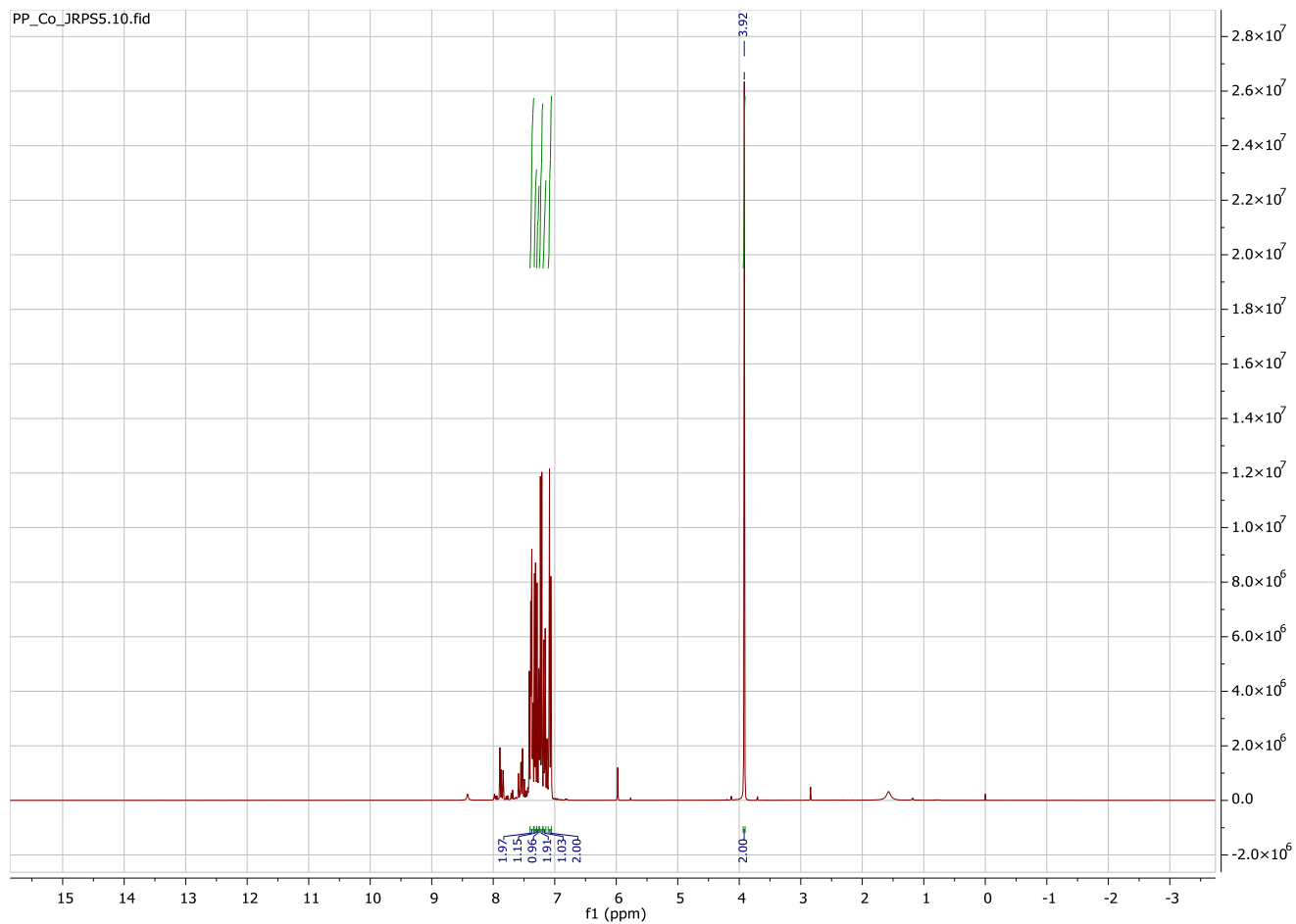
3g



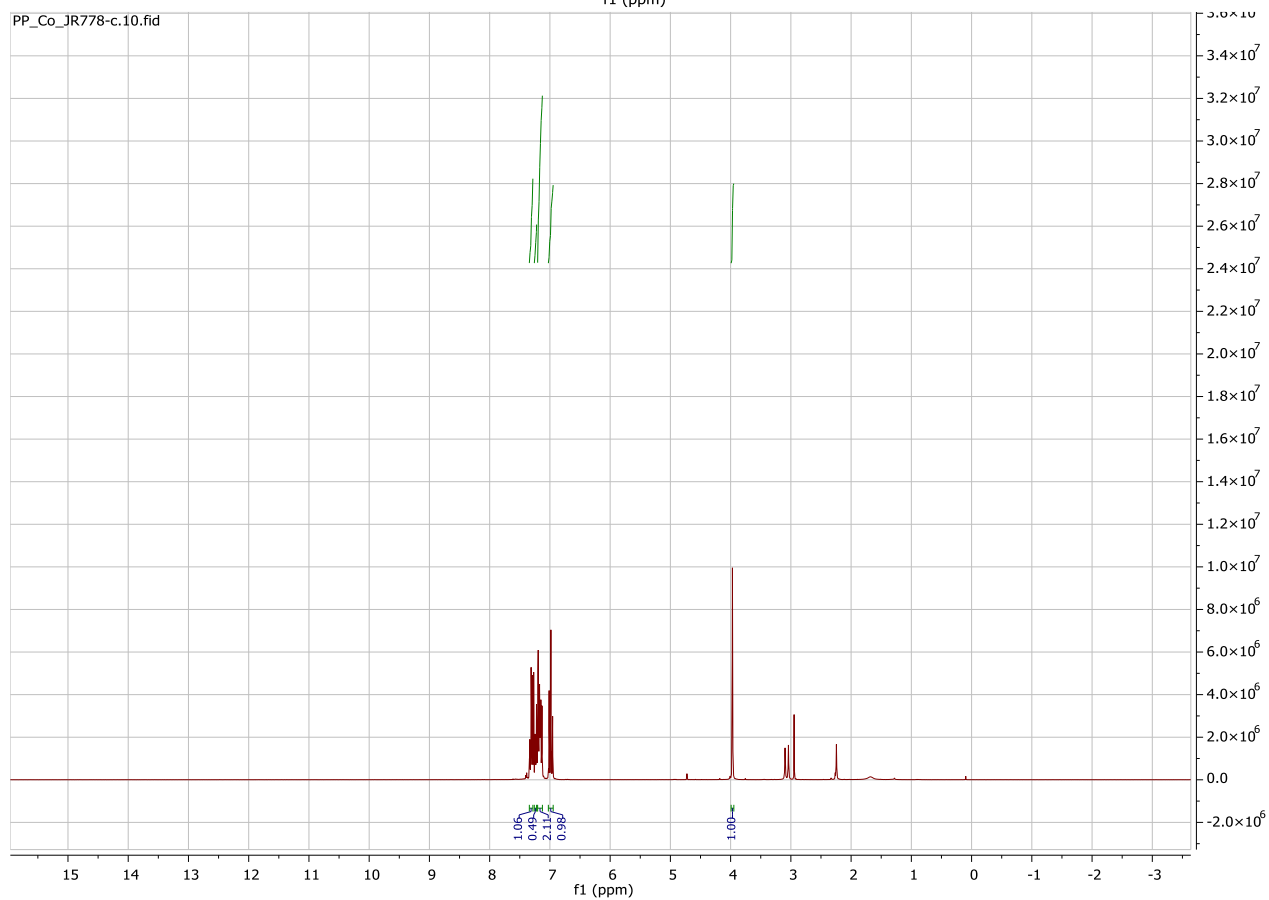
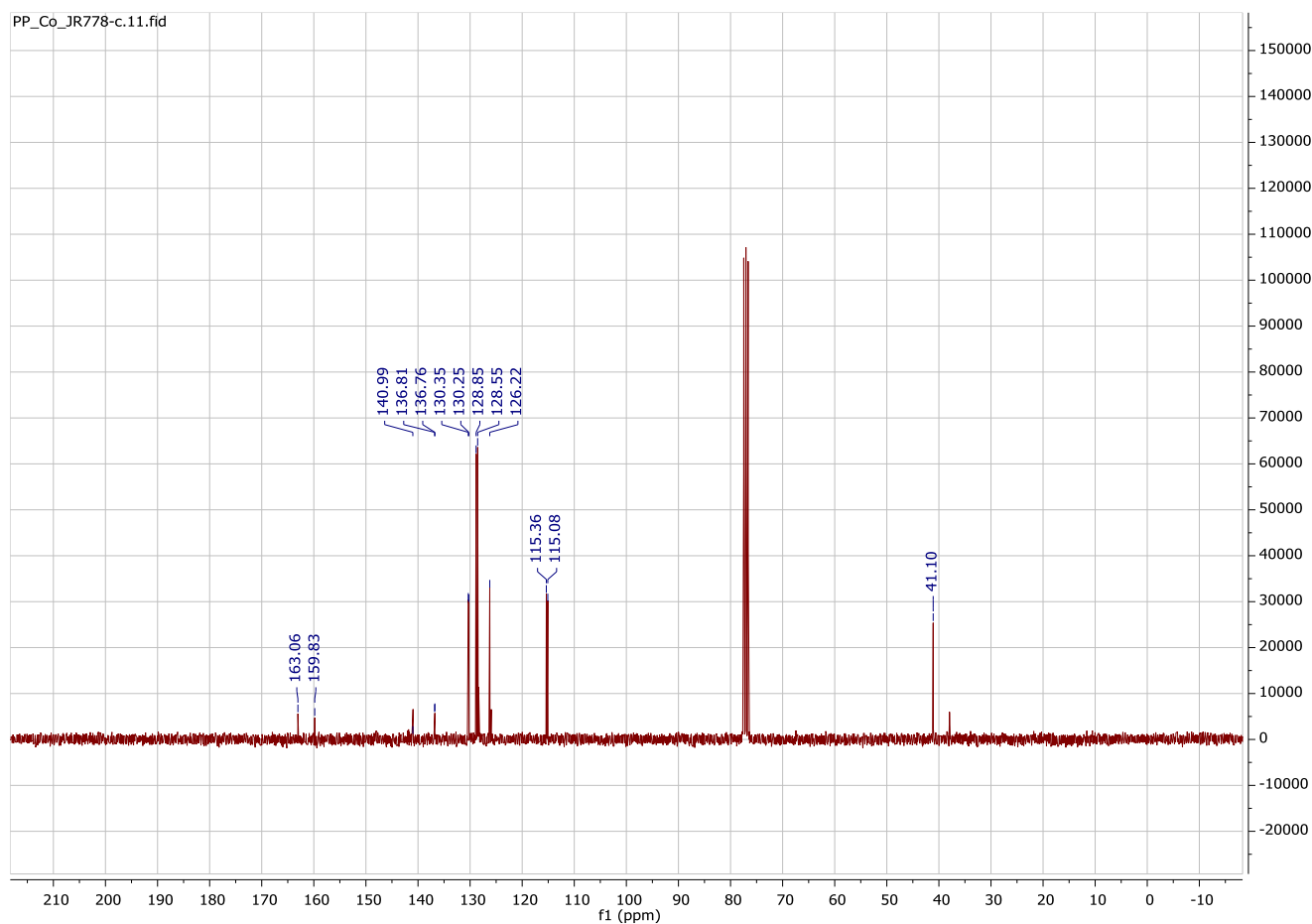


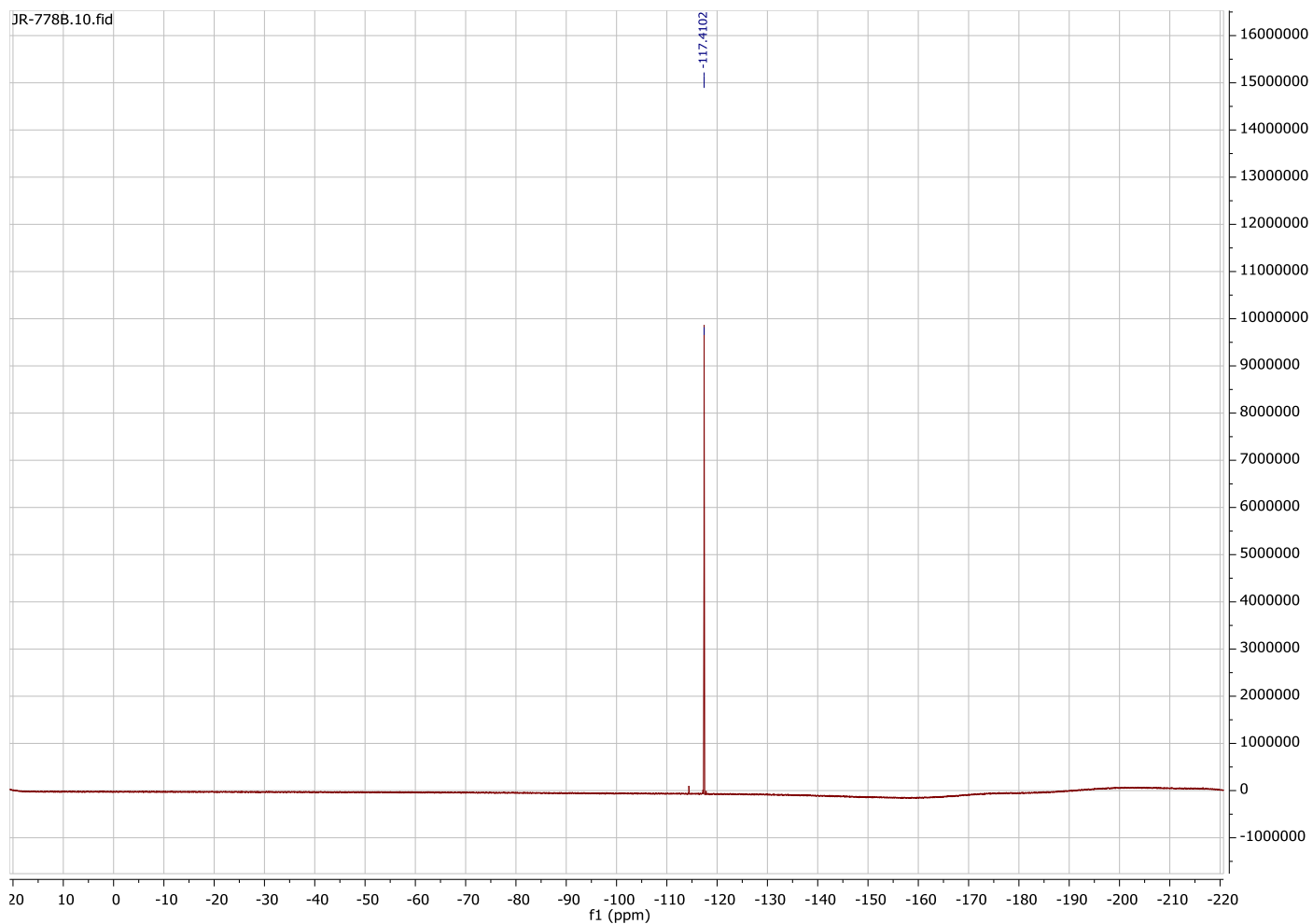
3h



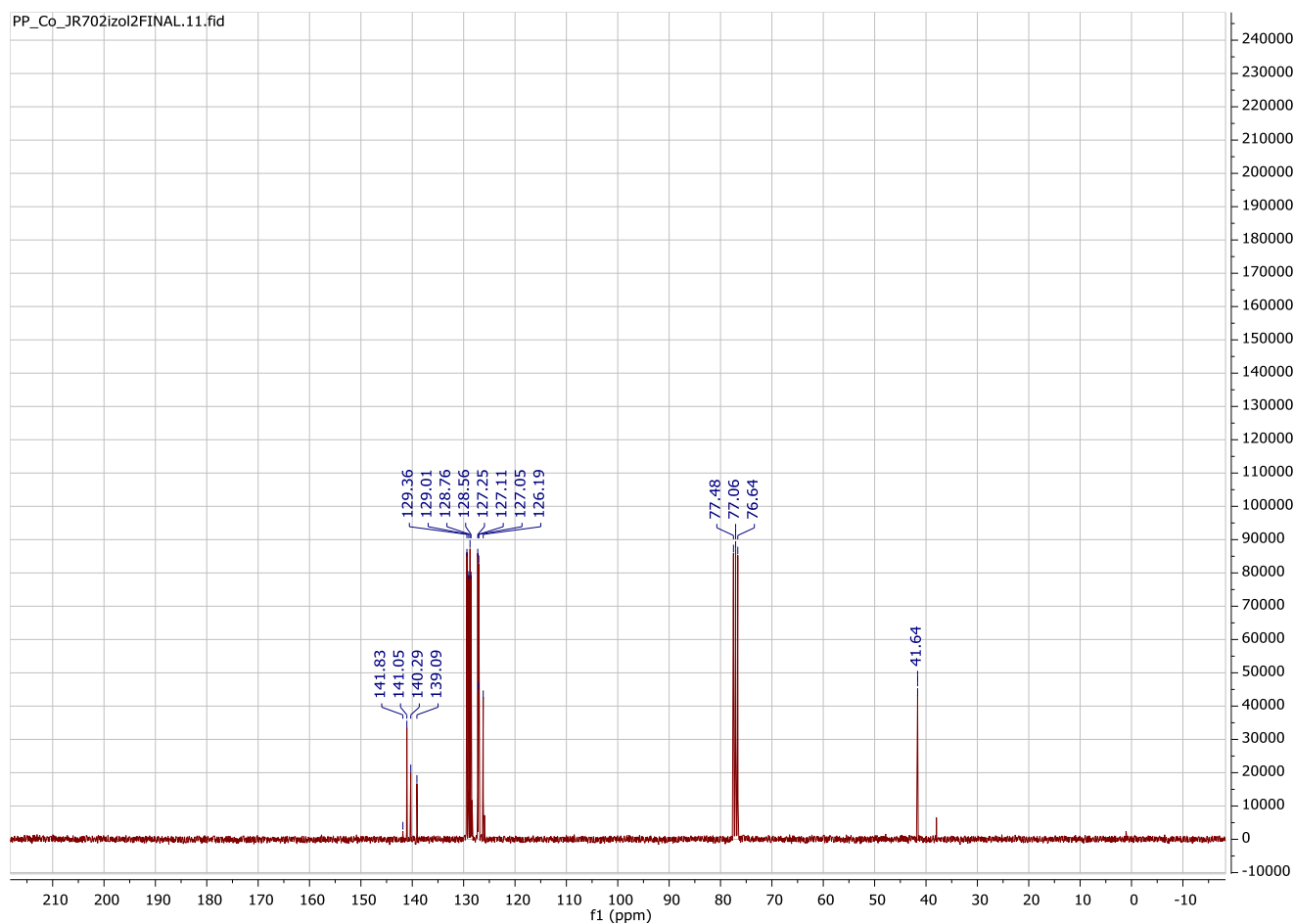
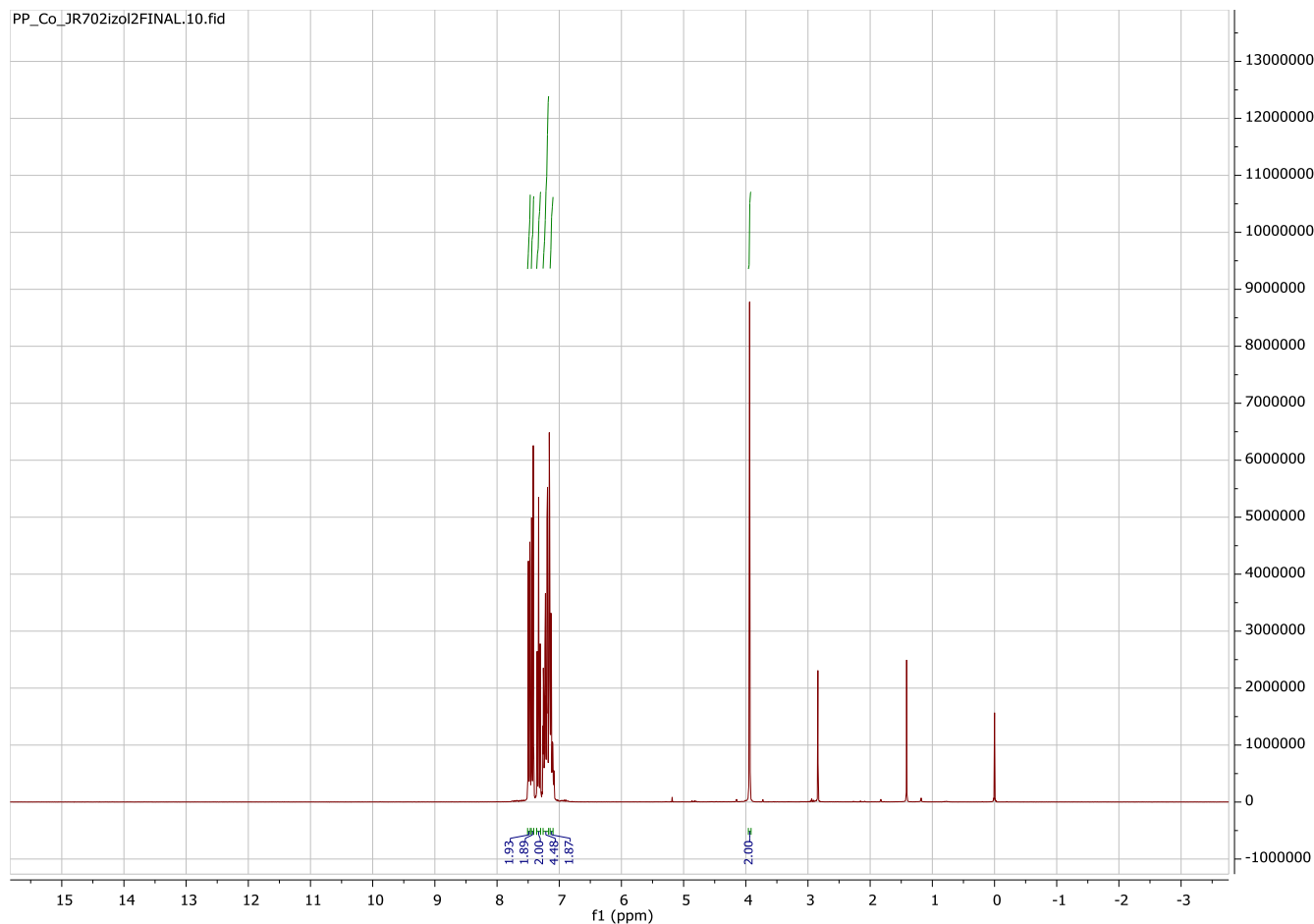


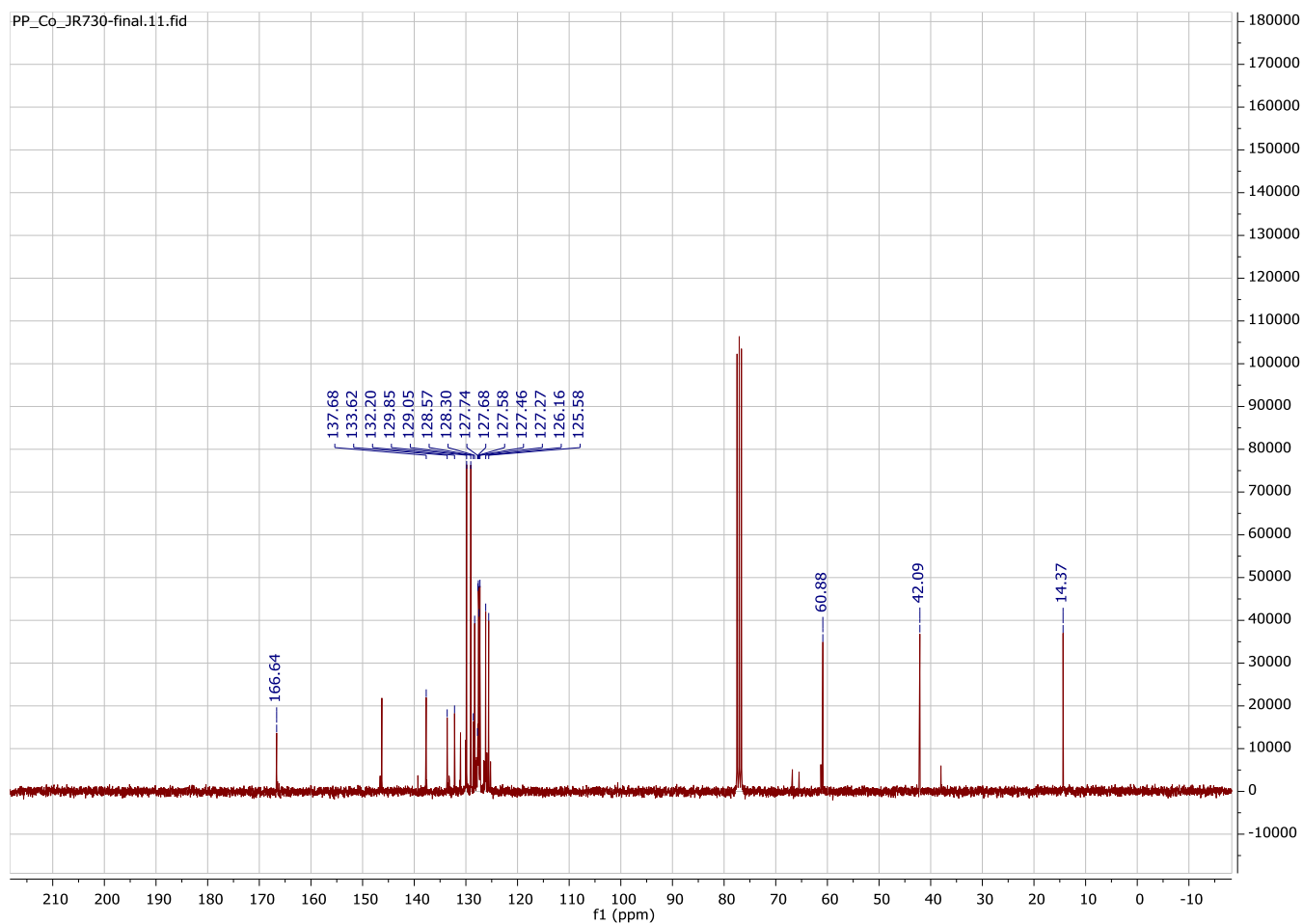
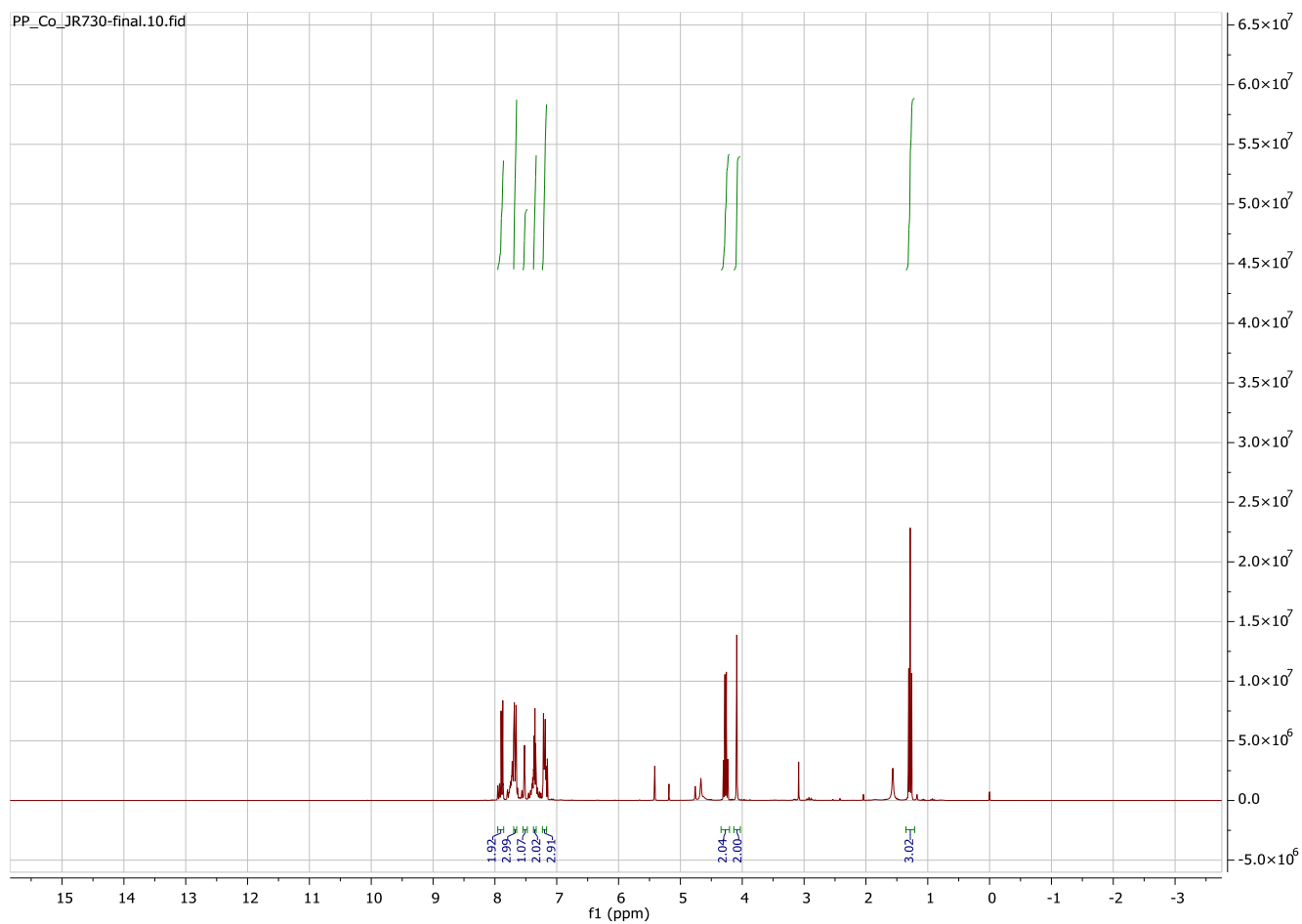
3j



