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Supporting Information

Rationale for the Sluggish Oxidative Addition of Aryl Halides to Au(I)

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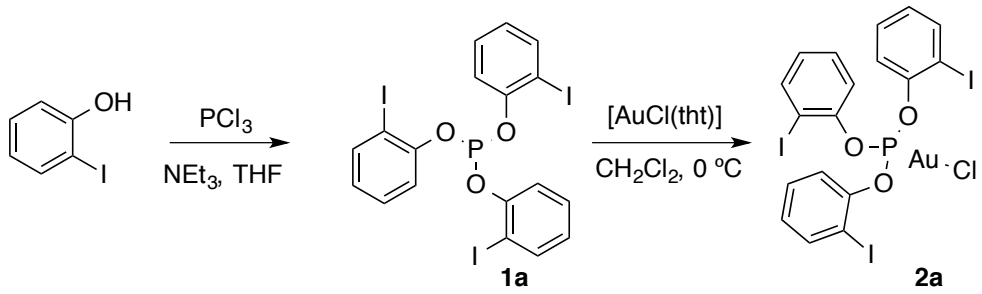
General methods

All reactions were carried out under Ar atmosphere. Solvents were dried using a Solvent Purification System (SPS). Analytical thin layer chromatography controls were carried out using TLC-aluminum sheets with 0.2 mm of silica gel (Merck GF234). Flash chromatography purifications were carried out using flash grade silica gel (SDS Chromatogel 60 ACC, 40-60. NMR spectra were recorded at 23 ºC (except stated) on the following spectrometers: Bruker Avance 400 Ultrashield (400 MHz for ^{1}H, and 100 MHz for ^{13}C) and Bruker Avance 500 Ultrashield (500 MHz for ^{1}H, and 125 MHz for ^{13}C) at the Institut Català d'Investigaciò Química (ICIQ). Mass spectra were recorded on a Waters LCT Premier (ESI) and Waters GCT (EI, CI) spectrometers at the ICIQ. Melting points were determined using a Büchi melting point apparatus.

X-Ray: Crystal structure determination were performed using a Bruker-Nonius diffractometer equipped with a APPEX 2 4K CCD area detector, a FR591 rotating anode with Mo_{K_α} radiation, Montel mirrors as monochromator and a Kryoflex low temperature device (T = 100 K). Fullsphere data collection omega and phi scans. Programs used: Data collection Apex2 V. 1.0-22 (Bruker-Nonius 2004), data reduction Saint + Version 6.22 (Bruker-Nonius 2001) and absorption correction SADABS V. 2.10 (2003). Crystal structure solutions were achieved using direct methods as implemented in SHELXTL Version 6.10 (Sheldrick, Universität Göttingen (Germany), 2000) and visualized using XP program. Missing atoms were subsequently located from difference Fourier synthesis and added to the atom list. Least-squares refinements on F2 using all measured intensities were carried out using the program SHELXTL Version 6.10 (Sheldrick, Universität Göttingen (Germany), 2000). All non-hydrogen atoms were refined including anisotropic displacement parameters.

Synthesis of Gold(I) Complex 2a