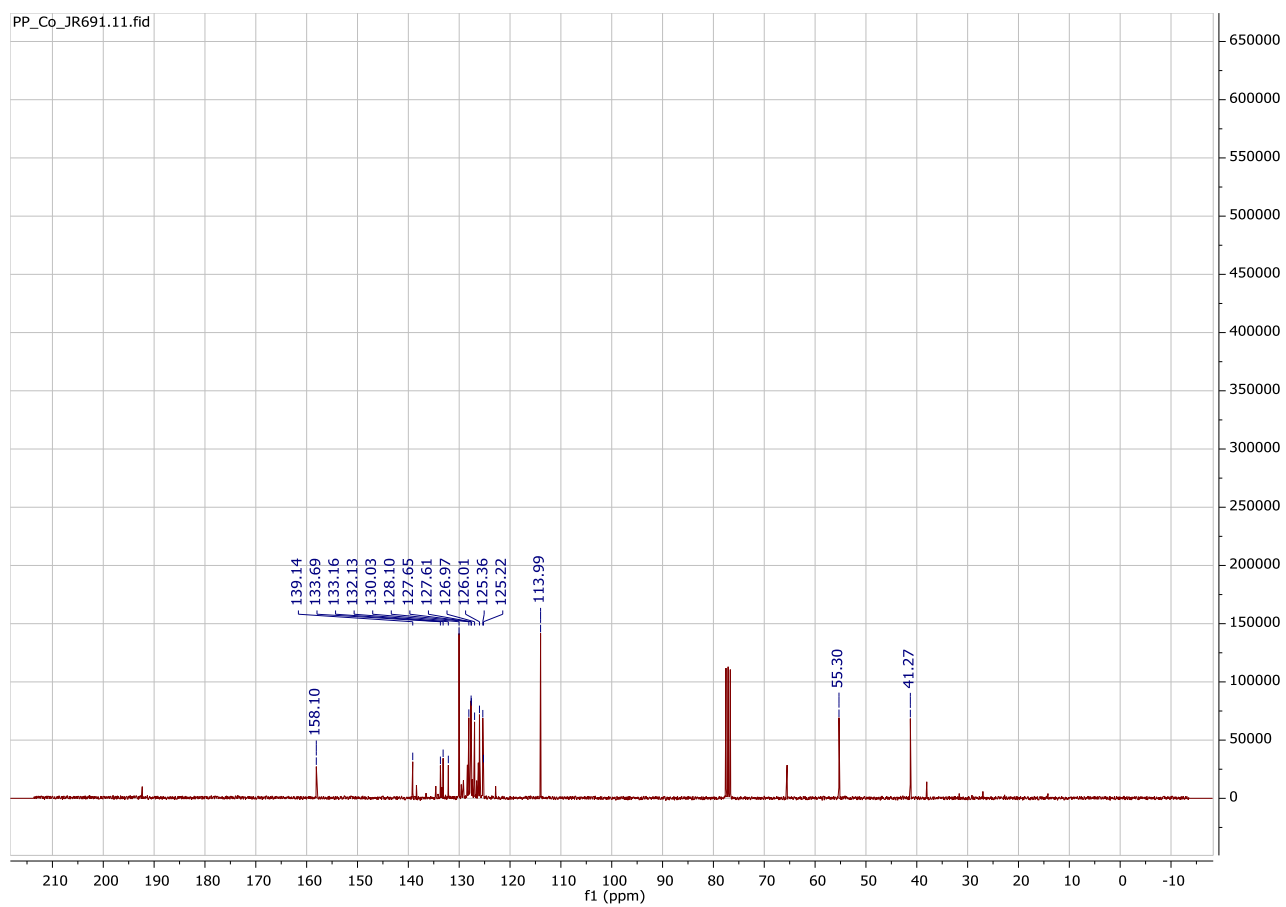
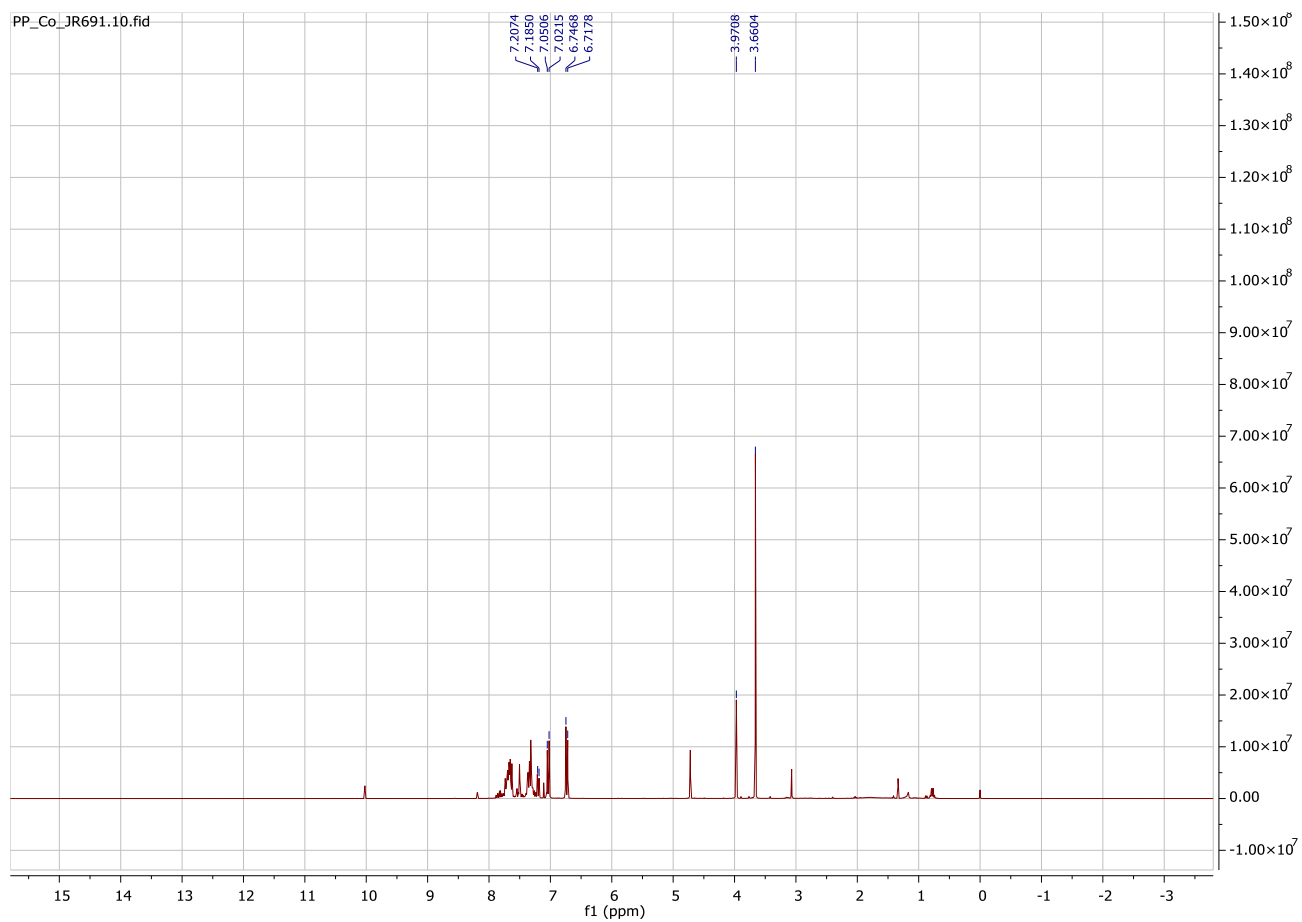


3k

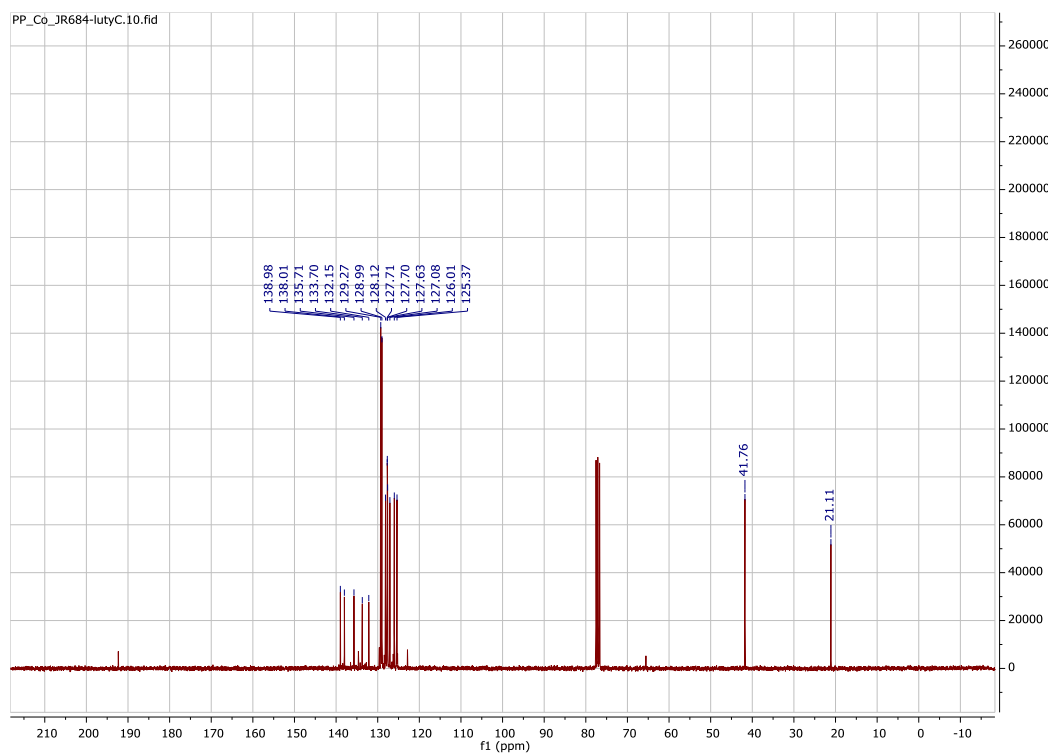
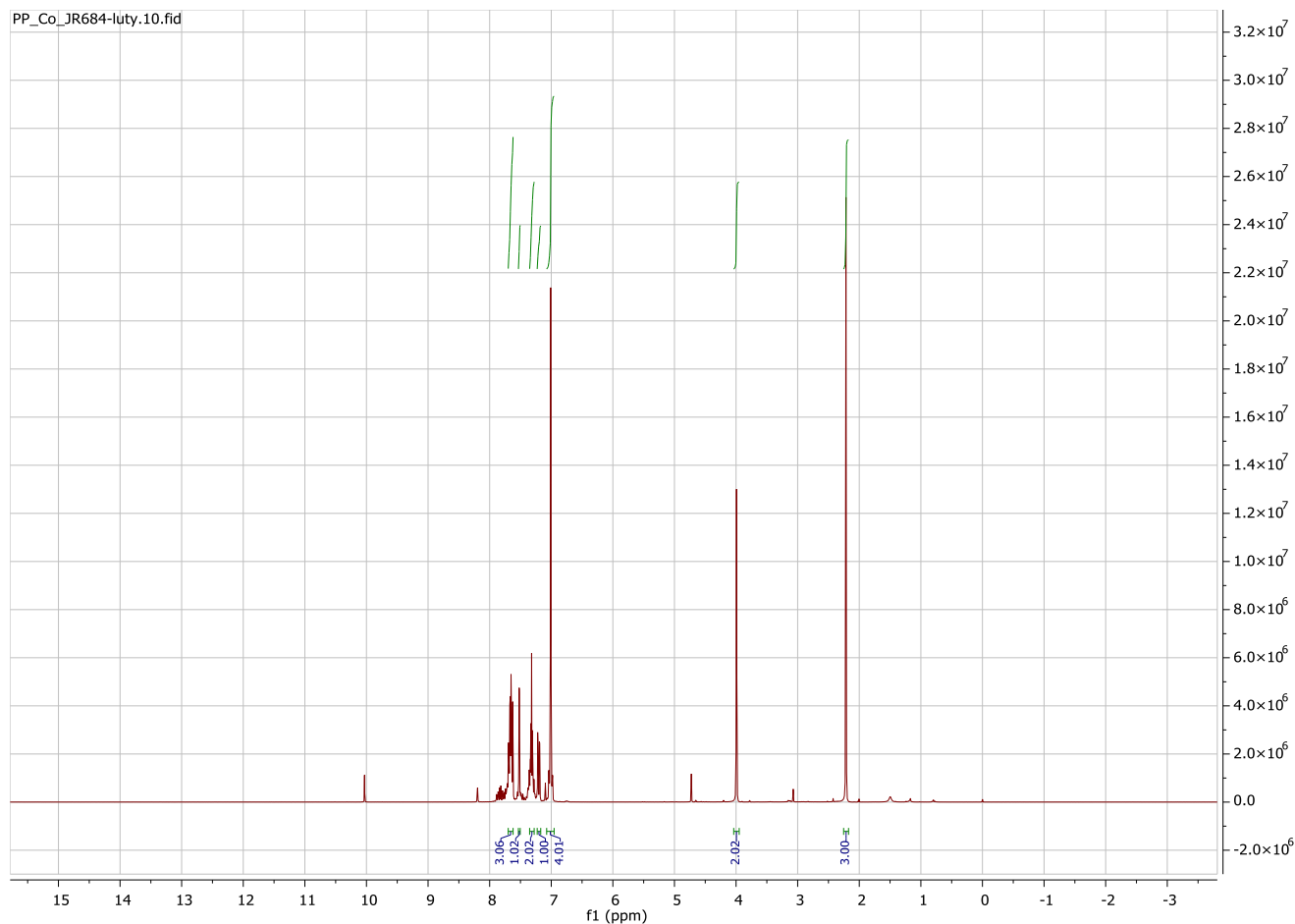


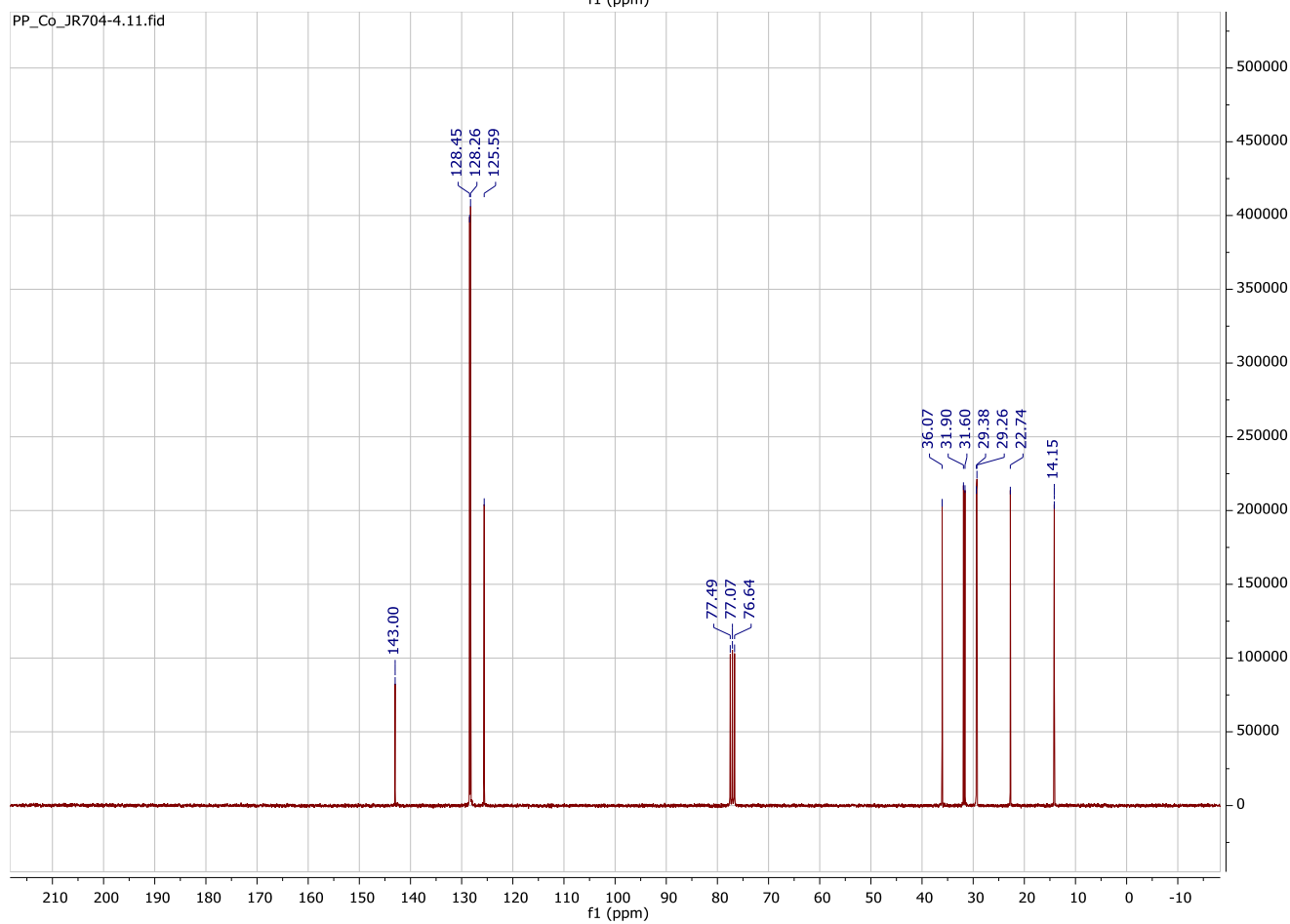
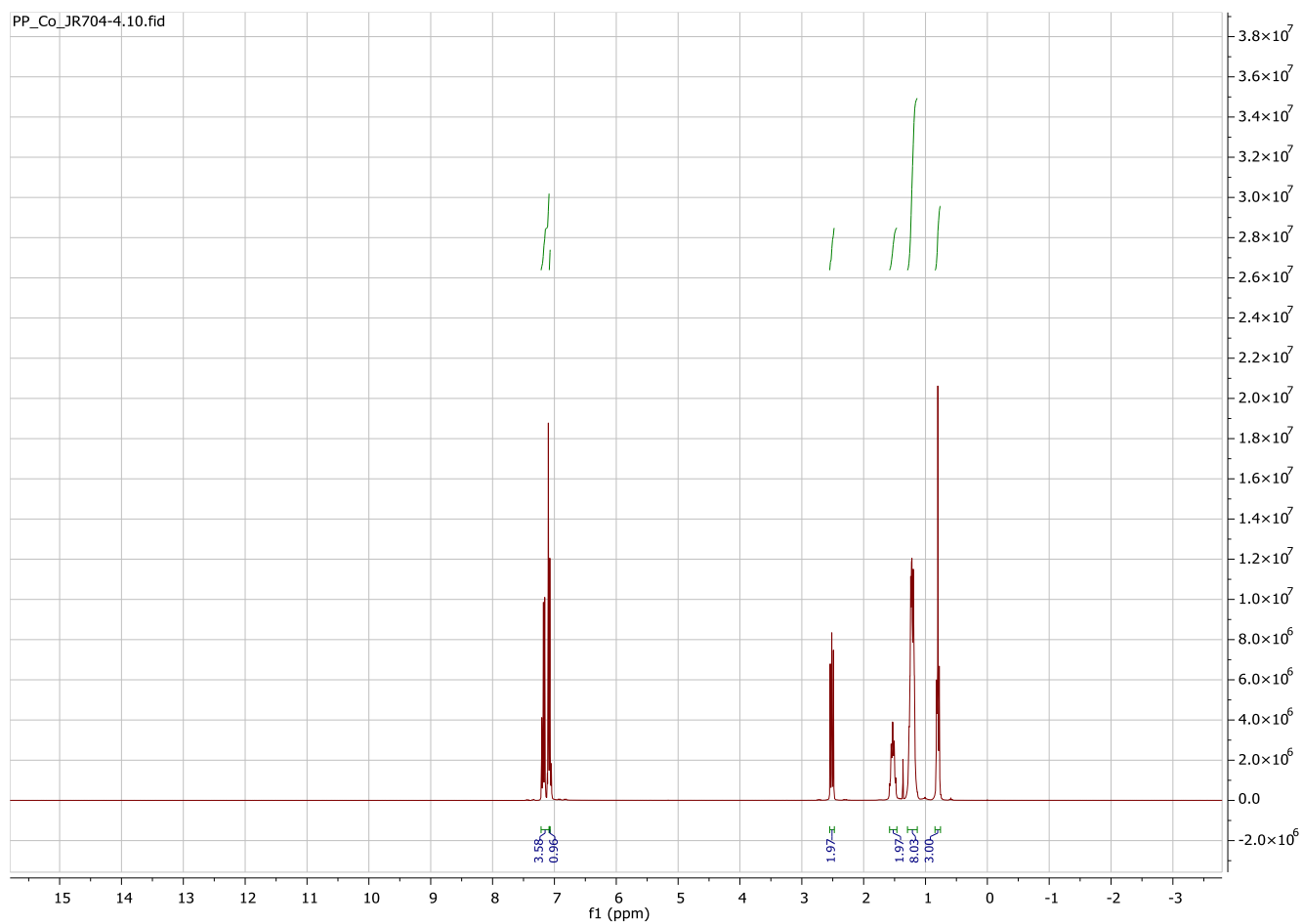


3m

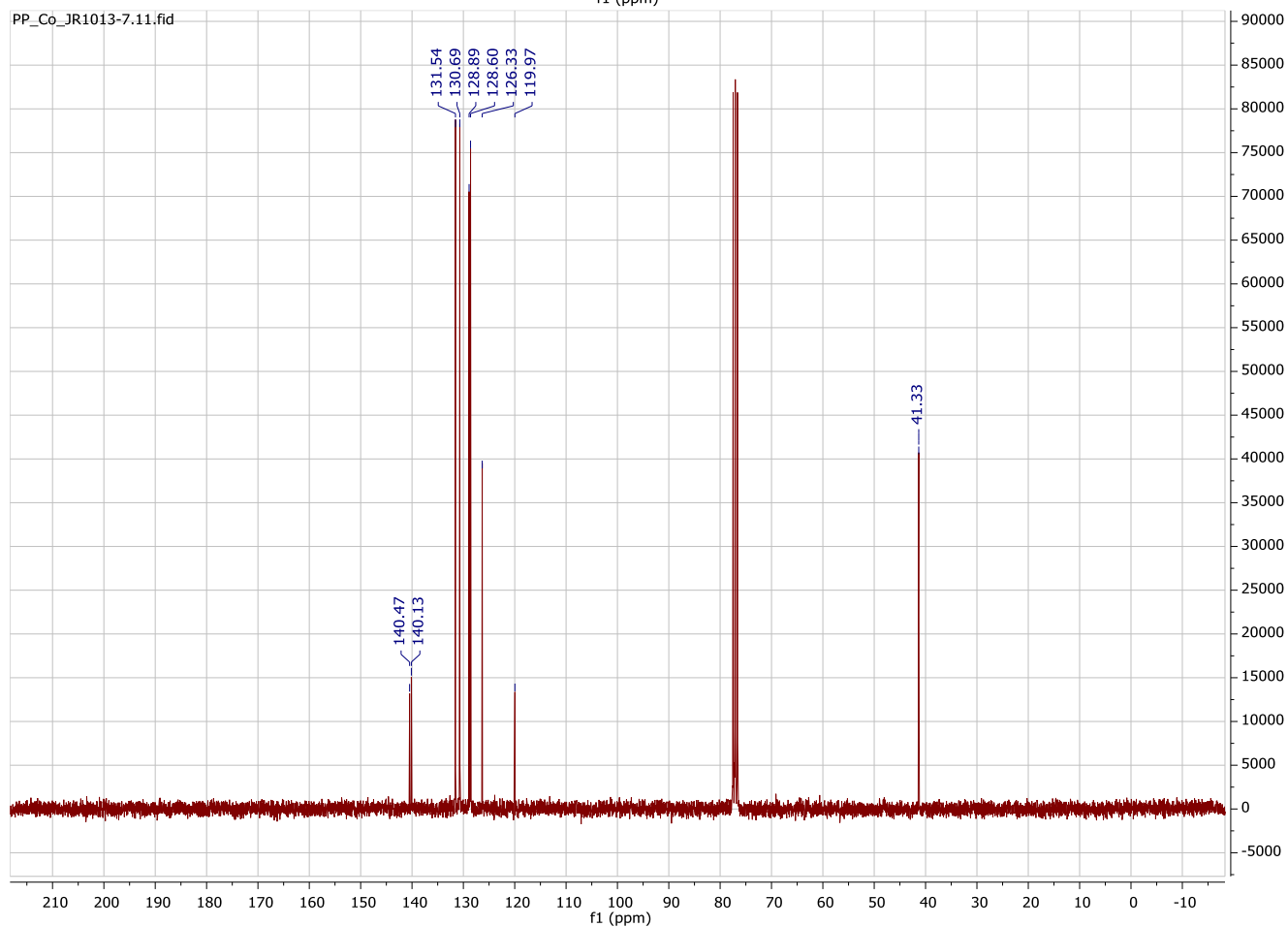
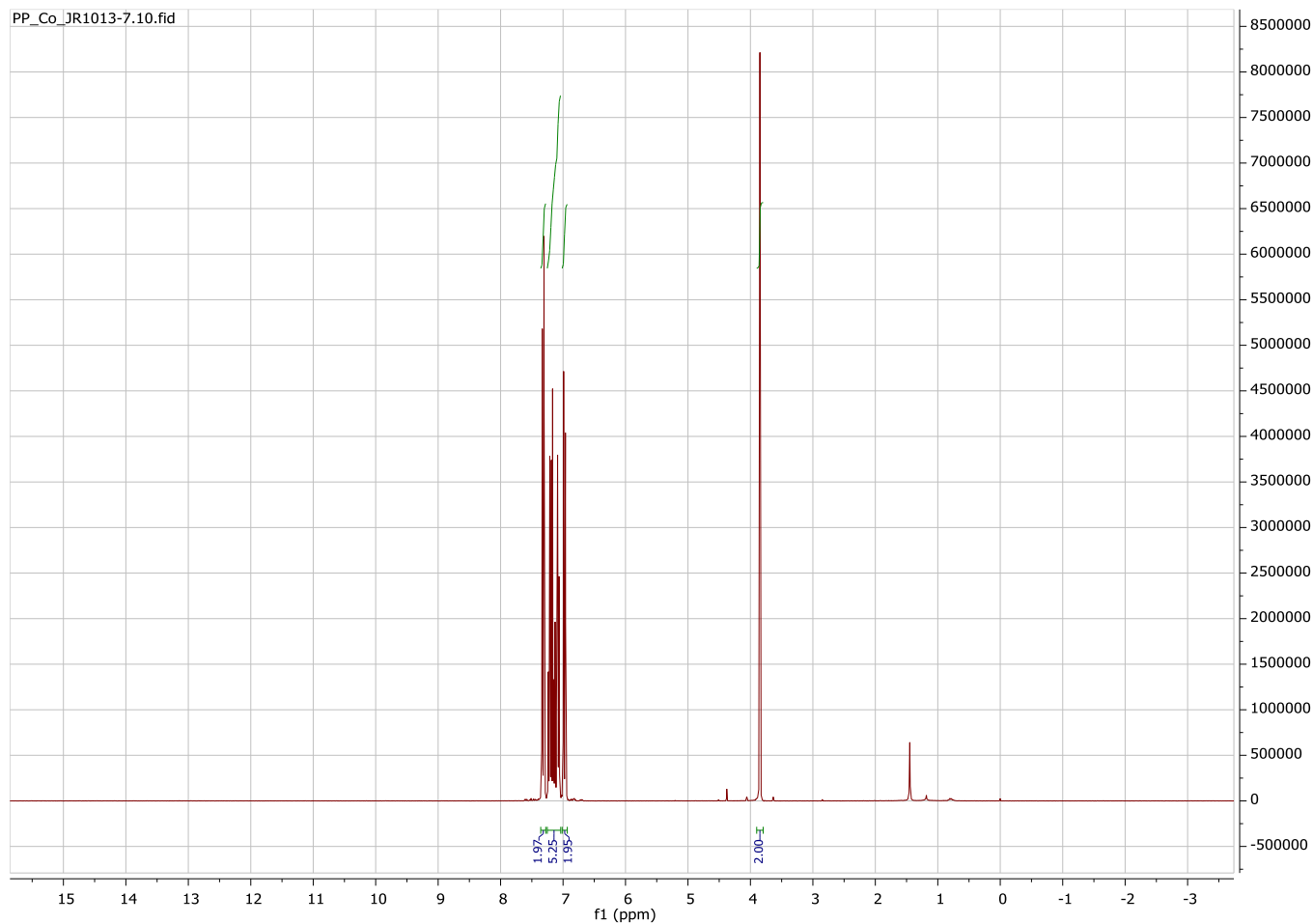


3n

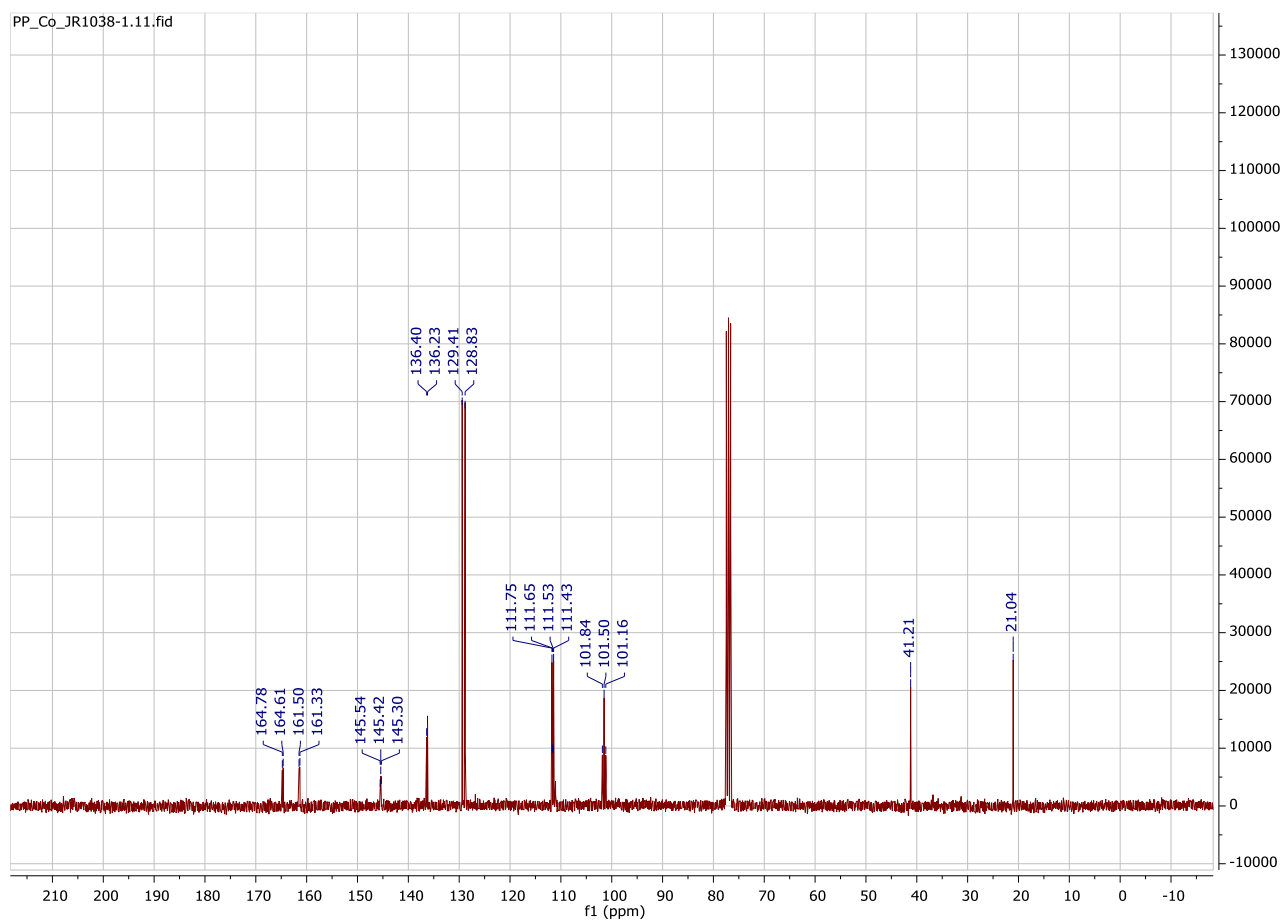
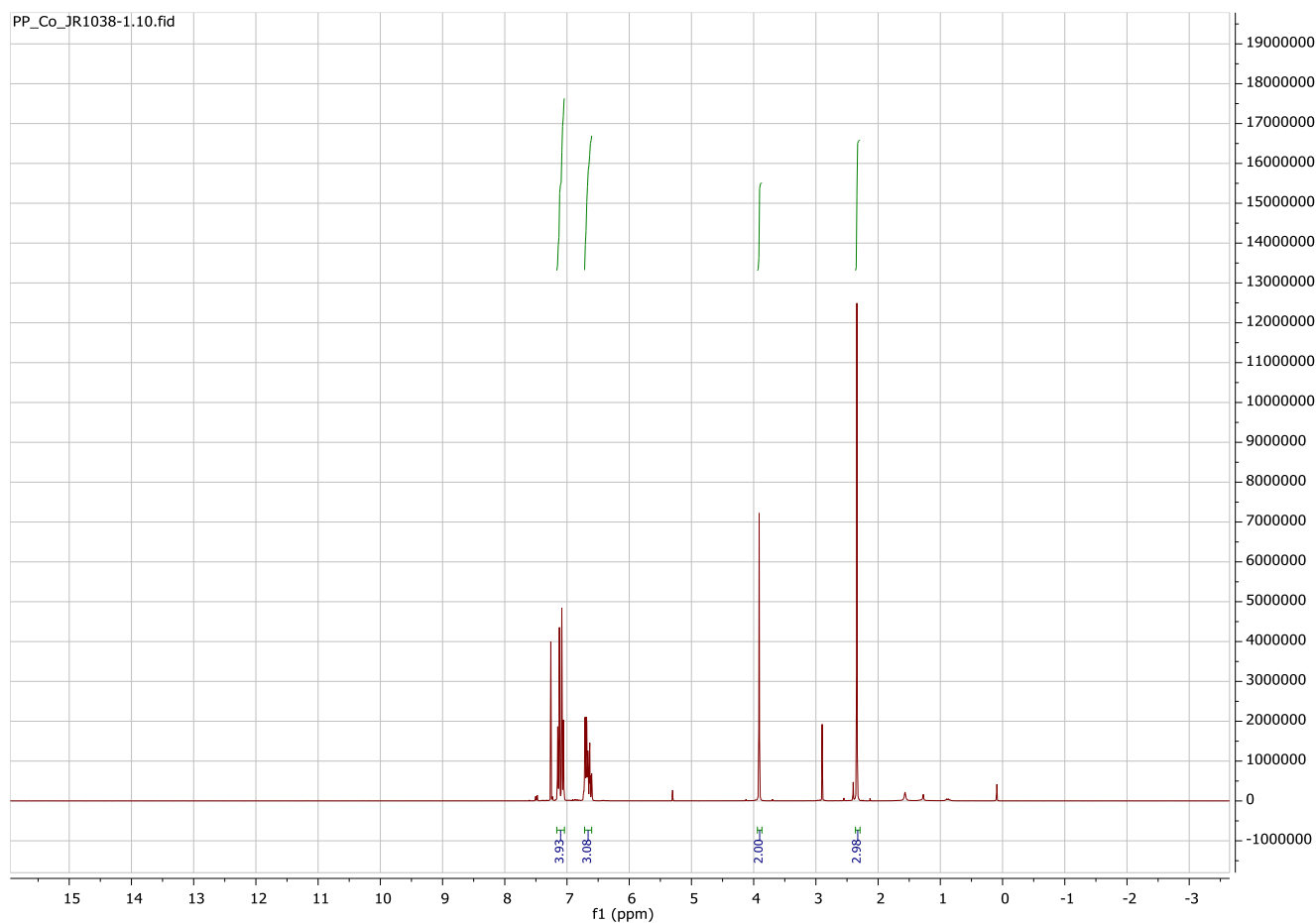


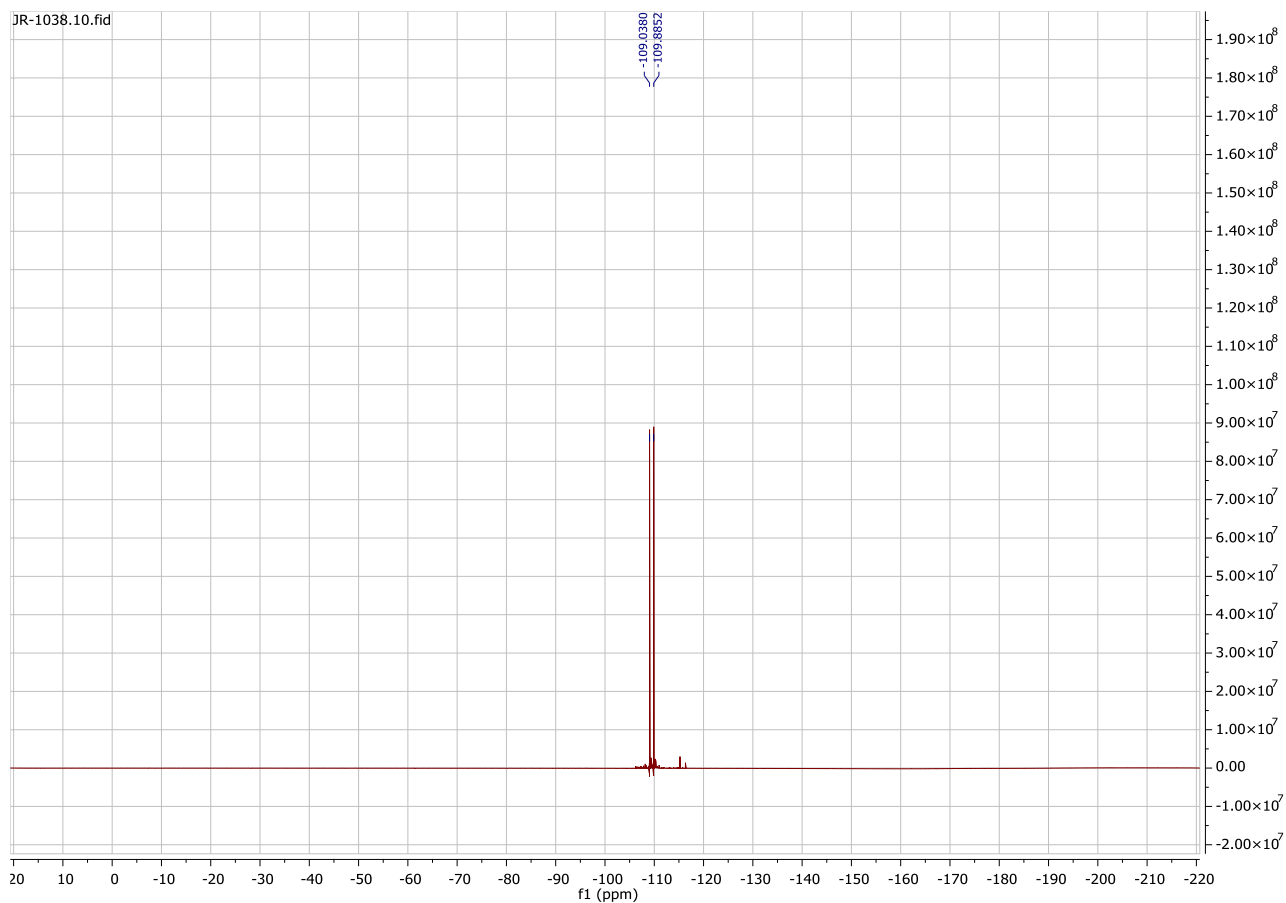


3q

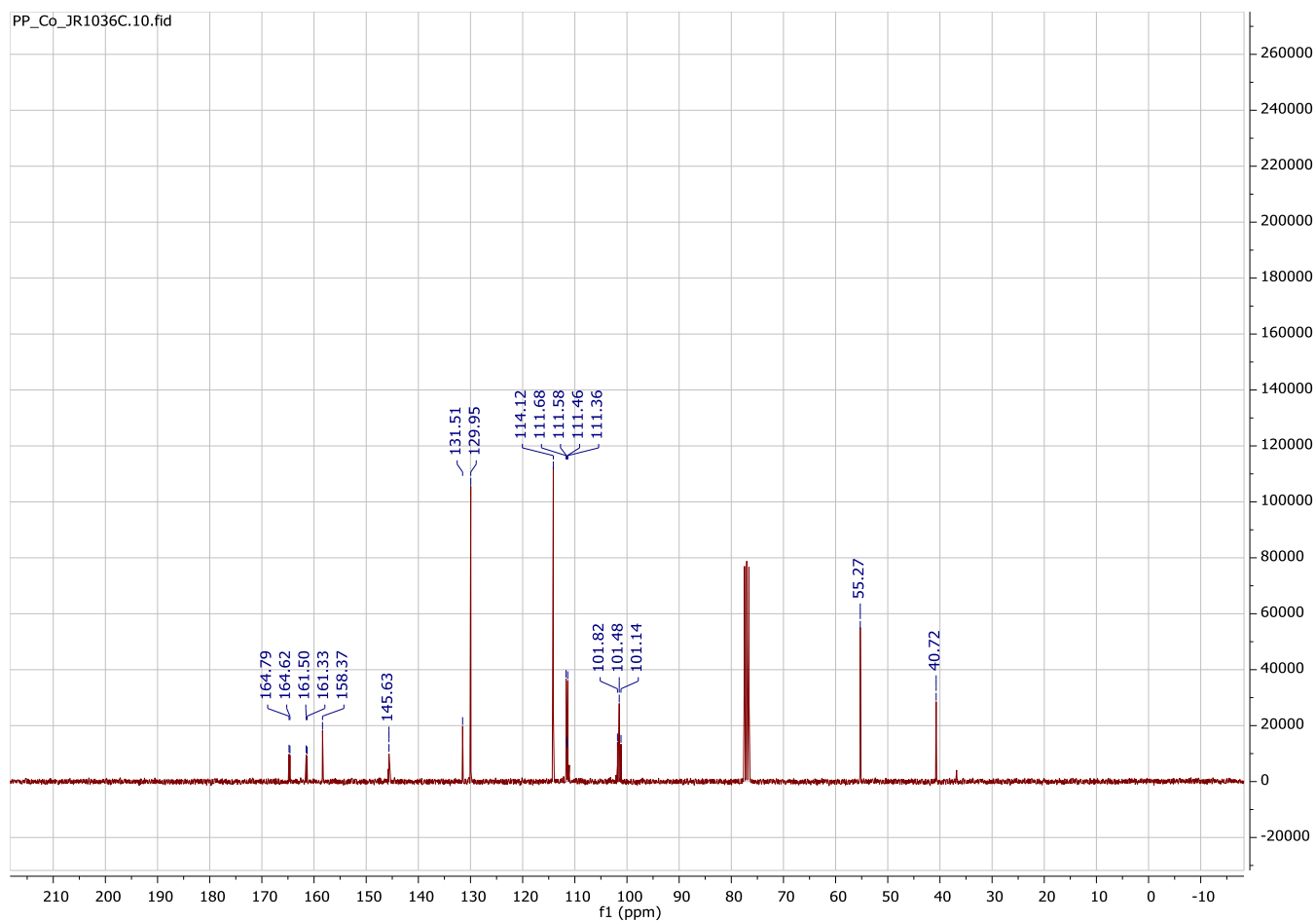
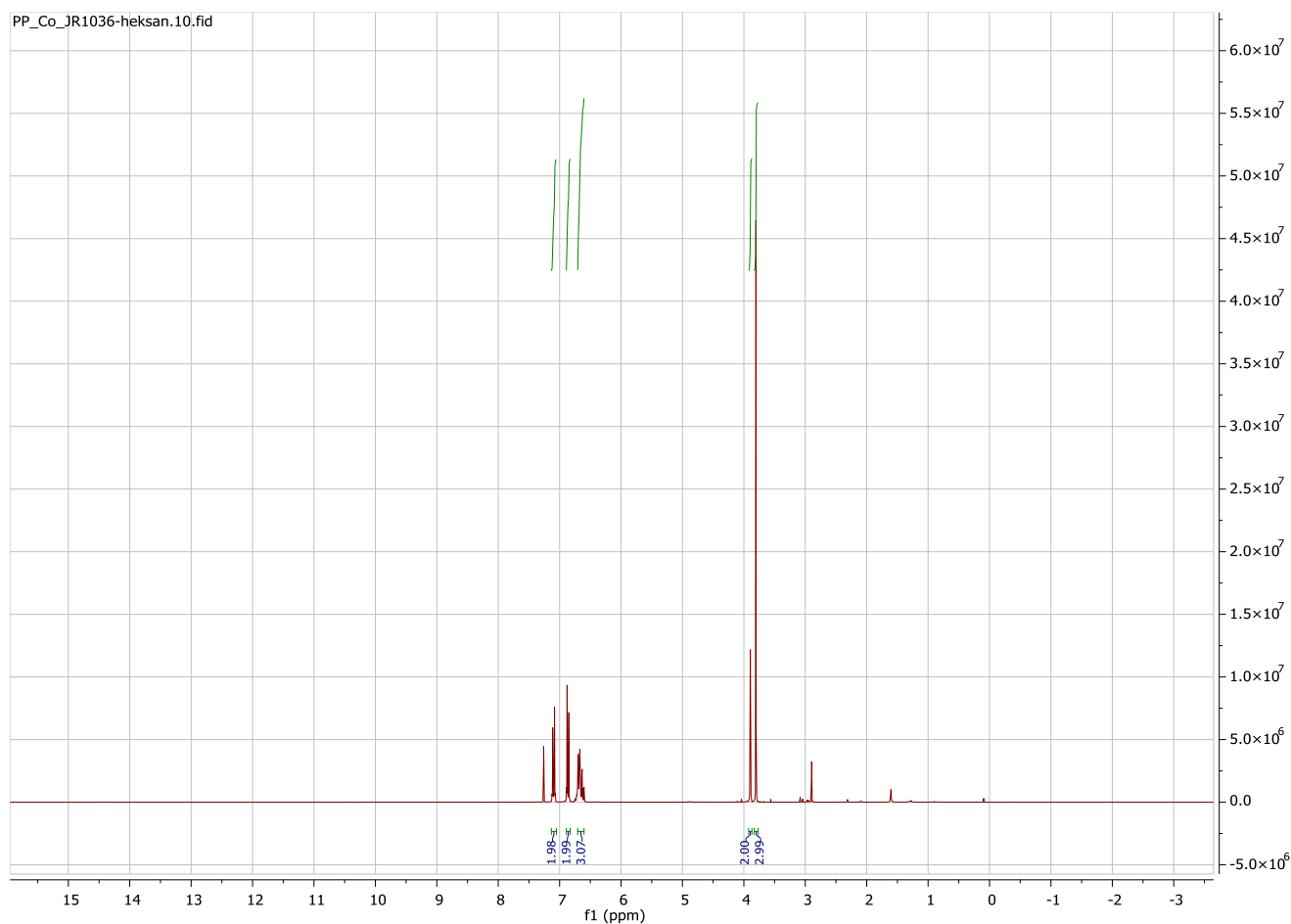


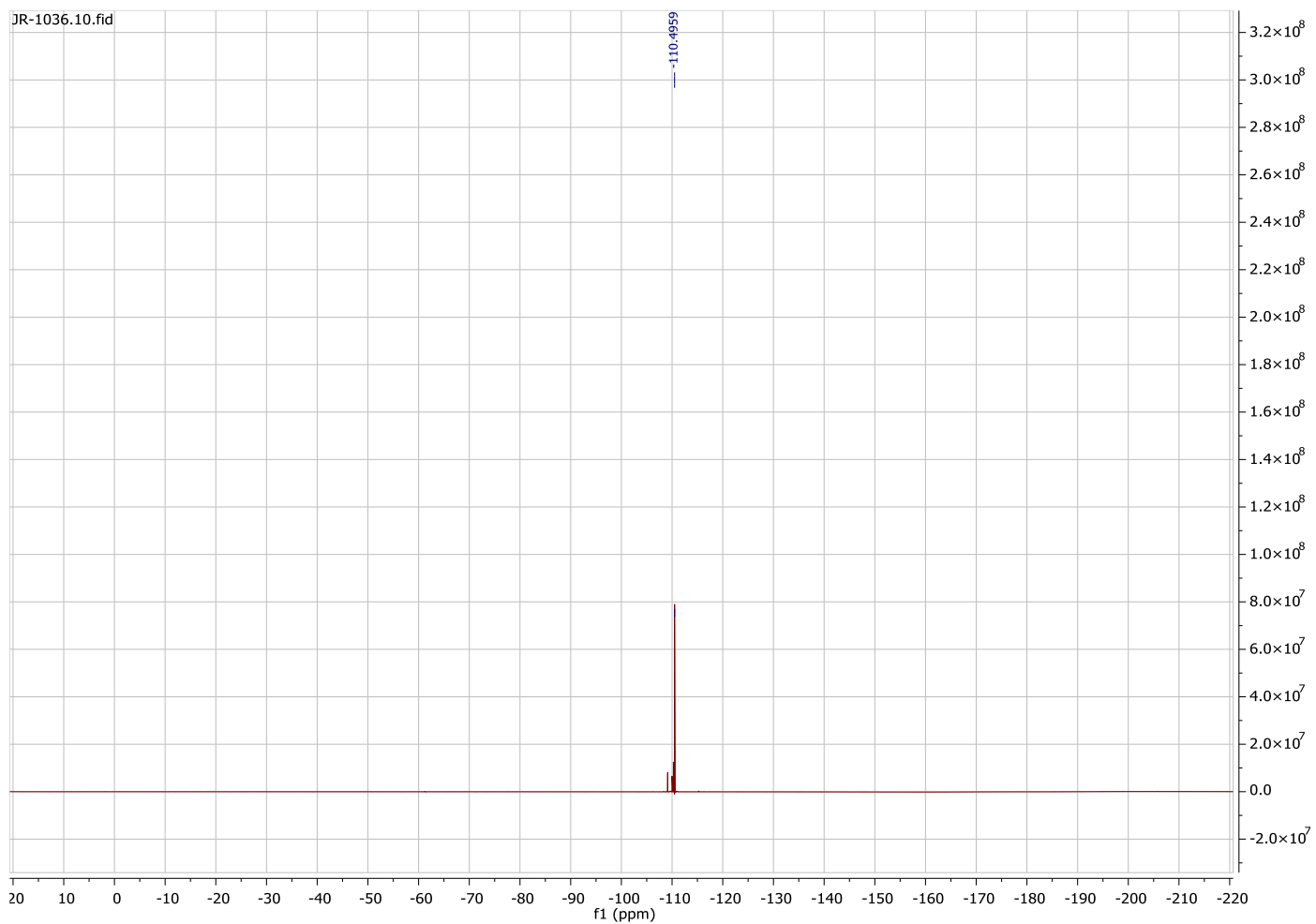
3r

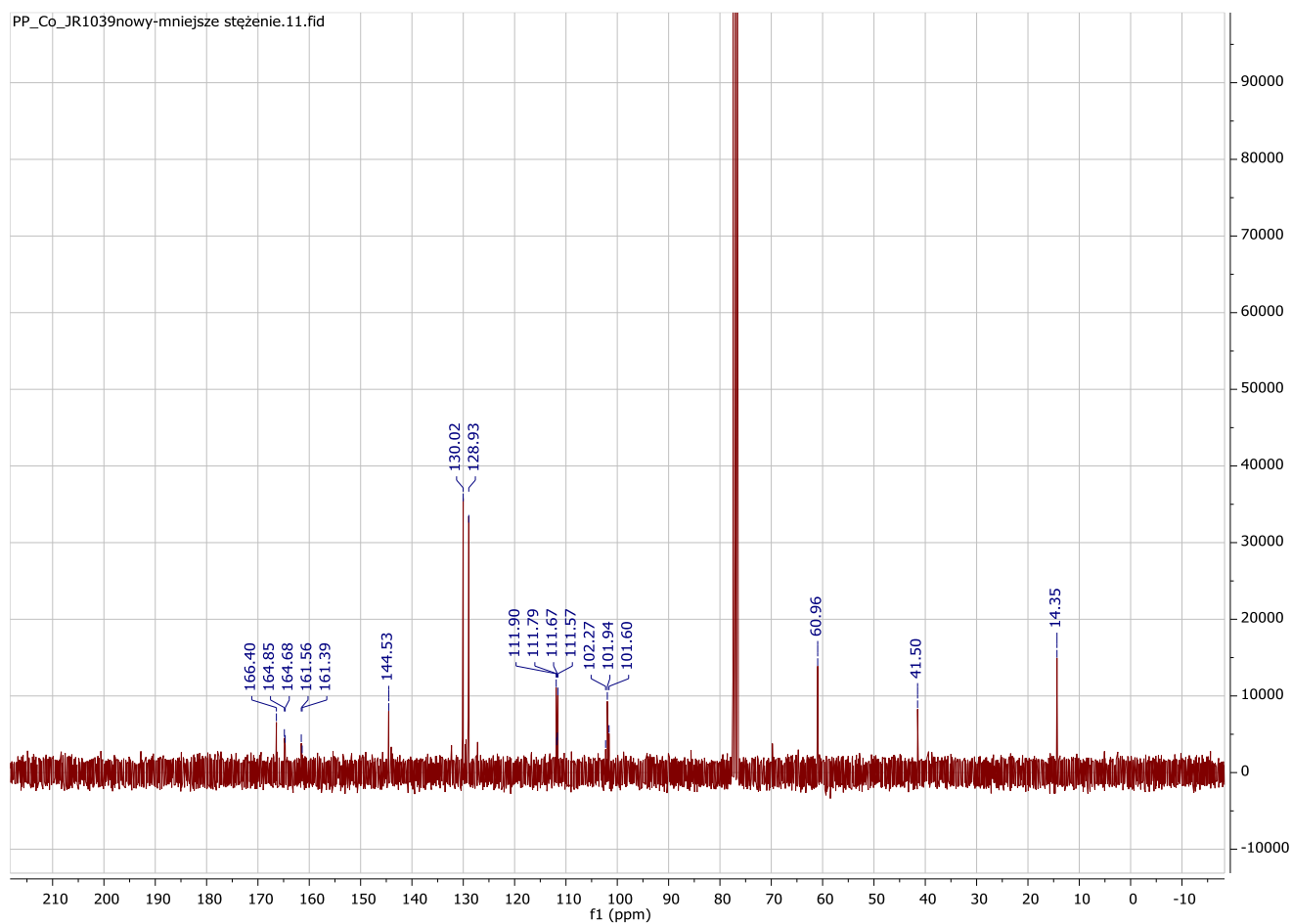
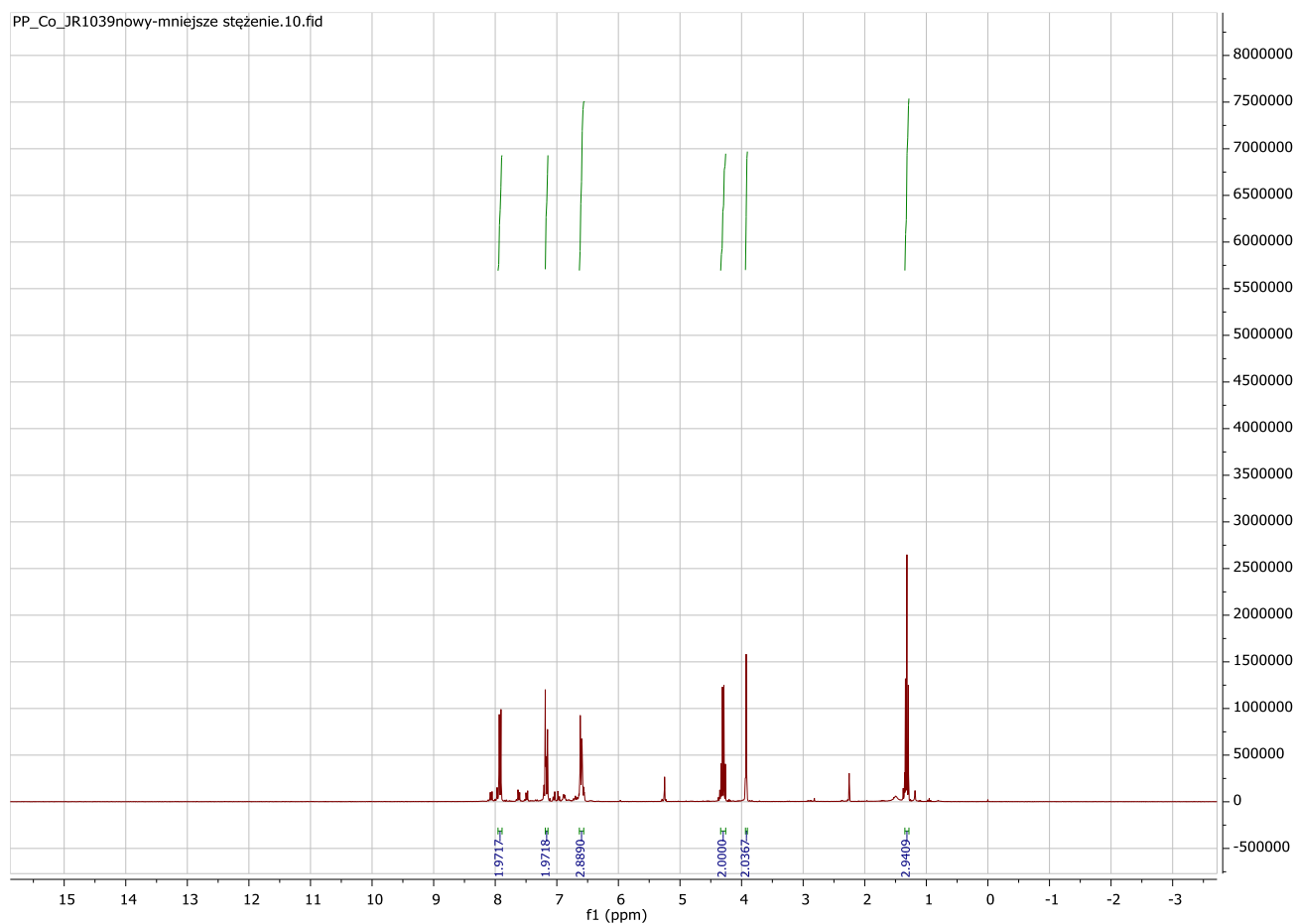


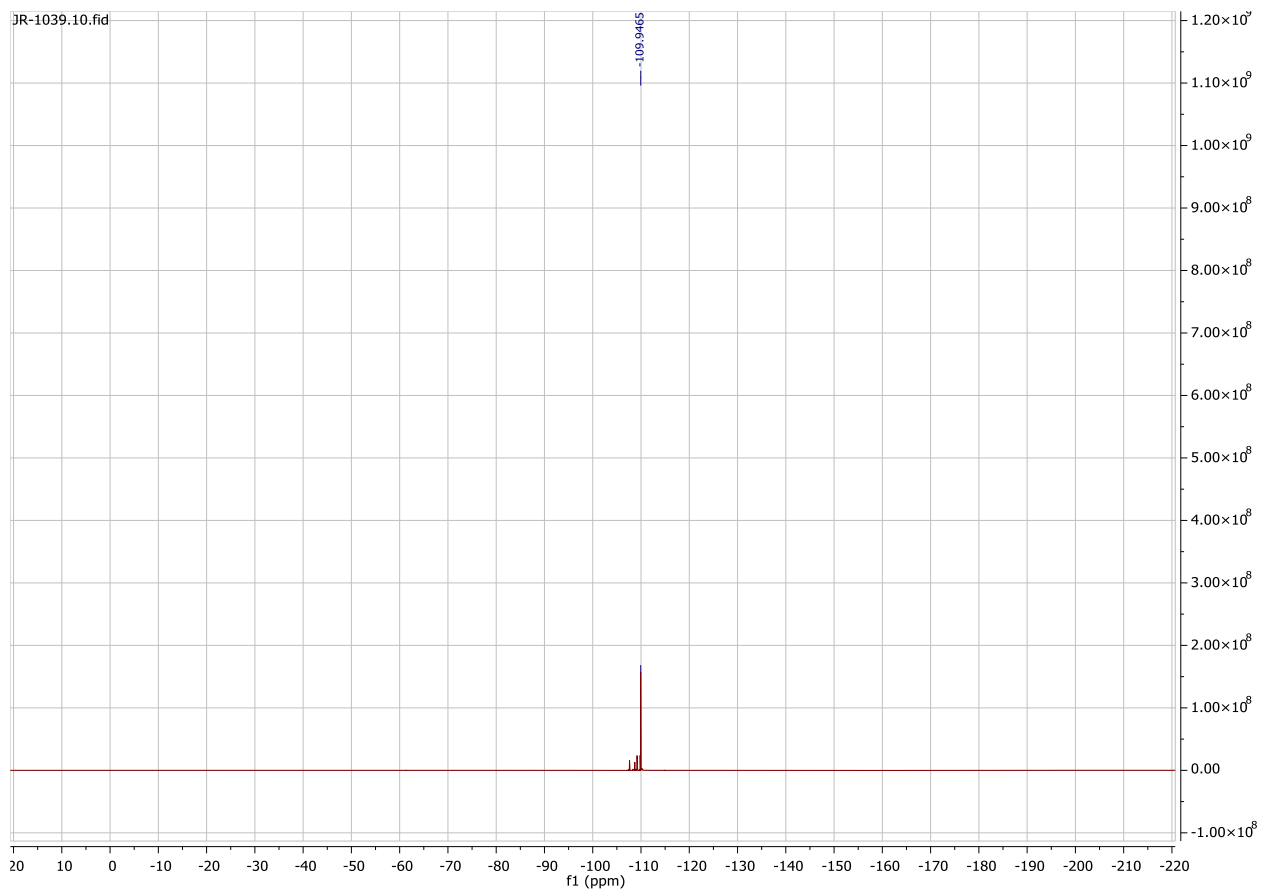


3s

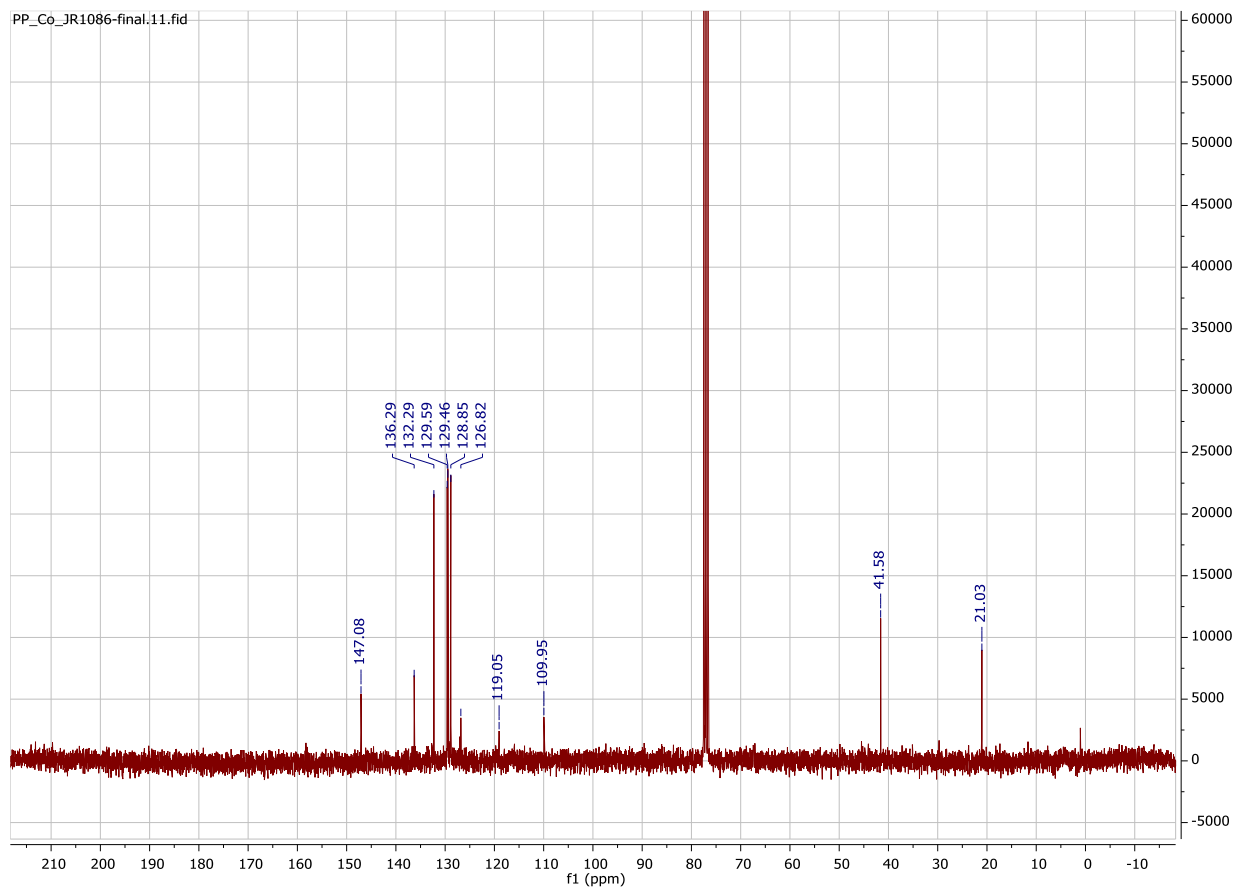
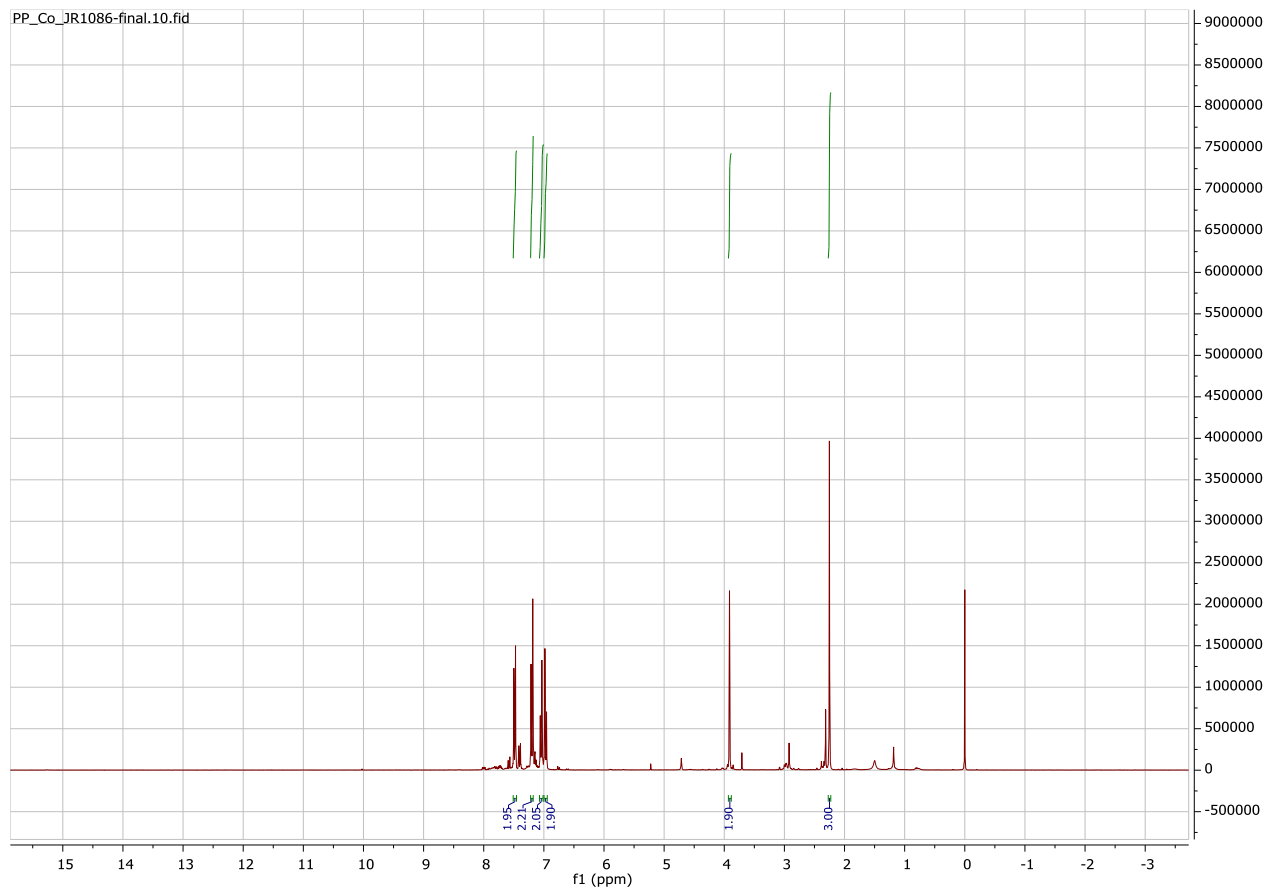




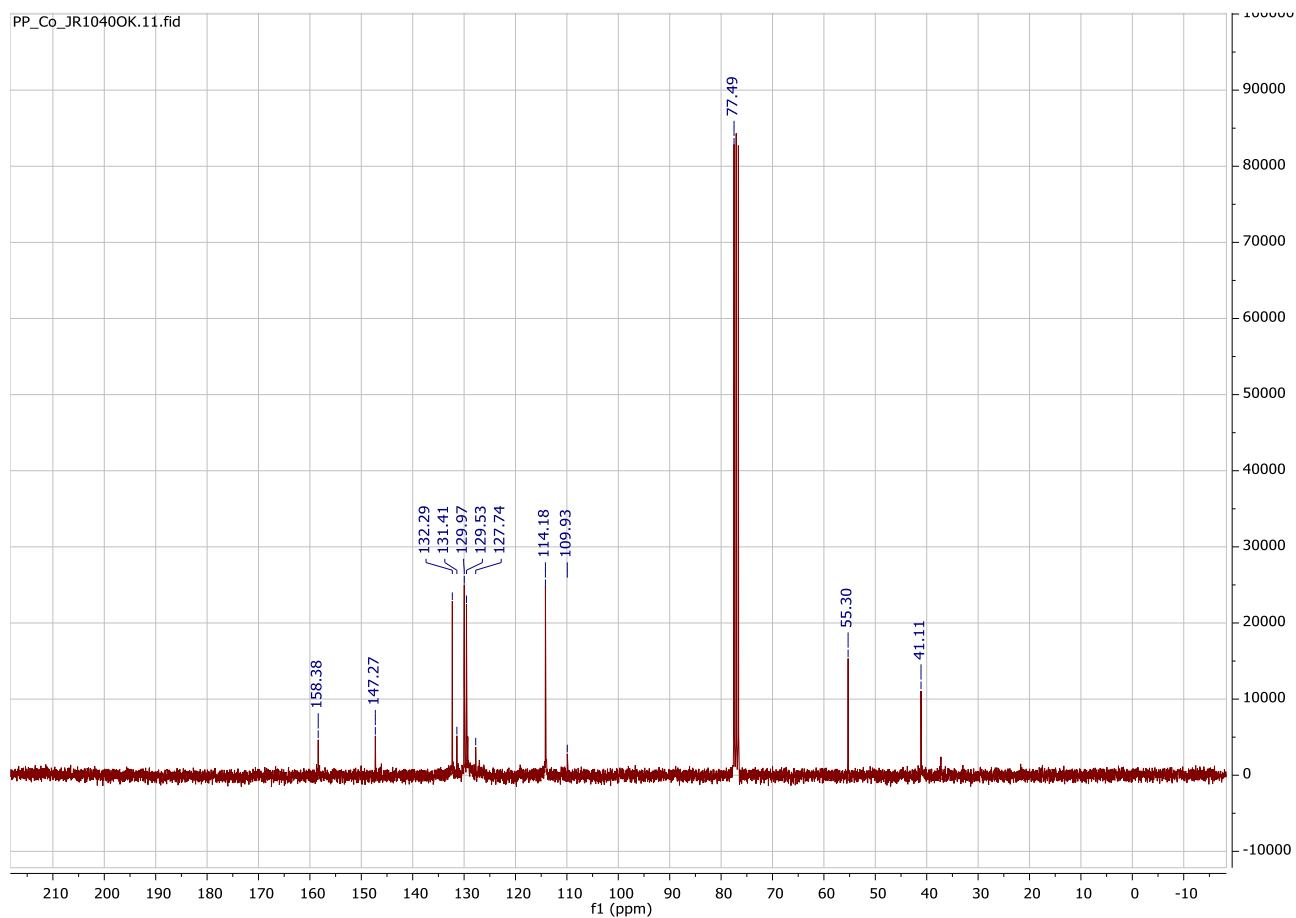
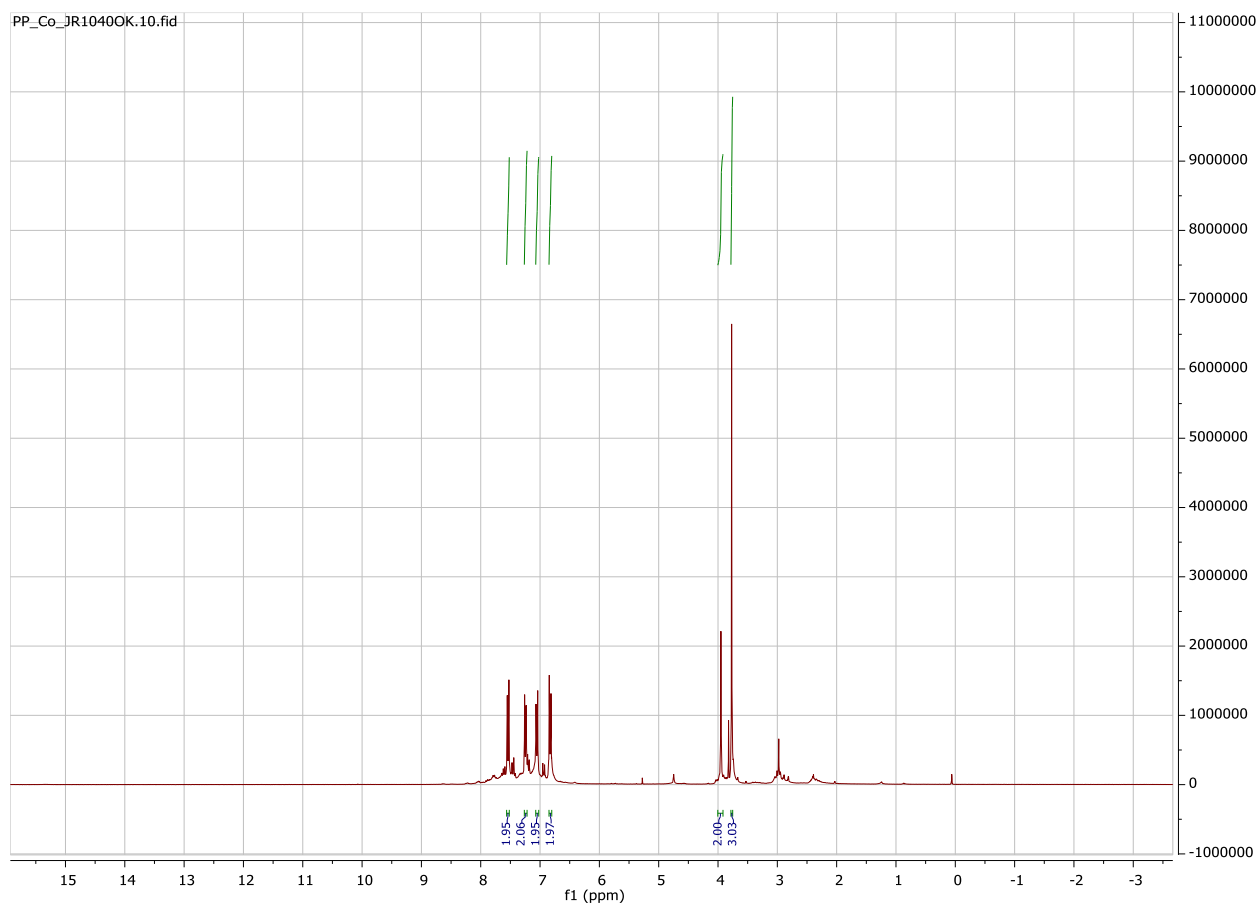




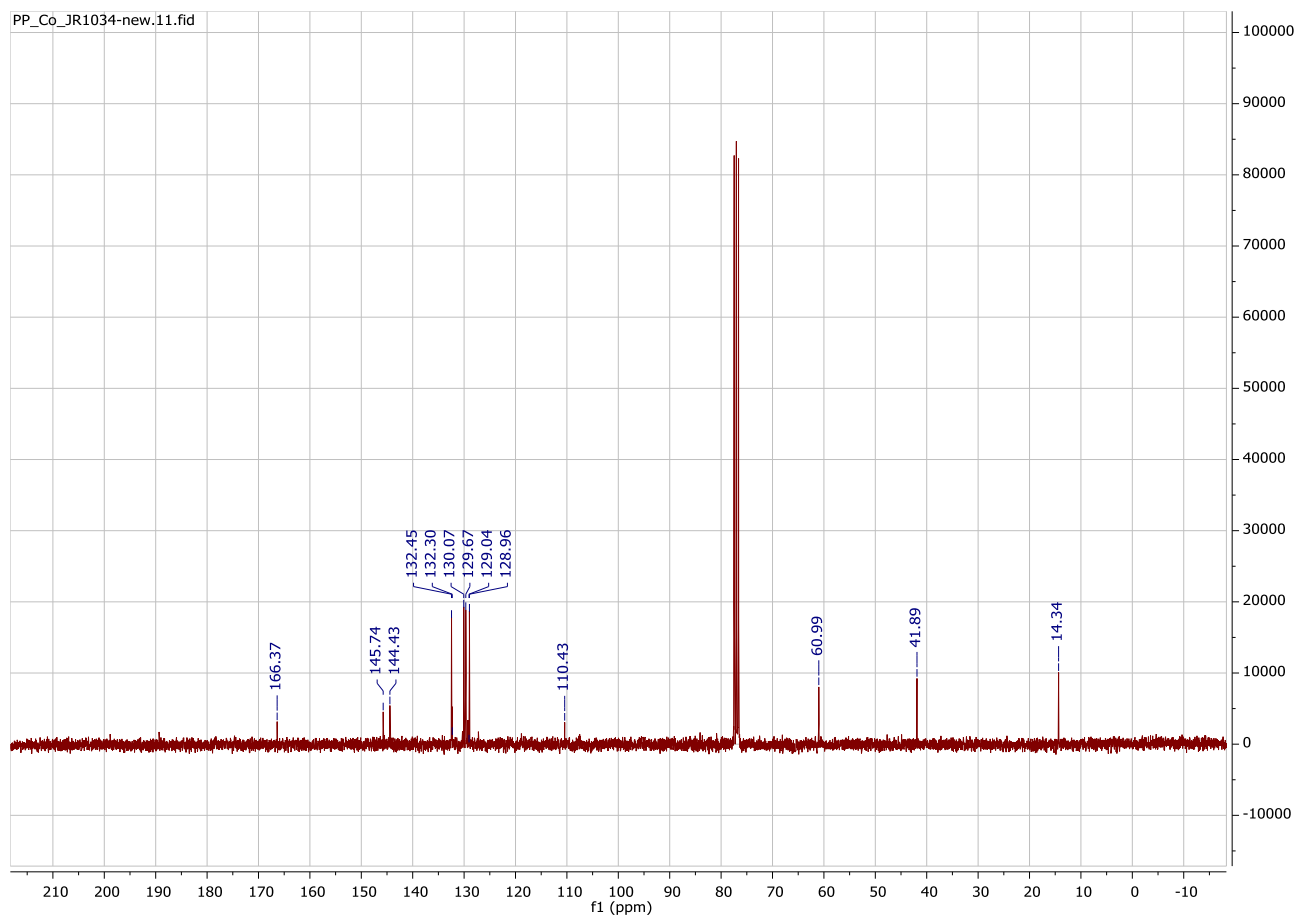
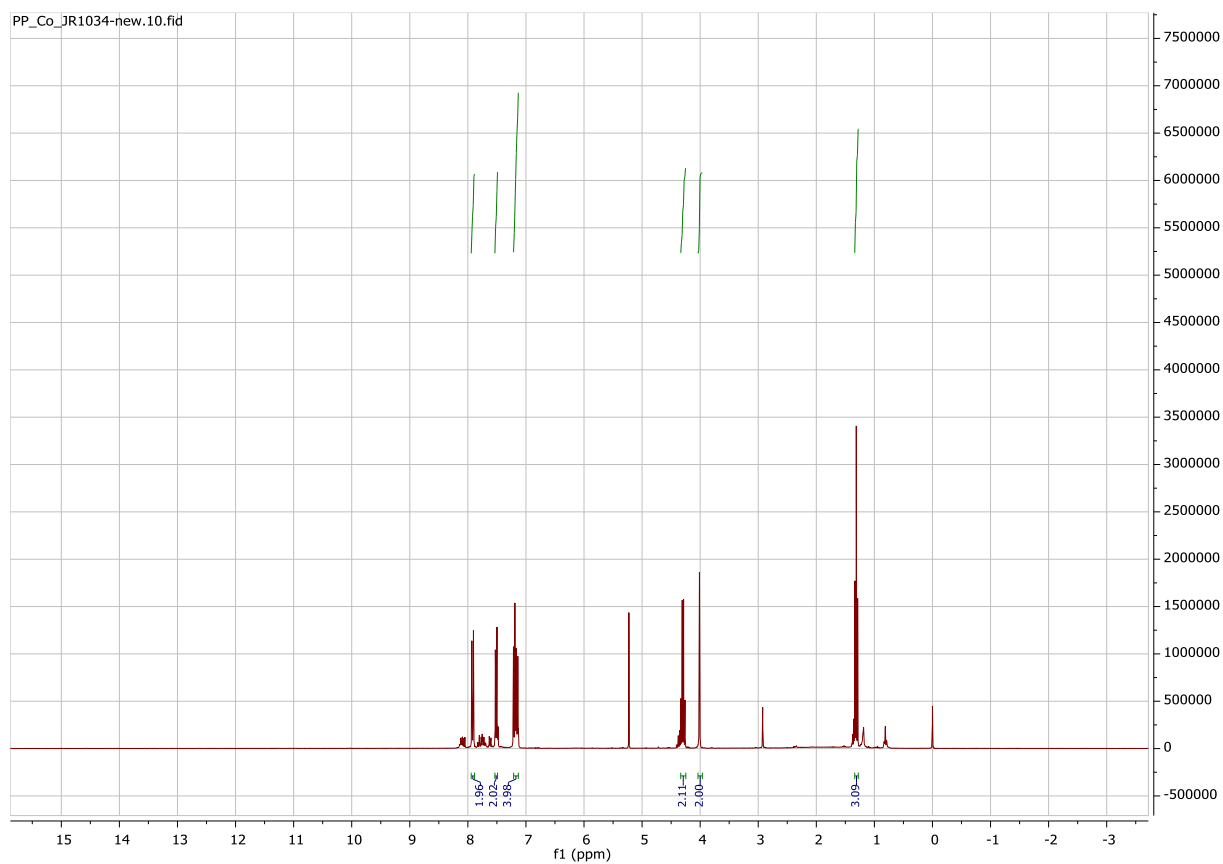
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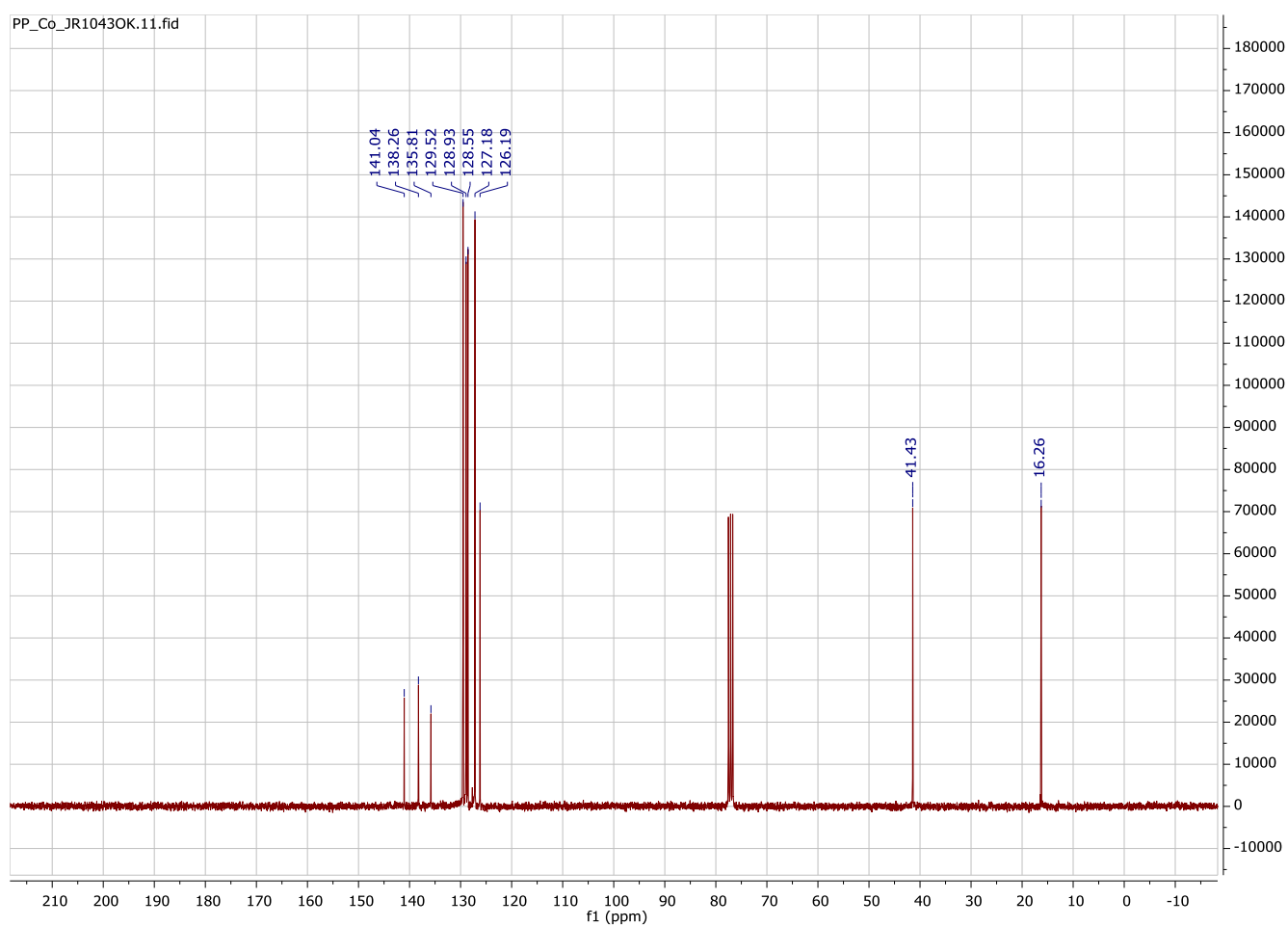
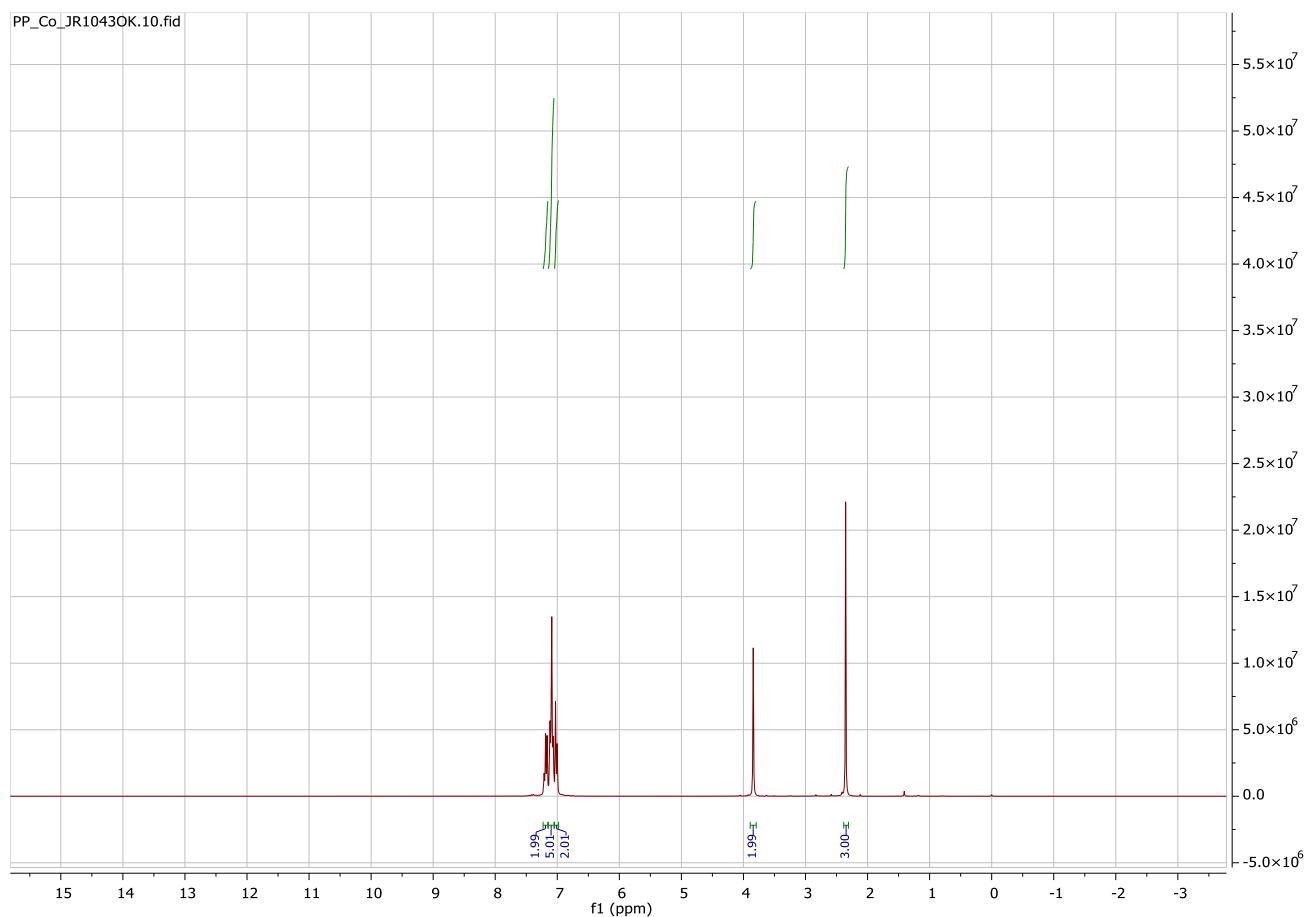
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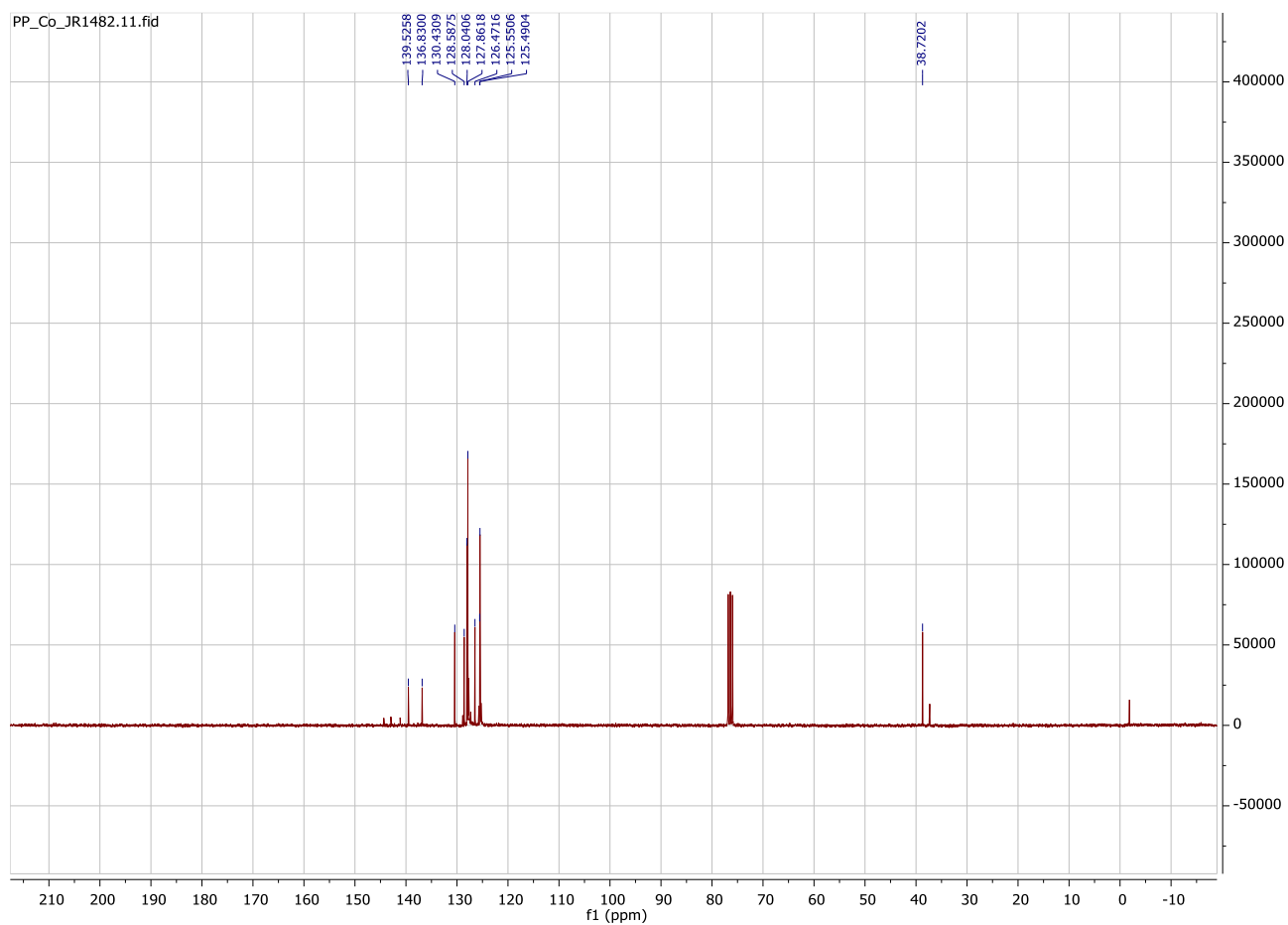
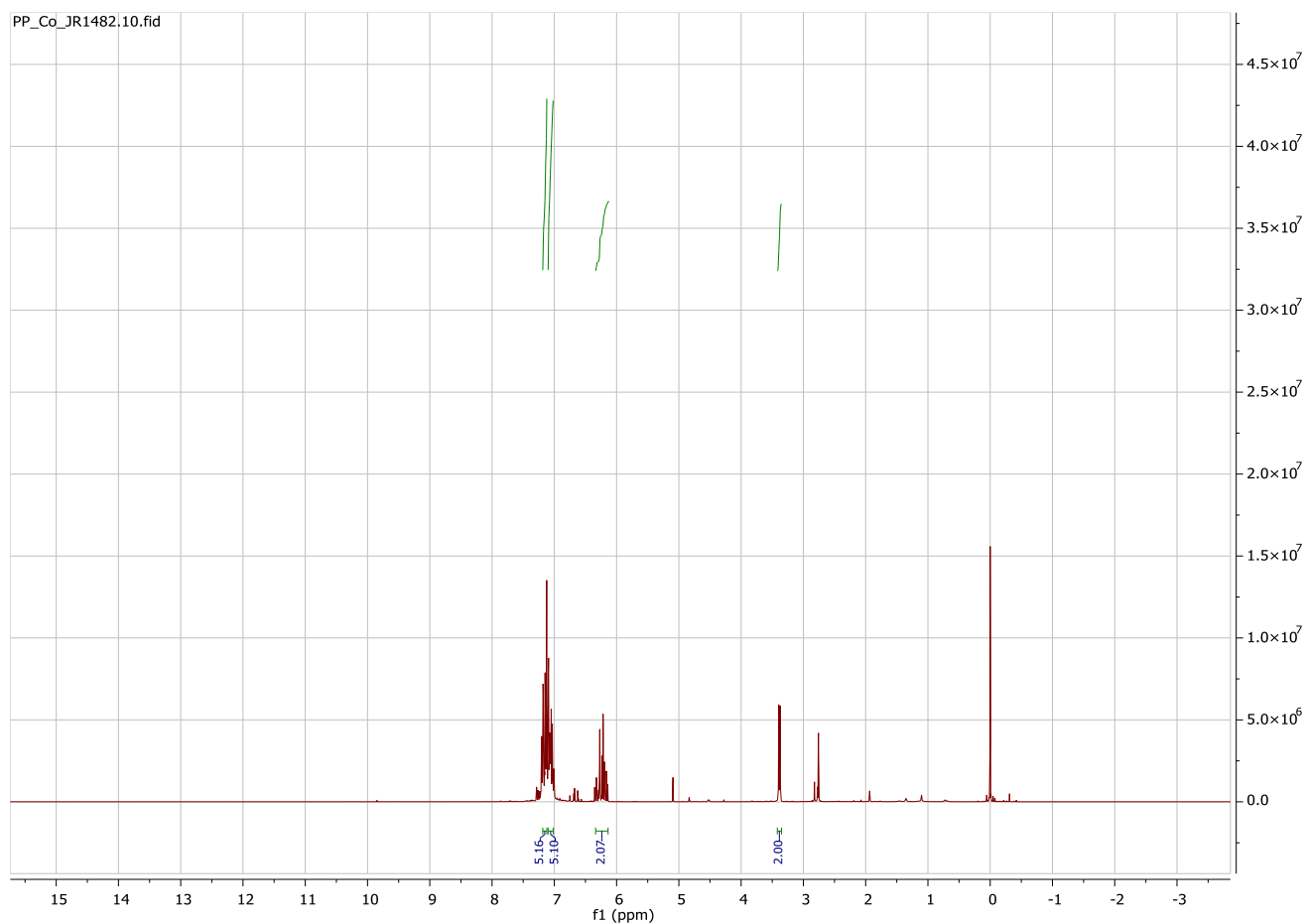
3w



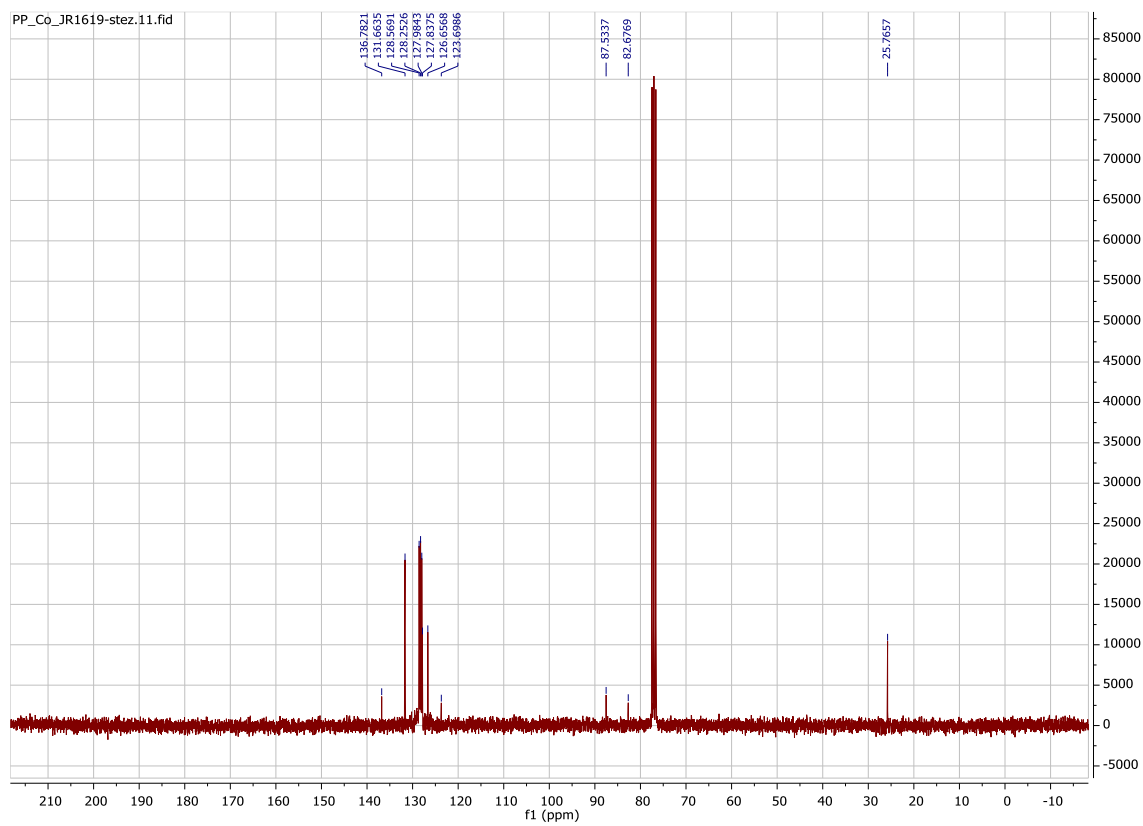
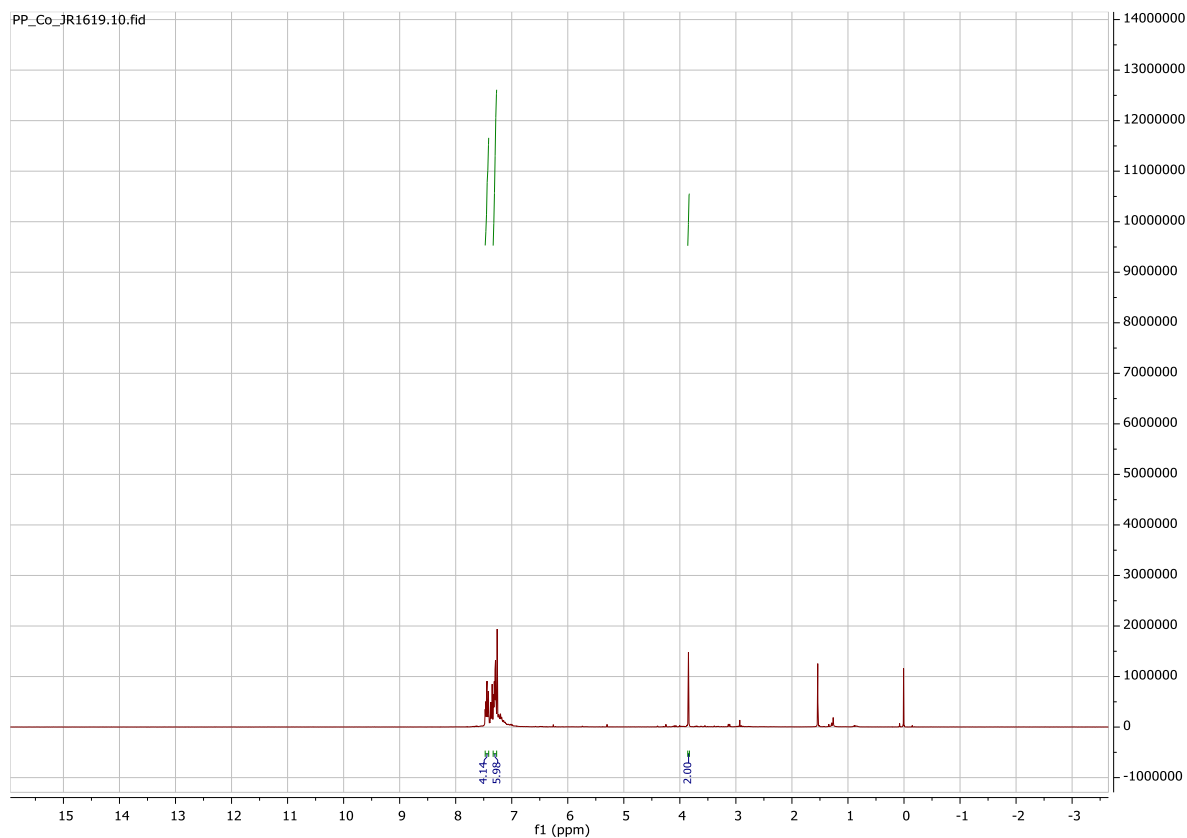
3y



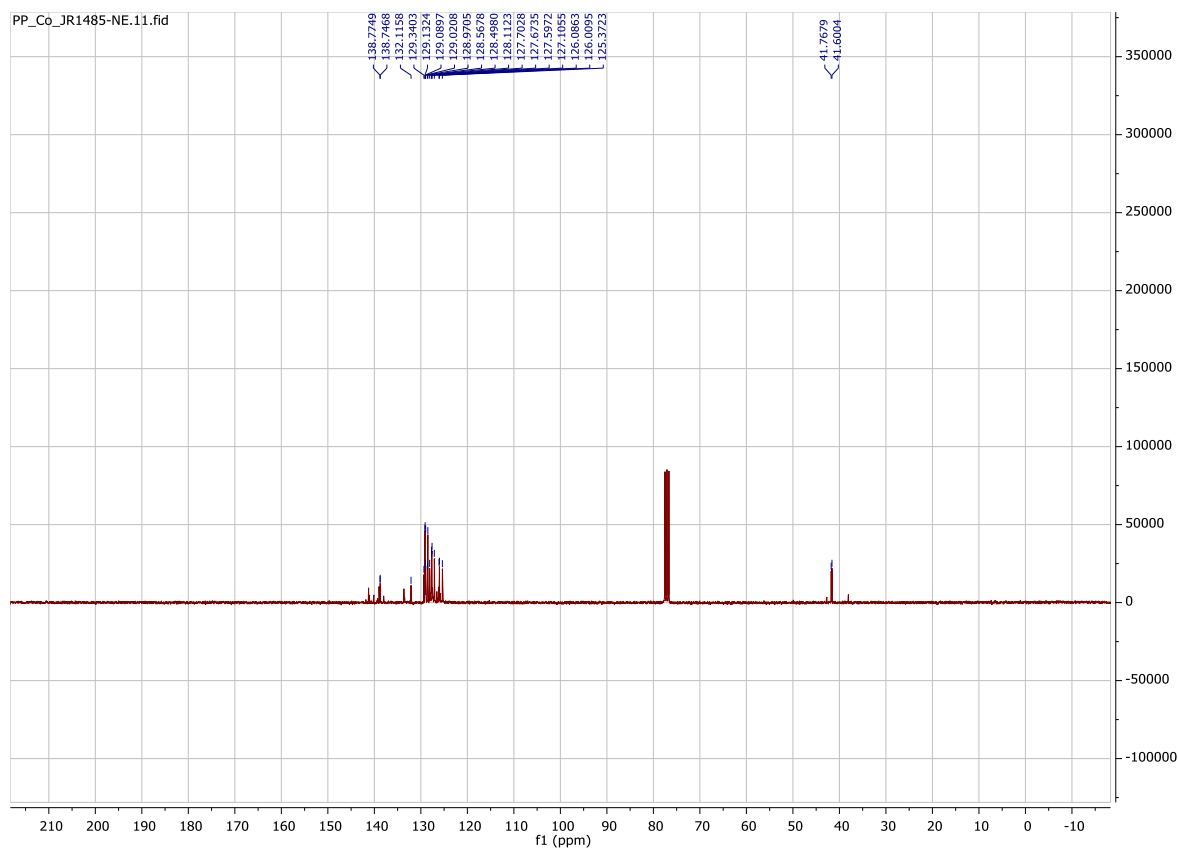
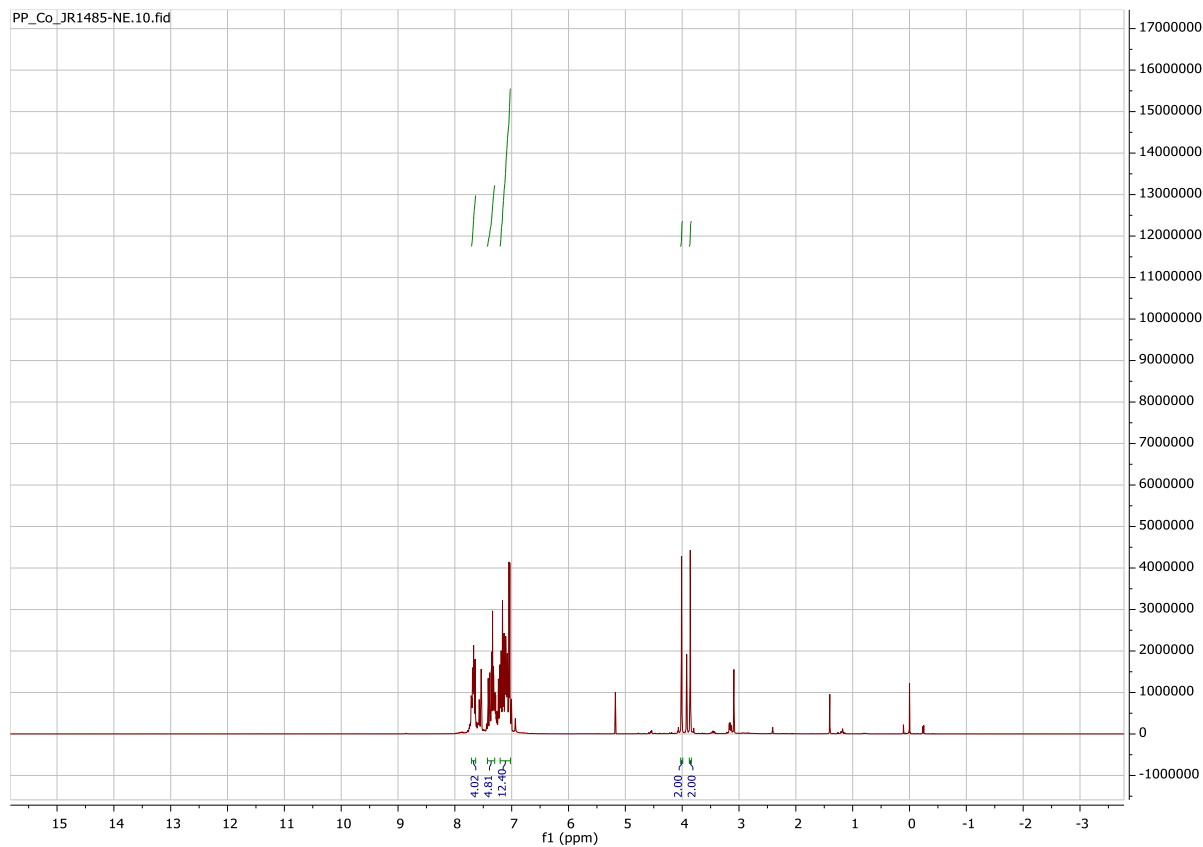
3x



3z



3aa

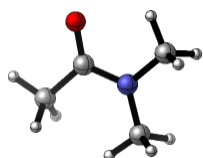


7. Computational methods

All calculations were conducted with Gaussian 16 package.¹⁷ Structures of minima and transition states were optimized employing BP86 functional, def2-SVP basis set¹⁸ Frequency analysis was performed at the same level of theory to provide correction to thermodynamic functions and confirm the nature of optimized structures (minima and transition states featured zero and one imaginary frequency, respectively). Single point energies were calculated with BP86 functional employing def2-TZVPP¹⁸ basis set and solvation (N,N-dimethylacetamide) with the SMD model.¹⁹ Molecular structures were visualized in CYLview.²⁰

Optimized geometries, energies and corrections to thermodynamic functions.

DMA



E (BP86/Def2-SVP) = -287.617611183

E (BP86/Def2-TZVPP/SMD(DMA)//BP86/Def2-SVP) = -287.954951993

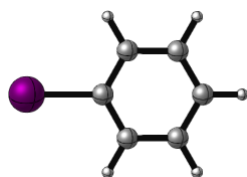
E (M06/Def2-TZVPP/SMD(DMA)//BP86/Def2-SVP) = -287.756571282

Zero-point correction=	0.125690 (Hartree/Particle)
Thermal correction to Energy=	0.133471
Thermal correction to Enthalpy=	0.134415
Thermal correction to Gibbs Free Energy=	0.094124

Charge = 0 Multiplicity = 1

C	-0.73332600	-0.29532600	-0.00005500
N	0.60274300	0.08570900	-0.00023100
C	1.08670000	1.45390700	0.00000600
H	1.71666800	1.65771200	-0.89698700
H	0.25154800	2.17569200	-0.00113300
H	1.71476500	1.65826500	0.89823000
C	1.62513300	-0.95021700	0.00008500
H	2.27523300	-0.87013900	-0.90043000
H	2.27459800	-0.87029100	0.90108300
H	1.11434400	-1.93080600	-0.00014300
C	-1.78221700	0.81850800	-0.00005100
H	-1.70661400	1.46851100	0.89675600
H	-1.70682600	1.46829400	-0.89703500
H	-2.77212000	0.32829400	0.00011700
O	-1.06981700	-1.48084100	0.00015600

PhI



E (BP86/Def2-SVP) = -529.308006841

E (BP86/Def2-TZVPP/SMD(DMA)//BP86/Def2-SVP) = -529.574190307

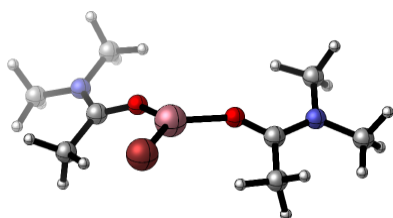
E (M06/Def2-TZVPP/SMD(DMA)//BP86/Def2-SVP) = -529.313711921

Zero-point correction=	0.087443 (Hartree/Particle)
Thermal correction to Energy=	0.093464
Thermal correction to Enthalpy=	0.094408
Thermal correction to Gibbs Free Energy=	0.055582

Charge = 0 Multiplicity = 1

C	3.37028600	0.00001800	0.00000000
C	2.66436100	1.21554800	0.00000200
C	1.25754200	1.22499600	-0.00000200
C	0.56711800	-0.00003300	0.00000100
C	1.25757000	-1.22501400	0.00000200
C	2.66441600	-1.21551600	-0.00000200
H	4.47145500	0.00006100	0.00000200
H	3.20866700	2.17353900	-0.00000100
H	0.70740500	2.17768800	-0.00000200
H	0.70751400	-2.17775300	0.00000400
H	3.20870900	-2.17351400	-0.00000300
I	-1.56587800	0.00000000	0.00000000

I



E (BP86/Def2-SVP) = -4532.24762354

E (BP86/Def2-TZVPP/SMD(DMA)//BP86/Def2-SVP) = -4533.44274602

E (M06/Def2-TZVPP/SMD(DMA)//BP86/Def2-SVP) = -4532.40012462

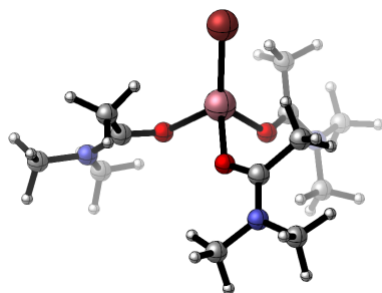
Zero-point correction=	0.253378 (Hartree/Particle)
Thermal correction to Energy=	0.275203
Thermal correction to Enthalpy=	0.276148
Thermal correction to Gibbs Free Energy=	0.195567

Charge = 0 Multiplicity = 3

Co	0.00014600	-0.54333900	0.32221900
O	1.44100400	0.74551700	0.09114900
C	2.63858700	0.64857400	-0.29783000
N	3.51546100	1.68382100	-0.05769400
C	3.11024600	-0.59218700	-1.02284500
C	4.90540000	1.69130100	-0.47866500
C	3.06849000	2.86019100	0.67523400
H	3.30386800	-0.39467400	-2.09969400
H	4.03378900	-1.02046700	-0.58152100
H	2.29650300	-1.34175300	-0.93678500
H	5.59410100	1.70383500	0.39788300
H	5.14178900	0.80390900	-1.09078500
H	5.12393000	2.59751200	-1.08817700
H	3.65197500	2.98598700	1.61504800

H	3.20090000	3.77970200	0.06198900
H	1.99933500	2.73565200	0.92254100
O	-1.43952200	0.74644600	0.08844100
C	-2.63779300	0.65004400	-0.29851100
N	-3.51409800	1.68518600	-0.05579400
C	-3.11110500	-0.59030900	-1.02313000
C	-4.90365700	1.69525900	-0.47787000
C	-3.06478000	2.86227300	0.67451400
H	-4.03317200	-1.01925400	-0.57931600
H	-3.30810700	-0.39212800	-2.09923400
H	-2.29701100	-1.33976900	-0.93982500
H	-5.11837400	2.59676400	-1.09584100
H	-5.14387000	0.80313100	-1.08152700
H	-5.59222300	1.71890200	0.39845400
H	-3.19155300	3.78048100	0.05801300
H	-3.65090700	2.99321000	1.61191000
H	-1.99685300	2.73448800	0.92543400
Br	-0.00205100	-2.85500000	0.27868100

II



E (BP86/Def2-SVP) = -4819.88111172

E (BP86/Def2-TZVPP/SMD(DMA)//BP86/Def2-SVP) = -4821.39532232

E (M06/Def2-TZVPP/SMD(DMA)//BP86/Def2-SVP) = -4820.16546759

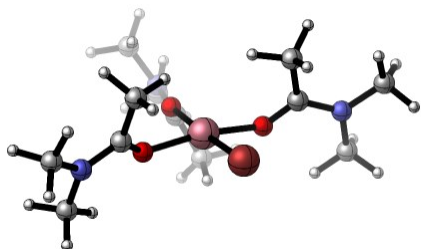
Zero-point correction=	0.378994 (Hartree/Particle)
Thermal correction to Energy=	0.410625
Thermal correction to Enthalpy=	0.411569
Thermal correction to Gibbs Free Energy=	0.305958

Charge = 0 Multiplicity = 3

Co	-0.02521200	0.13853300	0.63021800
O	-1.36216200	1.12154400	-0.51491800
C	-2.61634700	1.07187300	-0.43427700
N	-3.38873300	1.79843200	-1.32324500
C	-3.27933700	0.23288400	0.63590900
C	-4.83900900	1.77302600	-1.36926300
C	-2.74093200	2.66253000	-2.29847600
H	-4.20728500	0.67962200	1.04488200
H	-3.51505500	-0.78583400	0.26092900
H	-2.53555000	0.12050300	1.45585300
H	-5.18794500	1.57616400	-2.40874500
H	-5.24542900	0.97653600	-0.72168700
H	-5.28269700	2.74518200	-1.04842300

H	-3.00635700	2.35860700	-3.33677100
H	-3.05456900	3.72243500	-2.16114300
H	-1.64728700	2.58277500	-2.16355200
O	1.52914100	0.57757300	-0.57288300
C	2.43868200	1.44044700	-0.45830000
N	3.36979500	1.58813600	-1.47129100
C	2.52158100	2.31172300	0.77529500
C	4.43651800	2.57206100	-1.47055400
C	3.31254900	0.71775400	-2.63573000
H	3.55574000	2.44196900	1.15360400
H	2.09198100	3.32112800	0.59351600
H	1.90498500	1.81537900	1.55674200
H	4.41651900	3.16699600	-2.41231900
H	4.33100500	3.27415600	-0.62524900
H	5.44138000	2.09206300	-1.40232300
H	3.19934400	1.31366800	-3.56979700
H	4.24297800	0.11181700	-2.72795300
H	2.44423200	0.04347100	-2.52500700
Br	0.00072100	0.27815400	2.99758200
O	-0.37786500	-1.59197300	-0.33967900
C	0.26443100	-2.66985800	-0.23090000
N	-0.05610100	-3.74453900	-1.04298300
C	1.38224800	-2.78678200	0.78058800
C	0.62193700	-5.02747700	-1.01745200
C	-1.18185500	-3.64111800	-1.95849300
H	1.47509700	-3.79184400	1.23784800
H	2.36095800	-2.51531800	0.32964300
H	1.16637900	-2.03940500	1.57705200
H	0.85067700	-5.35809700	-2.05569800
H	1.57748100	-4.96356100	-0.46757900
H	-0.00102900	-5.82404900	-0.54466400
H	-0.86563400	-3.87979500	-2.99900200
H	-1.99714200	-4.34760900	-1.67815600
H	-1.56772200	-2.60647900	-1.92086100

III



E (BP86/Def2-SVP) = -4819.85388554

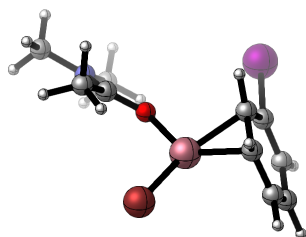
E (BP86/Def2-TZVPP/SMD(DMA)//BP86/Def2-SVP) = -4821.37283608

E (M06/Def2-TZVPP/SMD(DMA)//BP86/Def2-SVP) = -4820.16546759

Zero-point correction=	0.380846 (Hartree/Particle)
Thermal correction to Energy=	0.411288
Thermal correction to Enthalpy=	0.412232
Thermal correction to Gibbs Free Energy=	0.313760

Charge = 0 Multiplicity = 1

Co	-0.13231300	-0.09721700	-0.09400300
O	1.73381900	-0.38256300	-0.26109600
C	2.45579400	-1.14353600	0.44735500
N	3.66505600	-1.56071800	-0.05635400
C	2.01765500	-1.58503600	1.82284100
C	4.61507500	-2.37632500	0.67873800
C	4.06956700	-1.16142100	-1.39682100
H	1.71574000	-2.65350200	1.82044700
H	2.79758900	-1.41935800	2.59687600
H	1.10666900	-0.99373500	2.04931900
H	5.53885900	-1.80539700	0.93431200
H	4.17123100	-2.75639100	1.61508400
H	4.92187200	-3.25294900	0.06552600
H	4.89105400	-0.40828800	-1.36973300
H	4.43257600	-2.04647100	-1.96307800
H	3.19705500	-0.72553200	-1.91515900
O	0.13126100	1.74395900	0.29750800
C	0.87696700	2.59277700	-0.26860500
N	1.14296700	3.78688500	0.37758500
C	1.47119100	2.32860400	-1.63192400
C	1.90694600	4.86735300	-0.21733800
C	0.46883200	4.09254000	1.63080100
H	1.31002600	3.17311700	-2.33503500
H	2.56110100	2.11423200	-1.58996100
H	0.95987000	1.41773000	-2.00530000
H	2.54400600	5.34730700	0.55783800
H	2.57362800	4.49283900	-1.01509100
H	1.25515800	5.66413100	-0.65228200
H	1.19979500	4.45769400	2.38550900
H	-0.30825200	4.88113200	1.49485900
H	-0.02035400	3.17343200	2.00016200
Br	-0.53247600	-2.42951600	-0.36862600
O	-1.97594100	0.28836000	-0.28134100
C	-2.98483300	-0.15142000	0.33266000
N	-4.23159200	0.05374200	-0.21289700
C	-2.85659900	-0.86389800	1.65899100
C	-5.47005900	-0.40252800	0.39070700
C	-4.36540300	0.75990300	-1.47950800
H	-3.50607100	-0.41651300	2.44166800
H	-3.08507100	-1.94560800	1.56426400
H	-1.78852500	-0.78102400	1.94187000
H	-6.05066800	-1.01574900	-0.33521000
H	-5.27396700	-1.02616400	1.27990300
H	-6.11572600	0.45365900	0.69742300
H	-4.87624000	0.11884400	-2.23218000
H	-4.96460100	1.69011900	-1.35327600
H	-3.35656600	1.02090400	-1.84505000



E (BP86/Def2-SVP) = -4773.94534524

E (BP86/Def2-TZVPP/SMD(DMA)//BP86/Def2-SVP) = -4775.06345145

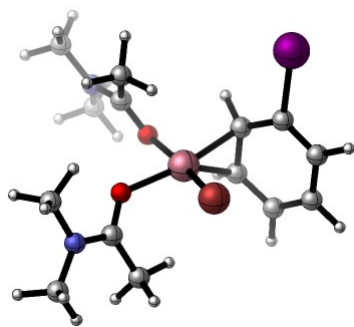
E (M06/Def2-TZVPP/SMD(DMA)//BP86/Def2-SVP) = -4773.96273581

Zero-point correction= 0.215049 (Hartree/Particle)
 Thermal correction to Energy= 0.234862
 Thermal correction to Enthalpy= 0.235807
 Thermal correction to Gibbs Free Energy= 0.159067

Charge = 0 Multiplicity = 3

Co	-1.16116400	-0.66569600	0.01891200
C	-0.47737900	-3.28842700	-0.15548400
C	-0.51569200	-2.34055000	0.92566200
C	0.52585000	-1.32893700	1.00793700
C	1.56454300	-1.36208400	0.01620800
C	1.56466300	-2.26300000	-1.04262500
H	-1.15338500	-2.54576200	1.80166400
H	0.68346700	-0.76271900	1.93943400
H	2.36627400	-2.24935500	-1.79525200
C	0.51925900	-3.23445100	-1.12298100
H	0.52114100	-3.95329900	-1.95742300
O	-0.54273700	1.21104900	-0.17850700
C	-1.01612900	2.33474200	0.14166700
N	-0.46148300	3.46587800	-0.38139900
C	-2.17539800	2.43774100	1.10919700
C	-0.89636900	4.81877500	-0.06069100
C	0.63941900	3.36954200	-1.33834000
H	-1.82823600	2.78532800	2.10559900
H	-2.96589300	3.12869700	0.75623400
H	-2.61542500	1.42525500	1.20684200
H	-1.31594000	5.32358600	-0.95941000
H	-1.66424700	4.81776400	0.73103900
H	-0.03281000	5.42212100	0.29509700
H	0.33875100	3.80207100	-2.31745300
H	1.52256000	3.92981200	-0.96363800
H	0.91136800	2.30797000	-1.46888700
H	-1.25974600	-4.06116400	-0.20917200
I	3.18996500	0.01331300	0.21464500
Br	-3.48711300	-0.88319300	-0.10962700

V



E (BP86/Def2-SVP) = -5061.55089043

E (BP86/Def2-TZVPP/SMD(DMA)//BP86/Def2-SVP) = -5062.99677873

E (M06/Def2-TZVPP/SMD(DMA)//BP86/Def2-SVP) = -5061.68928383

Zero-point correction= 0.342558 (Hartree/Particle)

Thermal correction to Energy= 0.371075

Thermal correction to Enthalpy= 0.372020

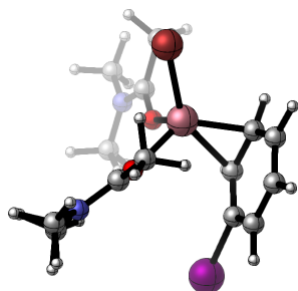
Thermal correction to Gibbs Free Energy= 0.277309

Charge = 0 Multiplicity = 1

Co	0.52823500	-0.06473300	0.51040000
C	-2.49683600	-0.47166800	0.61980400
C	-1.38522300	0.34761200	1.03243900
C	-0.57990400	-0.13719400	2.15942000
C	-0.93858000	-1.39506200	2.77544900
C	-1.98908900	-2.15037000	2.29424500
H	-1.49361500	1.43476000	0.86748700
H	-0.08164700	0.60466500	2.81273000
H	-2.24212200	-3.11592800	2.76170600
C	-2.78779300	-1.69297900	1.18938100
H	-3.62516100	-2.30652000	0.82681100
O	2.39202700	-0.14546200	-0.14520300
C	3.20799400	-1.10082900	-0.02332300
N	4.12498500	-1.32264400	-1.01037600
C	3.23542000	-1.95584500	1.22582800
C	5.19785500	-2.30262600	-0.92947200
C	4.03901900	-0.57236100	-2.25834400
H	3.17667800	-3.03632300	0.99192000
H	4.15425100	-1.76294500	1.82260700
H	2.34109400	-1.68692400	1.81723100
H	6.18313300	-1.81656800	-1.10610500
H	5.22513400	-2.78236200	0.06346800
H	5.06604900	-3.09648100	-1.69839900
H	4.81854400	0.22086400	-2.31279000
H	4.18151900	-1.26222800	-3.11638100
H	3.04033100	-0.10609700	-2.32462500
O	0.98035300	1.79534300	0.97000300
C	1.08195000	2.68309200	0.08001600
N	1.58235200	3.91360300	0.40984500
C	0.66041000	2.39349900	-1.34473000
C	1.72804000	5.01387400	-0.53084900
C	1.95014800	4.20769600	1.79120000

H	-0.02610200	3.16365300	-1.75055400
H	1.53788300	2.31128300	-2.01920400
H	0.13512800	1.41321100	-1.33008900
H	2.75817100	5.42947400	-0.47440400
H	1.55044000	4.68080000	-1.56779000
H	1.01733300	5.84005000	-0.30017700
H	3.00805100	4.54532900	1.84544200
H	1.30580600	5.01437700	2.20566400
H	1.82316000	3.29342100	2.39658100
Br	0.22345900	-2.17938500	-0.49299900
H	-0.37922200	-1.73442200	3.66355400
I	-3.73639900	0.26876200	-0.97135100

VI



E (BP86/Def2-SVP) = -5061.55131687

E (BP86/Def2-TZVPP/SMD(DMA)//BP86/Def2-SVP) = -5063.02241666

E (M06/Def2-TZVPP/SMD(DMA)//BP86/Def2-SVP) = -5061.73254078

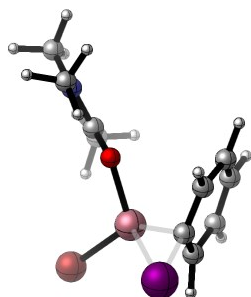
Zero-point correction=	0.342487 (Hartree/Particle)
Thermal correction to Energy=	0.371044
Thermal correction to Enthalpy=	0.371988
Thermal correction to Gibbs Free Energy=	0.277500

Charge = 0 Multiplicity = 3

Co	0.93548600	0.55006700	0.53028900
C	-0.34306300	1.56556500	2.89083600
C	0.28096300	0.35359600	2.42700900
C	-0.50797300	-0.58153800	1.64274400
C	-1.87549000	-0.24993500	1.39274500
C	-2.45815200	0.93783300	1.81556100
H	1.19212200	0.00060700	2.94484400
H	-0.17819000	-1.62301200	1.51612300
H	-3.51230200	1.16316100	1.59811100
C	-1.66474000	1.85519100	2.57586200
H	-2.12571600	2.79109600	2.93148900
O	-0.23451700	0.84239400	-1.11873400
C	-0.69263100	1.91484500	-1.58806900
N	-1.27124100	1.90504800	-2.83132400
C	-0.58561000	3.18618100	-0.78200200
C	-1.76506600	3.07025500	-3.55002300
C	-1.39649400	0.64045200	-3.55140900
H	0.49284200	3.44326000	-0.68800400
H	-1.15454000	4.05235900	-1.16180700

H	-0.92811000	2.95005800	0.24642300
H	-2.86650700	3.00956200	-3.70246400
H	-1.53626100	4.00580700	-3.01342800
H	-1.28836200	3.12908800	-4.55360200
H	-2.44898900	0.49071300	-3.87542100
H	-0.74821100	0.63537500	-4.45597800
H	-1.09437900	-0.18217800	-2.88046500
O	1.60959200	-1.27743100	-0.22457100
C	2.70152400	-1.89165000	-0.25409900
N	2.78166400	-3.09147200	-0.91782000
C	3.93689800	-1.34826100	0.43656300
C	3.98017100	-3.91209200	-0.99776500
C	1.60577700	-3.62761300	-1.59569200
H	4.21700800	-1.97410400	1.31041400
H	4.81004300	-1.30070900	-0.24498800
H	3.70822700	-0.31784700	0.77625800
H	4.30731800	-4.03492500	-2.05503800
H	4.81173400	-3.46459100	-0.42764700
H	3.78510500	-4.92775600	-0.58611000
H	1.80962800	-3.76106400	-2.68102800
H	1.32781200	-4.61740500	-1.17107100
H	0.76645900	-2.92290200	-1.46075200
H	0.24503300	2.26309500	3.50763600
I	-3.07651200	-1.67457900	0.33276700
Br	2.72385800	2.15432800	0.51397000

TS1



E (BP86/Def2-SVP) = -4773.94086764

E (BP86/Def2-TZVPP/SMD(DMA)//BP86/Def2-SVP) = -4775.05735643

E (M06/Def2-TZVPP/SMD(DMA)//BP86/Def2-SVP) = -4773.95226262

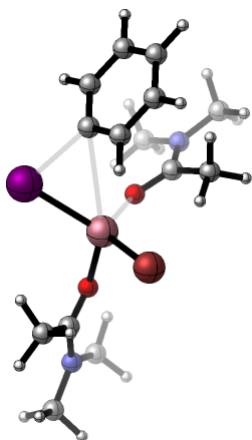
Zero-point correction=	0.214381 (Hartree/Particle)
Thermal correction to Energy=	0.233623
Thermal correction to Enthalpy=	0.234567
Thermal correction to Gibbs Free Energy=	0.159381

Charge = 0 Multiplicity = 3

Co	-0.17623300	0.66941400	0.40409900
C	-0.19320300	-1.22405100	2.89688300
C	0.41544000	0.02915000	2.73973500
C	1.30066700	0.29484800	1.63527500

C	1.45147800	-0.76107700	0.65888200
C	0.90575100	-2.05675500	0.88915200
H	0.26017100	0.81659900	3.49447000
H	1.98713100	1.15747400	1.66112700
H	1.11406700	-2.86746400	0.17465400
C	0.08748700	-2.28624600	1.99866000
H	-0.35306500	-3.28237400	2.15790000
O	-1.55116300	-0.64153000	-0.28574800
C	-2.80484300	-0.54285300	-0.19716400
N	-3.59283900	-1.34500000	-0.97295300
C	-3.39888800	0.46610700	0.75666400
C	-5.04839100	-1.40174400	-0.92924300
C	-2.96977000	-2.24252300	-1.94515600
H	-2.86031600	1.42410900	0.57864100
H	-4.48510100	0.63895800	0.66493400
H	-3.16558300	0.15415000	1.79619300
H	-5.37927000	-2.45860200	-0.83358400
H	-5.45126100	-0.84237100	-0.06856500
H	-5.49430100	-0.98901100	-1.86178600
H	-3.15811700	-3.30439100	-1.67373100
H	-3.39400400	-2.05959200	-2.95562400
H	-1.88209800	-2.05720400	-1.95959100
H	-0.86293800	-1.39483600	3.75524600
I	2.96129700	-0.55736400	-0.86422800
Br	-0.57088400	2.84082200	-0.34178200

TS2



E (BP86/Def2-SVP) = -5061.55978387

E (BP86/Def2-TZVPP/SMD(DMA)//BP86/Def2-SVP) = -5063.00653604

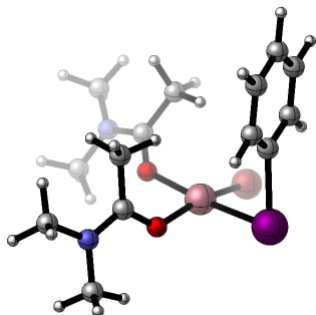
E (M06/Def2-TZVPP/SMD(DMA)//BP86/Def2-SVP) = -5061.71206288

Zero-point correction=	0.341163 (Hartree/Particle)
Thermal correction to Energy=	0.370575
Thermal correction to Enthalpy=	0.371519
Thermal correction to Gibbs Free Energy=	0.271460

Charge = 0 Multiplicity = 3

Co	0.55532000	-0.02556000	0.14857300
C	-4.75244800	-0.77229000	0.83416900
C	-3.70697200	-1.32379700	1.59865300
C	-2.44886300	-1.57661700	1.01128400
C	-2.26929900	-1.26919100	-0.34148100
C	-3.29509300	-0.72818800	-1.12562700
H	-3.86498300	-1.55888700	2.66477900
H	-1.61929000	-1.97599200	1.62037300
H	-3.13499700	-0.51280900	-2.19597600
C	-4.54598100	-0.47228800	-0.52632000
H	-5.36616300	-0.04690700	-1.12985400
O	-0.44741200	1.62905600	-0.35537400
C	-1.37191700	2.29401100	0.18005700
N	-2.02570100	3.24525200	-0.55907500
C	-1.77016000	2.05957100	1.61934400
C	-3.15050200	4.02970100	-0.07415600
C	-1.65573300	3.46971700	-1.95209200
H	-1.81027400	2.99961800	2.20604400
H	-2.76344600	1.56533700	1.67595000
H	-1.02178600	1.37672900	2.06988500
H	-4.05702100	3.83255800	-0.68933300
H	-3.38849400	3.78142900	0.97376400
H	-2.92860200	5.11876900	-0.13670600
H	-1.38353600	4.53581400	-2.11375300
H	-0.79462400	2.82486100	-2.19978400
H	-2.50447300	3.22162200	-2.62718200
O	2.36115100	0.73288100	-0.36896200
C	3.49977100	0.20981300	-0.24473300
N	4.61475900	0.99290400	-0.39461300
C	3.60638200	-1.26160700	0.06607400
C	5.99109100	0.54898700	-0.22827600
C	4.45930800	2.40716900	-0.72439900
H	2.87557600	-1.78404500	-0.58867600
H	4.60377400	-1.71596300	-0.06515500
H	3.24425300	-1.42021800	1.10623200
H	6.51517900	1.20489500	0.50124400
H	6.04050100	-0.48476800	0.15196800
H	6.54901600	0.59990500	-1.19072400
H	4.87647800	3.04432800	0.08621800
H	4.99954400	2.64536200	-1.66684800
H	3.38456200	2.62755400	-0.84598100
I	-0.22882900	-1.92415600	-1.45703900
Br	0.84134300	-0.59649600	2.46353000
H	-5.73472000	-0.58396800	1.29707600

TS3



E (BP86/Def2-SVP) = -5061.52496459

E (BP86/Def2-TZVPP/SMD(DMA)//BP86/Def2-SVP) = -5062.98295404

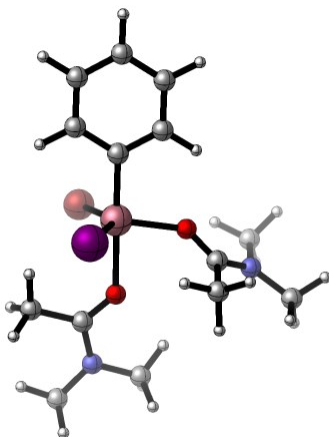
E (M06/Def2-TZVPP/SMD(DMA)//BP86/Def2-SVP) = -5061.67675593

Zero-point correction= 0.341862 (Hartree/Particle)
Thermal correction to Energy= 0.370415
Thermal correction to Enthalpy= 0.371359
Thermal correction to Gibbs Free Energy= 0.276706

Charge = 0 Multiplicity = 1

Co	0.20586100	-0.03763400	-0.72805300
C	-2.94465900	-1.00365900	3.48804200
C	-2.71935900	-1.96172500	2.47760200
C	-2.42632000	-1.56277900	1.16191500
C	-2.33870200	-0.18794800	0.87121700
C	-2.58935900	0.78260900	1.85928900
H	-2.77311500	-3.03743300	2.71451500
H	-2.22659200	-2.30713200	0.37359700
H	-2.55648700	1.85582800	1.61142800
C	-2.88225000	0.36558000	3.17238000
H	-3.07326200	1.12271600	3.95145800
O	1.96849900	-0.38728500	-0.05691600
C	2.41472400	-1.34088700	0.64204800
N	3.75969100	-1.60433000	0.60789700
C	1.52258700	-2.14794200	1.55796400
C	4.41119200	-2.63743600	1.39658300
C	4.62991500	-0.85582200	-0.29159300
H	1.49511000	-3.21762300	1.26975200
H	1.85087200	-2.06715700	2.61709700
H	0.49645400	-1.75066300	1.45200900
H	5.18596600	-2.19825900	2.06564200
H	3.68358900	-3.18391100	2.02001500
H	4.91762900	-3.37269000	0.73172600
H	5.17043400	-1.55154100	-0.96998600
H	4.01225500	-0.16430000	-0.89065200
H	5.38579400	-0.27387300	0.28214500
O	0.59559400	1.81729200	-0.54692400
C	1.04535300	2.49589000	0.41792100
N	1.56533900	3.74464400	0.16864500
C	1.01176000	1.96078800	1.83059400
C	2.07912200	4.63146300	1.19821600
C	1.52609200	4.29377900	-1.18166000

VII



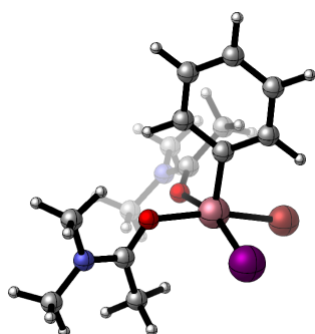
E (M06/Def2-TZVPP/SMD(DMA)//BP86/Def2-SVP) = -5061.71648894

Zero-point correction=	0.343217 (Hartree/Particle)
Thermal correction to Energy=	0.372533
Thermal correction to Enthalpy=	0.373477
Thermal correction to Gibbs Free Energy=	0.275405

Co	0.45025500	-0.08493700	0.20524200
C	5.07035000	0.90467500	0.55028700
C	4.60500400	-0.39313300	0.83402500
C	3.23690600	-0.69743800	0.73192600
C	2.31419200	0.29882200	0.34340900
C	2.78027500	1.59859100	0.06105400
H	5.31302800	-1.18122600	1.13977700
H	2.89111800	-1.71696600	0.96173000
H	2.07629500	2.38925600	-0.23752200
Br	0.28367600	-0.56335900	2.51307800
C	4.15408500	1.89664300	0.16487800
H	4.50446400	2.91825300	-0.05922200
O	-1.65938400	-0.47308100	0.05836500
C	-2.33290800	-1.49221500	0.33725300
N	-3.70012800	-1.39512300	0.42174500

C	-1.69473200	-2.84340100	0.58783800
C	-4.59310900	-2.51458400	0.68346100
C	-4.35669000	-0.11010700	0.22002300
H	-1.90245100	-3.19945900	1.61720800
H	-2.05828400	-3.60256100	-0.13489300
H	-0.60339100	-2.73938000	0.46810300
H	-5.28865700	-2.67358300	-0.17135200
H	-4.02937700	-3.44784000	0.84743200
H	-5.20900200	-2.31789700	1.58918600
H	-4.95318000	-0.10816500	-0.72011500
H	-5.04475100	0.10387400	1.06638900
H	-3.58610000	0.67837700	0.16519300
O	-0.20867800	1.81216500	-0.07086600
C	-1.08684500	2.37323100	-0.77213100
N	-1.75038100	3.45171200	-0.25666600
C	-1.39620600	1.90357700	-2.17724000
C	-2.65408100	4.30085200	-1.02049900
C	-1.45539100	3.89704900	1.10538700
H	-2.47974800	1.73481300	-2.33653100
H	-1.04804800	2.64694200	-2.92535500
H	-0.85539700	0.95306700	-2.34790500
H	-2.22688300	5.32141500	-1.14455300
H	-2.84528600	3.88227300	-2.02319900
H	-3.62667800	4.40397800	-0.49182500
H	-0.83839300	4.82281800	1.09673900
H	-2.40428800	4.11405300	1.63890200
H	-0.90060600	3.10142000	1.63354500
I	0.83847400	-1.41616700	-1.97576300
H	6.14387100	1.14009100	0.63090600

VIII



E (BP86/Def2-SVP) = -5061.60068385

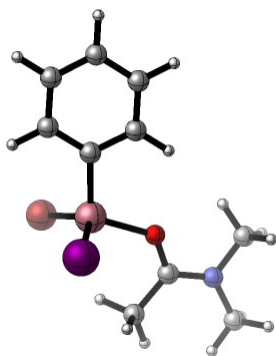
E (BP86/Def2-TZVPP/SMD(DMA)//BP86/Def2-SVP) = -5063.04847411

E (M06/Def2-TZVPP/SMD(DMA)//BP86/Def2-SVP) = -5061.73103107

Zero-point correction=	0.344084 (Hartree/Particle)
Thermal correction to Energy=	0.372866
Thermal correction to Enthalpy=	0.373811
Thermal correction to Gibbs Free Energy=	0.279359

Charge = 0 Multiplicity = 1

Co	-0.02688800	-0.15671800	0.27862800
C	-0.84226000	-2.73963700	-3.58166400
C	-0.62788000	-3.38556500	-2.35080000
C	-0.36526000	-2.64443000	-1.18240800
C	-0.31685100	-1.23273800	-1.23526400
C	-0.52961000	-0.58476700	-2.47311400
H	-0.65992600	-4.48644700	-2.29069500
H	-0.20178500	-3.16770700	-0.22960600
H	-0.49344900	0.51336200	-2.53653800
C	-0.79196500	-1.33612200	-3.63640100
H	-0.95655400	-0.81224200	-4.59364600
O	-1.49602900	1.13749900	0.01873700
C	-2.75312900	1.07560200	-0.07898600
N	-3.48141000	2.20288500	0.18838400
C	-3.48323300	-0.17391000	-0.51418500
C	-4.93395500	2.27858100	0.11331900
C	-2.81574000	3.43517200	0.59716800
H	-4.16158500	-0.53673500	0.28388400
H	-4.07817200	0.01514300	-1.43211200
H	-2.74201400	-0.96404200	-0.71808900
H	-5.25117300	3.02076800	-0.65314400
H	-5.37414300	1.30110300	-0.14373600
H	-5.35272100	2.60058100	1.09219600
H	-3.10565500	3.71138400	1.63476600
H	-1.72400000	3.28436200	0.55050400
H	-3.10356900	4.26954200	-0.07883400
O	1.07441700	1.13622800	-0.75025600
C	1.77305900	2.06183200	-0.26031500
N	2.70205400	2.67654300	-1.04769500
C	1.60515800	2.50019600	1.18065000
C	3.56982700	3.75960000	-0.60800700
C	2.90946300	2.22098500	-2.42142800
H	2.46696600	2.16350400	1.79286800
H	1.49900100	3.59958100	1.27952700
H	0.69723600	2.02051300	1.59126700
H	3.40944400	4.66989500	-1.22794900
H	3.38903200	4.01980600	0.44847300
H	4.63670200	3.46264900	-0.71107300
H	2.62899800	3.01799900	-3.14471800
H	3.97958900	1.96693600	-2.57649300
H	2.29032700	1.32482200	-2.60112500
I	2.14390700	-1.24776500	1.05201900
Br	-1.29160300	-1.28742400	1.88720900
H	-1.04488400	-3.32663900	-4.49203100



E (BP86/Def2-SVP) = -4773.97649560

E (BP86/Def2-TZVPP/SMD(DMA)//BP86/Def2-SVP) = -4775.09144495

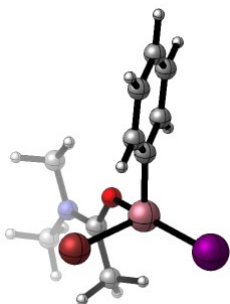
E (M06/Def2-TZVPP/SMD(DMA)//BP86/Def2-SVP) = -4773.96782926

Zero-point correction= 0.215786 (Hartree/Particle)
 Thermal correction to Energy= 0.235879
 Thermal correction to Enthalpy= 0.236823
 Thermal correction to Gibbs Free Energy= 0.159311

Charge = 0 Multiplicity = 3

Co	0.19981200	-0.05883000	0.35576400
C	3.82712000	2.32929800	-1.37942400
C	4.05037400	1.44288900	-0.30927200
C	2.98952000	0.69329200	0.23142500
C	1.69934500	0.84645800	-0.31029400
C	1.46208400	1.72373300	-1.38468000
H	5.06118100	1.33007900	0.11579600
H	3.17092700	0.00441300	1.07013800
H	0.45475300	1.82723400	-1.81694200
Br	0.23257900	0.51877700	2.58570300
C	2.53562600	2.46720000	-1.91552900
H	2.35320800	3.15492700	-2.75772300
O	-1.48378800	0.73274300	-0.41028100
C	-2.68596700	0.42039500	-0.17375100
N	-3.67931100	1.11534800	-0.79116500
C	-2.98693900	-0.70806100	0.78230400
C	-5.10114200	0.79313900	-0.72436200
C	-3.34160300	2.25331300	-1.64796600
H	-2.32037900	-0.57255200	1.66074200
H	-4.03170700	-0.77068400	1.13194300
H	-2.69513500	-1.66788500	0.30472900
H	-5.51502700	0.72506600	-1.75313600
H	-5.27431100	-0.17537900	-0.22683200
H	-5.66392000	1.58284300	-0.17945900
H	-3.45594400	1.98845500	-2.72185700
H	-4.02084600	3.10063700	-1.41965900
H	-2.29672100	2.55458500	-1.46108200
I	0.54660700	-2.26040800	-0.76311100
H	4.66356300	2.91182300	-1.79732900

X



E (BP86/Def2-SVP) = -4773.95355963

E (BP86/Def2-TZVPP/SMD(DMA)//BP86/Def2-SVP) = -4775.07682817

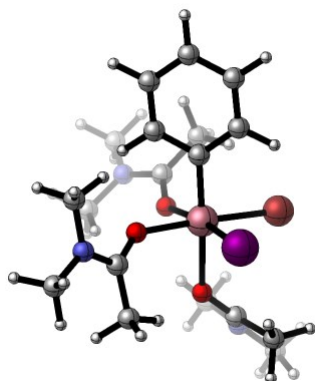
E (M06/Def2-TZVPP/SMD(DMA)//BP86/Def2-SVP) = -4773.96782926

Zero-point correction=	0.216264 (Hartree/Particle)
Thermal correction to Energy=	0.235913
Thermal correction to Enthalpy=	0.236857
Thermal correction to Gibbs Free Energy=	0.162830

Charge = 0 Multiplicity = 1

Co	0.13655700	-0.22829500	-0.16963100
C	1.99651000	4.04414400	0.02257400
C	2.36688800	3.10773600	1.00655700
C	1.81736300	1.81336700	1.00836500
C	0.87587500	1.45510400	0.01994200
C	0.48747500	2.39509600	-0.96000100
H	3.10057900	3.38222100	1.78253800
H	2.12178300	1.08599300	1.77534300
H	-0.25789700	2.13795100	-1.72955700
Br	-0.34476900	-0.86304600	1.96895700
C	1.06184500	3.68232300	-0.96204600
H	0.76317700	4.40676800	-1.73811400
O	-1.66939100	0.45741300	-0.46703400
C	-2.71081500	-0.25900200	-0.54096700
N	-3.92687200	0.34681300	-0.49694000
C	-2.60596600	-1.76223500	-0.68083500
C	-5.20324100	-0.35316100	-0.57973600
C	-4.01535000	1.80090500	-0.35329800
H	-2.71427300	-2.24707400	0.31142300
H	-3.34814900	-2.18964600	-1.38207800
H	-1.59065300	-2.00532900	-1.05379500
H	-5.74278500	-0.08853200	-1.51618200
H	-5.06838900	-1.44713200	-0.54454400
H	-5.84536800	-0.05997200	0.27818000
H	-4.49345800	2.24906600	-1.25109900
H	-4.62987500	2.05472500	0.53616500
H	-2.99957600	2.21452600	-0.23049500
I	2.13337600	-1.50585400	-0.75972000
H	2.43552200	5.05459400	0.02542700

XII



E (BP86/Def2-SVP) = -5349.22741350

E (BP86/Def2-TZVPP/SMD(DMA)//BP86/Def2-SVP) = -5350.99243400

E (M06/Def2-TZVPP/SMD(DMA)//BP86/Def2-SVP) = -5349.49561875

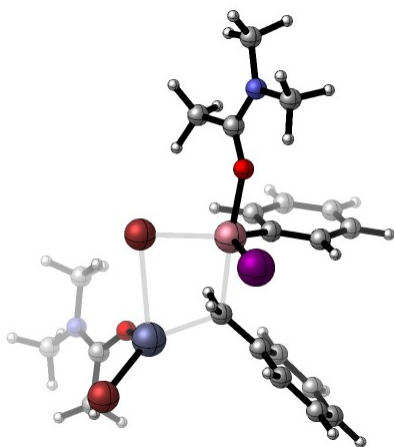
Zero-point correction=	0.471453 (Hartree/Particle)
Thermal correction to Energy=	0.509310
Thermal correction to Enthalpy=	0.510254
Thermal correction to Gibbs Free Energy=	0.396399

Charge = 0 Multiplicity = 1

Co	0.01898400	-0.04936100	-0.18123800
C	2.87000600	3.07481200	-2.39193900
C	2.30541700	2.01605200	-3.12629200
C	1.47432600	1.06675700	-2.50278400
C	1.17878500	1.15038900	-1.12094800
C	1.75840300	2.21787800	-0.39228700
H	2.51473100	1.91936400	-4.20515100
H	1.04454200	0.25387600	-3.10562800
H	1.56410500	2.31352500	0.68671700
C	2.59108600	3.16940800	-1.01842500
H	3.02523800	3.98899000	-0.41940100
O	-1.46433200	-1.20637900	0.98659800
C	-2.43127400	-1.90191800	0.59405800
N	-3.71470600	-1.50243500	0.86325200
C	-2.22720200	-3.21561500	-0.13416600
C	-4.90246600	-2.23319200	0.44756100
C	-3.95118000	-0.18708900	1.44434900
H	-2.54714500	-4.07564000	0.49324600
H	-2.79017000	-3.24433200	-1.08803400
H	-1.14881300	-3.31182000	-0.36401400
H	-5.36724000	-1.77206400	-0.45392300
H	-4.66538500	-3.28615100	0.21704100
H	-5.65593000	-2.22143700	1.26448700
H	-4.49940200	0.45927100	0.72387100
H	-4.55711400	-0.27353800	2.37328800
H	-2.97122300	0.27090200	1.66845100

O	1.26630100	0.00545500	1.40361400
C	1.78004600	-0.84867500	2.17262700
N	3.06460600	-0.66075400	2.59953800
C	1.00994400	-2.04763900	2.68337600
C	3.72993400	-1.49793000	3.58712500
C	3.87766500	0.41689900	2.04150900
H	1.54349300	-2.99546300	2.47246200
H	0.84339100	-1.96931500	3.77974900
H	0.03243000	-2.05581000	2.16977200
H	4.14219900	-0.87052300	4.40829700
H	3.03360100	-2.23020300	4.02918400
H	4.57733600	-2.05330800	3.12644900
H	4.04227400	1.22244400	2.79202200
H	4.86732500	0.01456200	1.73888500
H	3.36886600	0.84149900	1.15782200
O	-0.91846900	1.46852600	0.73715900
C	-1.27626800	2.64910200	0.49692500
N	-1.54506800	3.46931900	1.56673600
C	-1.42773000	3.20319500	-0.90120900
C	-2.01375600	4.84209100	1.45423000
C	-1.38387200	2.97008300	2.92847200
H	-2.42740500	3.66014200	-1.05076900
H	-0.65148300	3.96925600	-1.10565400
H	-1.31043500	2.36831900	-1.61697500
H	-1.33791700	5.52640600	2.01344500
H	-2.03935300	5.17128500	0.40210400
H	-3.03582900	4.95286300	1.88311600
H	-0.75309600	3.67035400	3.51777300
H	-2.36837000	2.87892400	3.43998600
H	-0.90038900	1.97806100	2.88803700
I	1.34834300	-2.11810100	-1.02953500
Br	-1.55834400	-0.16213500	-1.97977100
H	3.52142400	3.81502000	-2.88464700

TS4



E (BP86/Def2-SVP) = -9685.94018720

E (BP86/Def2-TZVPP/SMD(DMA)//BP86/Def2-SVP) = -9688.25826499

E (M06/Def2-TZVPP/SMD(DMA)//BP86/Def2-SVP) = -9686.07640913

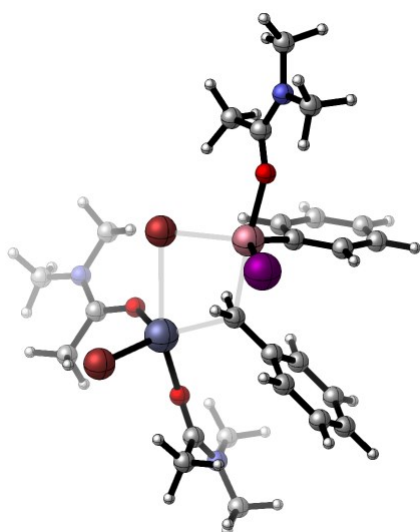
Zero-point correction=	0.457277 (Hartree/Particle)
Thermal correction to Energy=	0.498152
Thermal correction to Enthalpy=	0.499096
Thermal correction to Gibbs Free Energy=	0.367449

Charge = 0 Multiplicity = 3

Co	1.46390200	-0.05511400	-0.12831800
C	2.33943900	-0.74567500	4.47197300
C	1.65125300	-1.73041800	3.74161300
C	1.30841200	-1.50495700	2.39176100
C	1.65768200	-0.28873200	1.77017700
C	2.32977600	0.70675700	2.50570300
H	1.37081000	-2.68274300	4.22285000
H	0.76008200	-2.28217700	1.83230900
H	2.58387500	1.67175100	2.03680300
C	2.67529300	0.47131300	3.85112900
H	3.20489300	1.25445600	4.41863700
O	3.23400500	-0.83509200	-0.46875600
C	3.85298000	-1.92902000	-0.49415200
N	5.19449800	-1.90824500	-0.74218100
C	3.14783000	-3.24678000	-0.25855000
C	6.05587700	-3.08193900	-0.71543100
C	5.86559700	-0.63753000	-1.02059800
H	3.47637300	-4.03973100	-0.95806100
H	3.31997800	-3.59718200	0.78098700
H	2.06326400	-3.07722300	-0.39920000
H	6.89987800	-2.91671900	-0.01045900
H	5.50618100	-3.97891100	-0.38336700
H	6.48807100	-3.28193800	-1.72132900
H	6.46978800	-0.73076900	-1.94773000
H	5.10754000	0.15605900	-1.14968700
H	6.54458100	-0.36279900	-0.18383800
I	2.11682600	2.07489200	-1.55224500
Br	0.00780300	-1.61173400	-1.47069300
H	2.60406100	-0.92149200	5.52707400
C	-0.57076900	0.82950400	0.53526100
H	-0.16007200	1.04154900	-0.48244600
C	-0.76080700	1.95414400	1.46291300
C	-0.62991200	3.30094900	1.03085100
C	-1.11653600	1.72151200	2.81816900
C	-0.85283200	4.36450600	1.91720200
H	-0.34473600	3.50230900	-0.01398100
C	-1.34322100	2.78795200	3.69980500
H	-1.20642900	0.68337900	3.17768600
C	-1.21338400	4.11698700	3.25505100
H	-0.74497600	5.40064900	1.55782600
H	-1.61719900	2.58062500	4.74713800
H	-1.39034100	4.95512400	3.94792500
Zn	-2.22234200	0.19531500	-0.67270500
O	-3.16319500	-1.25757100	0.40258800
C	-4.35520400	-1.65021900	0.54181400

N	-4.58210000	-2.96007600	0.82890800
C	-5.49867400	-0.67188300	0.40991900
C	-5.88116900	-3.52808400	1.17269000
C	-3.45861900	-3.89941900	0.85647600
H	-6.46662900	-1.12805900	0.13594100
H	-5.62007300	-0.11417700	1.36299100
H	-5.21180100	0.06272700	-0.37332800
H	-5.80115700	-4.09100300	2.12735200
H	-6.64247100	-2.74121000	1.30548500
H	-6.22783600	-4.23446500	0.38658200
H	-3.21848700	-4.19560400	1.90104800
H	-3.72820100	-4.81202500	0.28524700
H	-2.57218600	-3.42181700	0.40296400
H	-0.65741800	-0.19024000	0.94061300
Br	-3.60516300	1.15278500	-2.28072700

TS5



E (BP86/Def2-SVP) = -9973.57711788

E (BP86/Def2-TZVPP/SMD(DMA)//BP86/Def2-SVP) = -9976.21531825

E (M06/Def2-TZVPP/SMD(DMA)//BP86/Def2-SVP) = -9973.85658995

Zero-point correction=	0.584835 (Hartree/Particle)
Thermal correction to Energy=	0.634970
Thermal correction to Enthalpy=	0.635914
Thermal correction to Gibbs Free Energy=	0.485467

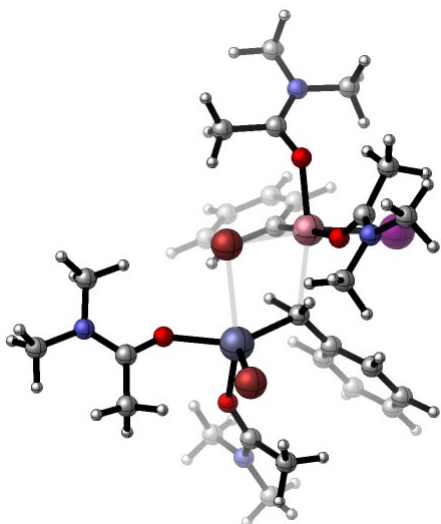
Charge = 0 Multiplicity = 3

Co	1.88123600	0.10524100	-0.09524800
C	2.38097100	1.46770100	4.41897200
C	1.84930900	0.19730100	4.13519200
C	1.62071300	-0.19613600	2.79974100
C	1.92547000	0.68168500	1.73759200
C	2.44560400	1.96080600	2.02546600
H	1.60386700	-0.49652100	4.95734700
H	1.19685200	-1.19354800	2.59135600
H	2.67071900	2.66565600	1.20771000
C	2.67651600	2.34663100	3.36035400

H	3.08640800	3.34848600	3.57188600
O	3.78485600	-0.39610400	-0.06387100
C	4.56233700	-1.26952000	0.39539300
N	5.90139000	-1.13078700	0.16397000
C	4.04578500	-2.44955600	1.18822000
C	6.92946200	-2.00022600	0.71667800
C	6.38649700	-0.01733600	-0.65236700
H	4.58163900	-3.39194600	0.96487800
H	4.12396200	-2.24281800	2.27658300
H	2.97543000	-2.57644700	0.93248100
H	7.68030100	-1.39531600	1.27114500
H	6.50108000	-2.73550700	1.41881300
H	7.46548500	-2.54894600	-0.09000700
H	7.06652000	-0.40213000	-1.44183400
H	5.52588100	0.49482600	-1.11996200
H	6.94944400	0.71037500	-0.02733000
I	2.30462400	1.56075800	-2.26355500
Br	0.79527000	-2.07855900	-0.62626800
H	2.55709500	1.77581300	5.46234200
C	-0.32643900	0.78609400	0.06406800
H	-0.03593900	0.53808300	-0.97755600
C	-0.70643400	2.16724000	0.38053400
C	-0.77284100	3.16578700	-0.62938500
C	-1.02258300	2.55389200	1.71080100
C	-1.14807100	4.48274100	-0.32139100
H	-0.50302700	2.89581000	-1.66273400
C	-1.40015800	3.87046100	2.01485100
H	-0.95224000	1.80449600	2.51546700
C	-1.46942100	4.84552900	1.00067500
H	-1.17942100	5.23809900	-1.12369400
H	-1.62413800	4.14450100	3.05925500
H	-1.75375900	5.88257400	1.24163400
Zn	-1.80931400	-0.63444700	-0.54602700
O	-3.43488600	0.38948200	0.40692500
C	-4.09696600	1.42468800	0.14232200
N	-4.75537700	2.07564800	1.14867800
C	-4.19010000	1.96216400	-1.27013100
C	-5.45850700	3.34082000	0.98814000
C	-4.64393900	1.59331400	2.52142500
H	-5.23375400	2.18505200	-1.56965500
H	-3.58979000	2.89097900	-1.36630800
H	-3.77520700	1.19714100	-1.95613200
H	-4.91407800	4.15702900	1.51290000
H	-5.54744200	3.61741200	-0.07563100
H	-6.48069000	3.27153400	1.42048100
H	-4.08311800	2.32352200	3.14469300
H	-5.65495300	1.45510800	2.96239400
H	-4.10059000	0.63250400	2.51621300
O	-2.20849200	-2.15749700	0.78403100
C	-3.01532800	-3.12261300	0.73514600
N	-2.69914200	-4.27337800	1.39524900

C	-4.30383300	-2.99671900	-0.04320200
C	-3.59759200	-5.40280900	1.59811100
C	-1.37880300	-4.39818500	2.01609700
H	-4.81919900	-3.94868800	-0.26024000
H	-4.99248300	-2.31878700	0.50207700
H	-4.05073600	-2.49418000	-1.00421300
H	-3.64618200	-5.65464100	2.67995400
H	-4.62115800	-5.16928100	1.25958600
H	-3.23843900	-6.30446300	1.05397300
H	-1.43317000	-4.22417100	3.11394800
H	-0.99157300	-5.42318700	1.84143000
H	-0.69081300	-3.66042800	1.56284500
H	-0.32148400	0.04866400	0.88316500
Br	-2.57870200	-1.09215300	-2.75945000

TS6



E (BP86/Def2-SVP) = -10261.1976068

E (BP86/Def2-TZVPP/SMD(DMA)//BP86/Def2-SVP) = -10264.1519050

E (M06/Def2-TZVPP/SMD(DMA)//BP86/Def2-SVP) = -10261.6170050

Zero-point correction=	0.712520 (Hartree/Particle)
Thermal correction to Energy=	0.771805
Thermal correction to Enthalpy=	0.772750
Thermal correction to Gibbs Free Energy=	0.604149

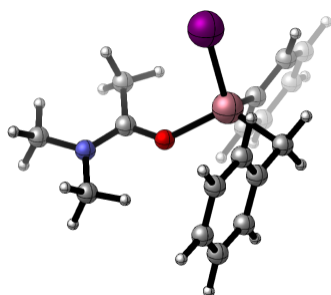
Charge = 0 Multiplicity = 3

Co	1.75625400	0.04777300	-0.02697600
C	1.60557800	1.18112500	-4.70530300
C	0.55791800	1.55506800	-3.84718600
C	0.57731200	1.18613400	-2.48672600
C	1.63998900	0.42256300	-1.93865500
C	2.68647700	0.05572900	-2.82183200
H	-0.28999700	2.14740200	-4.23176700

H	-0.24461900	1.54042900	-1.84332800
H	3.52255700	-0.55787800	-2.45316500
C	2.67141400	0.43039100	-4.18010200
H	3.50220100	0.11523900	-4.83451900
O	3.37162500	1.28944300	0.10389000
C	3.86738700	2.19876900	-0.61427500
N	5.17237600	2.10415600	-0.99954600
C	3.04592400	3.39728100	-1.03492700
C	5.88270000	3.13307900	-1.74567400
C	5.94493200	0.90523100	-0.67492400
H	3.48868100	4.34489500	-0.66248200
H	2.96269400	3.45589000	-2.13954400
H	2.03273200	3.28039200	-0.60419200
H	6.19468400	2.74840400	-2.74177400
H	5.24980600	4.02309300	-1.90042800
H	6.79906400	3.44603200	-1.19790000
H	6.65826000	1.10145800	0.15650800
H	5.25815300	0.08710300	-0.38486000
H	6.52643900	0.59099700	-1.56633700
O	1.70676200	-0.27437000	2.02134500
C	2.44555400	-0.29808300	3.03270700
N	1.86916800	-0.36912700	4.27049200
C	3.95422500	-0.24910800	2.91066600
C	2.59625200	-0.63280100	5.50292400
C	0.41120100	-0.31337700	4.38828200
H	4.44087800	0.32351400	3.72393000
H	4.36480300	-1.28057100	2.89047600
H	4.18529200	0.21705500	1.93663000
H	2.21301500	-1.56021800	5.98440800
H	3.67401600	-0.77385100	5.31230300
H	2.46992700	0.20136100	6.22917600
H	-0.03789000	-1.33045600	4.42487200
H	0.14376600	0.22105100	5.32256000
H	-0.02014300	0.22756600	3.52685400
I	3.08697700	-2.28228100	-0.23127600
Br	0.07429000	2.10063600	0.83370900
H	1.58976100	1.46669000	-5.76996500
C	-0.43287900	-0.94203500	-0.06158600
H	-0.12860500	-0.74266200	0.97765400
C	-0.66073900	-2.32743700	-0.45934800
C	-0.67455600	-3.37447900	0.50419000
C	-0.88734400	-2.68744800	-1.81703500
C	-0.91407500	-4.70459300	0.13310800
H	-0.49020600	-3.12450800	1.56115100
C	-1.12283200	-4.01937600	-2.18714700
H	-0.85086800	-1.90022900	-2.58722400
C	-1.14408900	-5.04004700	-1.21589600
H	-0.91135800	-5.49331000	0.90342400
H	-1.27158600	-4.27004400	-3.25094100
H	-1.31895600	-6.08761100	-1.50919100
Zn	-2.10484000	0.36720200	0.52892700

O	-3.50632600	-0.60644700	-0.82308100
C	-4.04025200	-1.73807700	-0.90918300
N	-4.49654100	-2.17841100	-2.12465100
C	-4.21571700	-2.62616200	0.30473200
C	-5.03208100	-3.50986600	-2.36571400
C	-4.28407900	-1.36295200	-3.31505000
H	-5.26373900	-2.97060800	0.42138800
H	-3.55726000	-3.51687100	0.23154800
H	-3.92667300	-2.04203500	1.20019700
H	-4.30894600	-4.12679600	-2.94522600
H	-5.24405100	-4.03347400	-1.41836000
H	-5.97664600	-3.44358100	-2.94889600
H	-3.56034400	-1.85430400	-4.00250100
H	-5.24227600	-1.22010000	-3.86053500
H	-3.87815300	-0.38408200	-3.00497600
O	-2.89643400	2.06696600	-0.38438700
C	-3.90063500	2.78723200	-0.16538900
N	-3.84285400	4.11199400	-0.49549500
C	-5.14959500	2.19714900	0.45116500
C	-4.97721000	5.02494300	-0.50435500
C	-2.57259500	4.67261400	-0.96005200
H	-5.82566700	2.93083500	0.92595700
H	-5.70871600	1.63064400	-0.32240800
H	-4.81413200	1.46569300	1.21848900
H	-5.07324600	5.50127500	-1.50504500
H	-5.92127000	4.49523200	-0.29095000
H	-4.84671800	5.83631500	0.24625700
H	-2.55227500	4.76123300	-2.06946300
H	-2.44383500	5.68557600	-0.52535600
H	-1.74081100	4.01931900	-0.63347200
H	-0.36850200	-0.17755500	-0.84914400
Br	-3.07234200	0.07842600	2.73132300

XIII



E (BP86/Def2-SVP) = -2470.57575974

E (BP86/Def2-TZVPP/SMD(DMA)//BP86/Def2-SVP) = -2471.669451

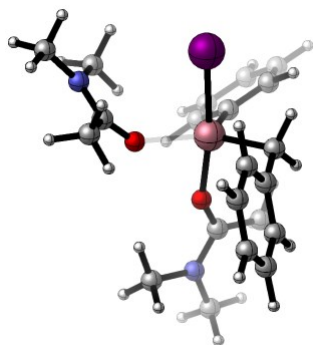
E (M06/Def2-TZVPP/SMD(DMA)//BP86/Def2-SVP) = -2470.702157

Zero-point correction=	0.329066 (Hartree/Particle)
Thermal correction to Energy=	0.354102
Thermal correction to Enthalpy=	0.355046
Thermal correction to Gibbs Free Energy=	0.266358

Charge = 0 Multiplicity = 3

Co	0.40543300	-0.45559500	-0.15952100
C	4.66711900	0.18491400	-2.08502400
C	3.52483000	0.79437100	-2.63382400
C	2.25856700	0.57426300	-2.05740900
C	2.12003100	-0.25592500	-0.91879200
C	3.27294300	-0.87414700	-0.38071200
H	3.61641400	1.44612500	-3.51899600
H	1.37341400	1.05907400	-2.50391800
H	3.18854500	-1.52479900	0.50499100
C	4.53609800	-0.64833500	-0.95828900
H	5.42707300	-1.12905500	-0.52106600
I	0.46537100	-0.60045100	2.41402000
H	5.65787300	0.35665000	-2.53572700
C	0.03044200	-2.09847200	-1.15238200
H	0.44462400	-2.88185800	-0.48515700
C	-1.44068200	-1.98954500	-1.17009800
C	-2.12723900	-1.52450800	-2.32824000
C	-2.21930900	-2.28863000	-0.01679800
C	-3.52017200	-1.37653600	-2.33486500
H	-1.54487100	-1.29146800	-3.23505700
C	-3.61415200	-2.13827600	-0.02666100
H	-1.71154600	-2.64186700	0.89496600
C	-4.27324000	-1.68113200	-1.18247400
H	-4.02880500	-1.03070500	-3.24966400
H	-4.19320900	-2.38389700	0.87806200
H	-5.36932400	-1.56954600	-1.19022600
H	0.50837800	-2.12401600	-2.14974100
O	-0.66890200	1.19529500	-0.50148600
C	-0.61909600	2.37325700	-0.05215700
N	-1.72626500	3.16157000	-0.14119600
C	0.64397300	2.91875000	0.57885300
C	-1.80723000	4.52531200	0.36618100
C	-2.95343400	2.64143700	-0.74368600
H	0.92967700	3.90588500	0.16354400
H	0.52145900	3.01617500	1.67759200
H	1.46166600	2.19885700	0.39402100
H	-2.63924600	4.60989900	1.09876200
H	-0.87367300	4.82359600	0.87172400
H	-2.00757600	5.24176800	-0.46107100
H	-3.77604000	2.64055700	0.00336300
H	-3.25827600	3.28043200	-1.60033900
H	-2.77955900	1.60899900	-1.09356500

XIV



E (BP86/Def2-SVP) = -2758.20204461

E (BP86/Def2-TZVPP/SMD(DMA)//BP86/Def2-SVP) = -2759.61845597

E (M06/Def2-TZVPP/SMD(DMA)//BP86/Def2-SVP) = -2758.45653196

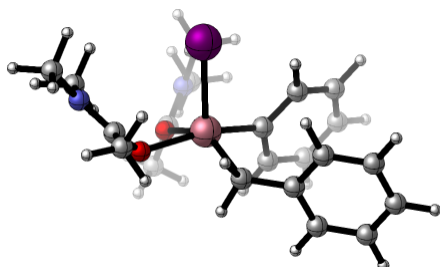
Zero-point correction=	0.457756 (Hartree/Particle)
Thermal correction to Energy=	0.491248
Thermal correction to Enthalpy=	0.492192
Thermal correction to Gibbs Free Energy=	0.388111

Charge = 0 Multiplicity = 1

Co	-0.00756600	0.12413700	0.26666800
C	-0.85740600	4.69324800	1.04547800
C	-0.57029100	4.17560900	-0.23004500
C	-0.31742600	2.79996000	-0.39958700
C	-0.35745900	1.90338100	0.70095500
C	-0.65245100	2.43991800	1.97772800
H	-0.53820900	4.84689400	-1.10553800
H	-0.07560700	2.42251900	-1.40773400
H	-0.70977400	1.77639900	2.85440100
C	-0.89460400	3.81629300	2.14562100
H	-1.12565800	4.20513700	3.15187700
O	-0.60968900	-0.46565200	-1.66812000
C	-1.56000300	-1.13167100	-2.15088500
N	-2.73436700	-0.54582800	-2.52101600
C	-1.40119200	-2.63121100	-2.32907500
C	-3.91702200	-1.28907300	-2.93537800
C	-2.95387700	0.87874900	-2.28502700
H	-2.04542000	-3.16731500	-1.60033200
H	-1.65837700	-2.98122900	-3.34962900
H	-0.34929700	-2.88661900	-2.11004800
H	-4.40127100	-0.77735600	-3.79433100
H	-3.66257100	-2.31709300	-3.24512100
H	-4.65638200	-1.34497200	-2.10472000
H	-3.69659000	1.02498700	-1.47160200
H	-2.00803800	1.34945700	-1.96959600
H	-3.32809000	1.36107600	-3.21377000
O	1.65267400	0.48996000	-0.67663700
C	2.66708400	1.23216300	-0.69430700
N	3.55046000	1.08735900	-1.73238000
C	2.95207600	2.26918000	0.37201700
C	4.80996700	1.80646500	-1.84694000
C	3.28713300	0.09917600	-2.77628200

H	3.88071900	2.02709700	0.93064900
H	3.06727800	3.28163900	-0.06550700
H	2.10119600	2.29585400	1.07367900
H	4.86032300	2.35151000	-2.81560700
H	4.93049800	2.54006100	-1.03207800
H	5.67140700	1.10190900	-1.81094300
H	3.44263700	0.56019200	-3.77487800
H	3.97239600	-0.77210700	-2.68061900
H	2.24444400	-0.25279300	-2.68257700
I	-2.29244200	-0.67934100	1.18966800
H	-1.05352200	5.76903400	1.18126500
C	0.92533400	-0.32446400	1.92516300
H	0.18170500	-0.44482200	2.73669800
C	1.60749400	-1.60018200	1.57360900
C	3.00397000	-1.64944900	1.31263300
C	0.88613600	-2.82099600	1.46593300
C	3.64725800	-2.84657800	0.96544200
H	3.59664200	-0.72510100	1.41569400
C	1.52813800	-4.01994300	1.11691600
H	-0.19766000	-2.81329000	1.66720200
C	2.91110800	-4.04175300	0.85964000
H	4.73516000	-2.85200000	0.78550400
H	0.94182700	-4.95136700	1.05241100
H	3.41422600	-4.98383900	0.58843400
H	1.64934700	0.47143100	2.19456700

XV



E (BP86/Def2-SVP) = -2758.19012026

E (BP86/Def2-TZVPP/SMD(DMA)//BP86/Def2-SVP) = -2759.60710871

E (M06/Def2-TZVPP/SMD(DMA)//BP86/Def2-SVP) = -2758.46725072

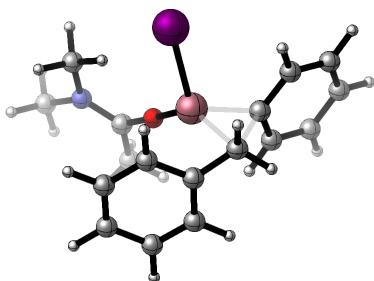
Zero-point correction=	0.456422 (Hartree/Particle)
Thermal correction to Energy=	0.490500
Thermal correction to Enthalpy=	0.491444
Thermal correction to Gibbs Free Energy=	0.384096

Charge = 0 Multiplicity = 3

Co	0.40543300	-0.45559500	-0.15952100
C	4.66711900	0.18491400	-2.08502400
C	3.52483000	0.79437100	-2.63382400
C	2.25856700	0.57426300	-2.05740900
C	2.12003100	-0.25592500	-0.91879200
C	3.27294300	-0.87414700	-0.38071200
H	3.61641400	1.44612500	-3.51899600

H	1.37341400	1.05907400	-2.50391800
H	3.18854500	-1.52479900	0.50499100
C	4.53609800	-0.64833500	-0.95828900
H	5.42707300	-1.12905500	-0.52106600
I	0.46537100	-0.60045100	2.41402000
H	5.65787300	0.35665000	-2.53572700
C	0.03044200	-2.09847200	-1.15238200
H	0.44462400	-2.88185800	-0.48515700
C	-1.44068200	-1.98954500	-1.17009800
C	-2.12723900	-1.52450800	-2.32824000
C	-2.21930900	-2.28863000	-0.01679800
C	-3.52017200	-1.37653600	-2.33486500
H	-1.54487100	-1.29146800	-3.23505700
C	-3.61415200	-2.13827600	-0.02666100
H	-1.71154600	-2.64186700	0.89496600
C	-4.27324000	-1.68113200	-1.18247400
H	-4.02880500	-1.03070500	-3.24966400
H	-4.19320900	-2.38389700	0.87806200
H	-5.36932400	-1.56954600	-1.19022600
H	0.50837800	-2.12401600	-2.14974100
O	-0.66890200	1.19529500	-0.50148600
C	-0.61909600	2.37325700	-0.05215700
N	-1.72626500	3.16157000	-0.14119600
C	0.64397300	2.91875000	0.57885300
C	-1.80723000	4.52531200	0.36618100
C	-2.95343400	2.64143700	-0.74368600
H	0.92967700	3.90588500	0.16354400
H	0.52145900	3.01617500	1.67759200
H	1.46166600	2.19885700	0.39402100
H	-2.63924600	4.60989900	1.09876200
H	-0.87367300	4.82359600	0.87172400
H	-2.00757600	5.24176800	-0.46107100
H	-3.77604000	2.64055700	0.00336300
H	-3.25827600	3.28043200	-1.60033900
H	-2.77955900	1.60899900	-1.09356500

TS8



E (BP86/Def2-SVP) = -2470.56110440

E (BP86/Def2-TZVPP/SMD(DMA)//BP86/Def2-SVP) = -2471.64787941

E (M06/Def2-TZVPP/SMD(DMA)//BP86/Def2-SVP) = -2470.69220758

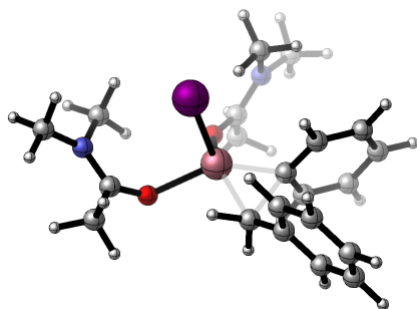
Zero-point correction=	0.329042 (Hartree/Particle)
Thermal correction to Energy=	0.352993
Thermal correction to Enthalpy=	0.353937
Thermal correction to Gibbs Free Energy=	0.270230

Charge = 0 Multiplicity = 3

Co	0.36321700	-0.01889300	0.24987900
C	3.76508800	-2.30240600	-1.95358800
C	2.57954100	-2.95936600	-1.57268300
C	1.69403200	-2.35390700	-0.66566300
C	1.95904100	-1.05925400	-0.14802100
C	3.16769200	-0.41901800	-0.51510400
H	2.34288400	-3.95555500	-1.98215400
H	0.77822900	-2.88943000	-0.36352700
H	3.39870000	0.57899500	-0.11108900
C	4.05296900	-1.03367800	-1.41808200
H	4.97850600	-0.50925700	-1.70752600
I	0.93351200	2.54545900	0.18080600
H	4.46303700	-2.78053000	-2.65915200
C	1.48157800	-0.83904500	1.82171500
H	1.94858100	0.07479700	2.23097000
C	0.05915400	-1.06209200	2.14540400
C	-0.52272100	-2.37101800	2.14279100
C	-0.81534000	0.06224400	2.32219100
C	-1.89932700	-2.54576900	2.28788000
H	0.13862200	-3.24718600	2.04571400
C	-2.20989200	-0.13740600	2.46442900
H	-0.39229400	1.06565400	2.48295700
C	-2.75466400	-1.42524100	2.43404100
H	-2.32204400	-3.56351800	2.30078900
H	-2.86158900	0.73639700	2.62523900
H	-3.83956200	-1.57294100	2.55744700
H	2.12086800	-1.72294100	1.97502400
O	-1.16889500	-0.53133600	-0.92911900
C	-2.27832200	-0.67477800	-1.49203900
N	-3.07391300	0.39122900	-1.79525400
C	-2.74304300	-2.07512300	-1.86087800
C	-4.35878500	0.28481000	-2.47403700
C	-2.65316200	1.75469800	-1.47307300

H	-3.70359100	-2.33597600	-1.37109800
H	-2.87302600	-2.19122200	-2.95688300
H	-1.96915700	-2.78454100	-1.51980300
H	-4.33422600	0.83281300	-3.44215400
H	-4.62738100	-0.76562800	-2.67701800
H	-5.16279000	0.73656900	-1.85202200
H	-2.55169100	2.35439600	-2.40337500
H	-3.41108500	2.24313300	-0.82372700
H	-1.67846700	1.74691200	-0.95004600

TS9



E (BP86/Def2-SVP) = -2758.17839155

E (BP86/Def2-TZVPP/SMD(DMA)//BP86/Def2-SVP) = -2759.59446886

E (M06/Def2-TZVPP/SMD(DMA)//BP86/Def2-SVP) = -2758.46020928

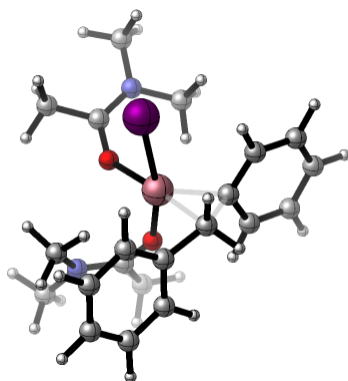
Zero-point correction=	0.455965 (Hartree/Particle)
Thermal correction to Energy=	0.489468
Thermal correction to Enthalpy=	0.490413
Thermal correction to Gibbs Free Energy=	0.384743

Charge = 0 Multiplicity = 3

Co	-0.30417300	0.02144200	-0.56085100
C	3.36439800	2.86545700	0.19483800
C	2.78963800	2.78433500	-1.08751200
C	1.88168400	1.75579400	-1.39592000
C	1.49370200	0.79542300	-0.41976800
C	2.12126200	0.86420800	0.85348500
H	3.06277400	3.51956700	-1.86349200
H	1.45464500	1.70349600	-2.41246600
H	1.87859400	0.10519600	1.61408900
C	3.02551700	1.89352400	1.15849000
H	3.48002100	1.93201000	2.16268800
O	-1.19357500	1.86798200	-0.77010300
C	-1.03138400	3.09697100	-0.55614300
N	-0.75571600	3.60111400	0.67614800
C	-1.15850400	4.05351700	-1.73211600
C	-0.46378100	5.00523400	0.93762600
C	-0.70249600	2.73437600	1.85307000
H	-1.85633700	4.89289600	-1.53709300
H	-0.16768900	4.47988100	-1.99621200
H	-1.52538100	3.47139500	-2.59593800
H	0.56857800	5.10943800	1.33761700
H	-0.54297900	5.61679700	0.02329800

H	-1.16789200	5.41167100	1.69662800
H	-1.50667500	3.01703400	2.56730000
H	-0.83093000	1.67645400	1.55789500
H	0.27951200	2.84228400	2.35736300
O	-1.80338700	-0.79117900	-1.88695600
C	-2.65617000	-1.66240600	-1.57387800
N	-3.81604200	-1.32603100	-0.94012100
C	-2.38394600	-3.12222200	-1.88736900
C	-4.71614500	-2.29086900	-0.32142000
C	-4.06420500	0.06914800	-0.58619300
H	-2.04365800	-3.63807600	-0.96295300
H	-3.26128200	-3.66654600	-2.28953900
H	-1.56472100	-3.16139100	-2.62780100
H	-5.77105700	-1.99637000	-0.50724100
H	-4.56271900	-3.30513100	-0.72818500
H	-4.54765500	-2.32690300	0.77851900
H	-5.12134700	0.32491200	-0.81272100
H	-3.86969300	0.23183000	0.49673600
H	-3.37987600	0.71727400	-1.16121000
I	-1.10216100	-1.19659500	1.74041800
H	4.08972600	3.65994400	0.43288800
C	1.32842800	-0.96883300	-1.25231200
H	1.42671100	-0.70660200	-2.32511000
C	2.55603500	-1.66380800	-0.74962600
C	2.50177700	-2.51373400	0.38062000
C	3.79568500	-1.50144400	-1.41125000
C	3.65252200	-3.18196100	0.82887200
H	1.54341000	-2.63880200	0.91269400
C	4.94531400	-2.17036000	-0.96271900
H	3.85448400	-0.83654900	-2.28886300
C	4.87897600	-3.01461000	0.16044300
H	3.58932700	-3.84146200	1.70958000
H	5.90073000	-2.03206000	-1.49440100
H	5.78056400	-3.54090100	0.51297800
H	0.46618900	-1.68711700	-1.13924200

TS10



E (BP86/Def2-SVP) = -5034.43966907

E (BP86/Def2-TZVPP/SMD(DMA)//BP86/Def2-SVP) = -2759.5656

E (M06/Def2-TZVPP/SMD(DMA)//BP86/Def2-SVP) = -2758.41803247

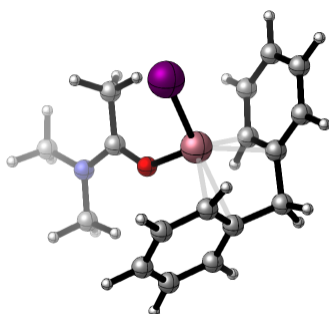
Zero-point correction=	0.458081 (Hartree/Particle)
Thermal correction to Energy=	0.490320
Thermal correction to Enthalpy=	0.491265
Thermal correction to Gibbs Free Energy=	0.392656

Charge = 0 Multiplicity = 1

Co	0.04535300	0.21564000	-0.02490200
C	2.30651600	3.71189900	2.01715400
C	0.97163900	3.43141900	2.37899600
C	0.14561600	2.66433900	1.55137900
C	0.62107300	2.07667700	0.32570400
C	1.95623700	2.44902200	-0.04947700
H	0.56143200	3.83305200	3.32135100
H	-0.89633500	2.49189900	1.85481200
H	2.35200900	2.10280700	-1.01613300
C	2.77666200	3.22354400	0.78365500
H	3.80358100	3.45492000	0.45337900
O	0.41505000	-1.58166000	0.63889100
C	1.42181500	-2.32350300	0.81566100
N	2.60521000	-1.87048600	1.30249800
C	1.26694000	-3.79708300	0.49099600
C	3.83246900	-2.65852900	1.29712200
C	2.78365800	-0.46803600	1.67235300
H	1.76399900	-4.01702300	-0.47776200
H	1.68349200	-4.47038400	1.26642700
H	0.18901600	-4.00313700	0.36828900
H	4.34172300	-2.57398600	2.28071100
H	3.63340700	-3.72448800	1.09544900
H	4.52596200	-2.27822100	0.51414400
H	3.44642600	0.04616100	0.94497200
H	1.80640500	0.05040400	1.65932500
H	3.23475200	-0.40979100	2.68562700
O	-1.26249800	0.23470300	1.46079600
C	-2.10608500	-0.47479100	2.06169300
N	-2.74199000	-1.55277200	1.51749600
C	-2.44665000	-0.07977300	3.49317200
C	-3.71640800	-2.36180500	2.23993200
C	-2.57657700	-1.92110800	0.11502600
H	-3.52696700	0.13769500	3.62391600
H	-2.16916600	-0.87566700	4.21589700
H	-1.86466100	0.82590500	3.73820100
H	-3.48086600	-3.43992100	2.10531900
H	-3.71192700	-2.14410300	3.32129600
H	-4.74495300	-2.19156400	1.84853400
H	-2.16550800	-2.94921200	0.02938200
H	-3.55662000	-1.87594900	-0.40459600
H	-1.88361900	-1.21611600	-0.37827600
I	1.65572200	-0.46627900	-2.02892500
H	2.95228600	4.32103600	2.66914300
C	-0.47283100	2.10413300	-1.04485300
H	0.17487600	2.08765000	-1.93978500

C	-1.76547700	1.35828800	-1.30581100
C	-2.94654400	1.67924200	-0.57382300
C	-1.92133400	0.53321700	-2.45576100
C	-4.19603700	1.15606200	-0.93551500
H	-2.87533900	2.37050400	0.28136700
C	-3.17523300	0.02178200	-2.82168600
H	-1.03554400	0.30337100	-3.06870900
C	-4.32421600	0.31906700	-2.06188500
H	-5.08951600	1.43275000	-0.35094500
H	-3.25716500	-0.60785400	-3.72295500
H	-5.31029600	-0.07249500	-2.35912600
H	-0.75305500	3.15636600	-0.85551700

XVI



E (BP86/Def2-SVP) = -2470.60087840

E (BP86/Def2-TZVPP/SMD(DMA)//BP86/Def2-SVP) = -2471.69355064

E (M06/Def2-TZVPP/SMD(DMA)//BP86/Def2-SVP) = -2470.75160855

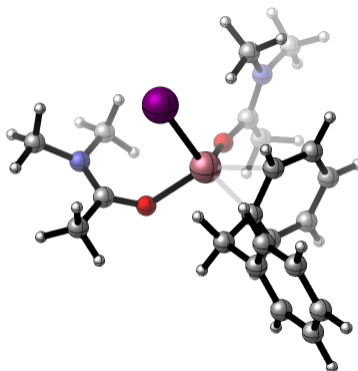
Zero-point correction=	0.330689 (Hartree/Particle)
Thermal correction to Energy=	0.354882
Thermal correction to Enthalpy=	0.355826
Thermal correction to Gibbs Free Energy=	0.272418

Charge = 0 Multiplicity = 3

Co	0.33955200	0.29431900	-0.01687600
C	2.60187800	-0.92123100	2.50732900
C	1.24638800	-0.61630300	2.64776100
C	0.70824100	0.59396200	2.12078600
C	1.57963800	1.51381200	1.44535500
C	2.96100400	1.18140800	1.32957100
H	0.58325000	-1.30304000	3.19839700
H	-0.30309900	0.91371200	2.41927400
H	3.63675400	1.89074000	0.82406800
C	3.46472500	-0.01279900	1.84883300
H	4.53343500	-0.25208900	1.73555500
I	1.57267700	-1.41676200	-1.50586100
H	3.00016300	-1.86584400	2.90933500
C	1.03576000	2.87487900	1.03086600
H	1.84959300	3.49090200	0.59031400
C	-0.07931300	2.65420000	0.02146900
C	-1.41454200	3.07096000	0.25840200
C	0.24842100	2.05961400	-1.24500700
C	-2.40382800	2.92051400	-0.72015900

H	-1.66175100	3.54282400	1.22426900
C	-0.77437500	1.92147000	-2.23248200
H	1.30319900	1.97945800	-1.55928300
C	-2.08156900	2.33190300	-1.96917700
H	-3.42868300	3.27507200	-0.52448700
H	-0.51099900	1.49468000	-3.21298900
H	-2.85897100	2.21936800	-2.74191900
H	0.65547900	3.43073300	1.91537200
O	-1.59465100	-0.24967100	0.43069800
C	-2.18055300	-1.34915800	0.59474800
N	-3.54761200	-1.37755900	0.67517900
C	-1.41228800	-2.64999600	0.71126700
C	-4.33425800	-2.58375500	0.88844400
C	-4.31506600	-0.14226300	0.54975300
H	-1.53436200	-3.10514000	1.71648300
H	-1.73966300	-3.39157700	-0.04546700
H	-0.34232200	-2.43196200	0.53046900
H	-5.02069200	-2.76205300	0.03067800
H	-3.68879300	-3.47042900	1.00529000
H	-4.95807300	-2.48408900	1.80466500
H	-5.05578100	-0.23374500	-0.27408400
H	-4.86784200	0.07170000	1.49127300
H	-3.62173200	0.68952100	0.33069100

XVII



E (BP86/Def2-SVP) = -2758.19872136

E (BP86/Def2-TZVPP/SMD(DMA)//BP86/Def2-SVP) = -2759.64607223

E (M06/Def2-TZVPP/SMD(DMA)//BP86/Def2-SVP) = -2758.51680138

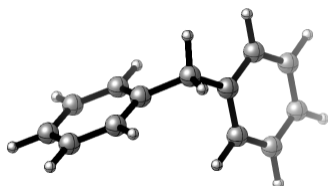
Zero-point correction=	0.455949 (Hartree/Particle)
Thermal correction to Energy=	0.490678
Thermal correction to Enthalpy=	0.491622
Thermal correction to Gibbs Free Energy=	0.378886

Charge = 0 Multiplicity = 3

Co	-0.38222000	0.06837300	-0.32085400
C	0.73325400	3.46700000	-0.25429300
C	1.06726300	2.94491300	-1.53397100
C	1.45633800	1.61369600	-1.67464600
C	1.51714900	0.71688500	-0.54676100
C	1.12552500	1.25125600	0.74258100

H	1.03624400	3.59946800	-2.42040100
H	1.74908500	1.23151600	-2.66700700
H	1.34273700	0.67821100	1.65742900
C	0.77226500	2.62733800	0.86116400
H	0.55499900	3.03401000	1.86286100
O	-1.81125000	1.42050800	-0.78920000
C	-2.45597300	2.47041300	-0.55855400
N	-2.87216100	2.81840300	0.69547400
C	-2.82290400	3.36896900	-1.73085200
C	-3.63041700	4.02386300	0.99928700
C	-2.58006500	1.96328500	1.84361500
H	-3.92191300	3.46510900	-1.85701300
H	-2.40077100	4.38832700	-1.61706600
H	-2.39753600	2.91366200	-2.64239300
H	-3.06300800	4.67517300	1.70117500
H	-3.85251000	4.60698600	0.08958400
H	-4.59459000	3.76231700	1.48964000
H	-3.51846900	1.53236500	2.25710900
H	-1.91011700	1.13607500	1.54062600
H	-2.08562200	2.55499300	2.64285700
O	-0.71872200	-1.30316500	-1.83188300
C	-1.16611300	-2.47635900	-1.71081700
N	-2.48417600	-2.70778700	-1.45895700
C	-0.21851400	-3.65061400	-1.84539800
C	-3.01226800	-3.99336000	-1.01786200
C	-3.38846500	-1.57259600	-1.29385100
H	0.05065800	-4.01622100	-0.83040400
H	-0.63311400	-4.49645500	-2.42864700
H	0.70341700	-3.28706500	-2.33370400
H	-3.98868900	-4.19025400	-1.50912900
H	-2.32351500	-4.81807500	-1.26883900
H	-3.16203200	-3.98881200	0.08531900
H	-4.38364500	-1.83747500	-1.70766600
H	-3.49078300	-1.31360200	-0.21631800
H	-2.97744500	-0.69476100	-1.82267300
I	-0.89147800	-1.60808000	1.74247700
H	0.47113500	4.53142900	-0.14179300
C	2.37402100	-0.55417700	-0.63171900
H	2.30548500	-0.95412000	-1.66533300
C	3.83296300	-0.31969000	-0.26363900
C	4.31430700	-0.65333300	1.02104700
C	4.73326100	0.25984800	-1.18504400
C	5.65314000	-0.41309700	1.37685900
H	3.62725300	-1.11391500	1.75024600
C	6.07185400	0.50107900	-0.83383000
H	4.37863500	0.52593500	-2.19456200
C	6.53736700	0.16620100	0.45058300
H	6.00789900	-0.68421800	2.38447200
H	6.75806300	0.95139700	-1.56946500
H	7.58750600	0.35336100	0.72666800
H	1.94913600	-1.32536900	0.04587700

PhBn



E (BP86/Def2-SVP) = -502.244150526

E (BP86/Def2-TZVPP/SMD(DMA)//BP86/Def2-SVP) = -502.793829659

E (M06/Def2-TZVPP/SMD(DMA)//BP86/Def2-SVP) = -502.395627521

Zero-point correction=	0.203568 (Hartree/Particle)
Thermal correction to Energy=	0.214211
Thermal correction to Enthalpy=	0.215155
Thermal correction to Gibbs Free Energy=	0.164731

Charge = 0 Multiplicity = 1

C	-3.68597300	0.88224500	0.14633300
C	-2.66050800	1.14490700	1.07374900
C	-1.47116500	0.39977600	1.04261000
C	-1.28233600	-0.62538600	0.08813700
C	-2.31702400	-0.87626300	-0.83730100
H	-2.78872700	1.93888000	1.82712600
H	-0.66924900	0.61781000	1.76710300
H	-2.18674100	-1.67154500	-1.59051800
C	-3.50996000	-0.13089100	-0.81048500
H	-4.30462700	-0.34374300	-1.54362300
H	-4.61855600	1.46829000	0.16954900
C	-0.00055000	-1.44798000	0.07572700
H	-0.04638600	-2.16458300	-0.77387000
C	1.28195800	-0.63252800	-0.02257100
C	2.31203900	-0.77824500	0.93012700
C	1.47596000	0.27946300	-1.08479500
C	3.50540600	-0.04034800	0.82604400
H	2.17780600	-1.48447700	1.76678200
C	2.66570100	1.01664200	-1.19315300
H	0.67776100	0.41491200	-1.83315800
C	3.68652200	0.85948500	-0.23713000
H	4.29641800	-0.16992000	1.58221800
H	2.79798900	1.72138100	-2.02996400
H	4.61944600	1.43938100	-0.32119600
H	0.04444800	-2.07164100	0.99579700

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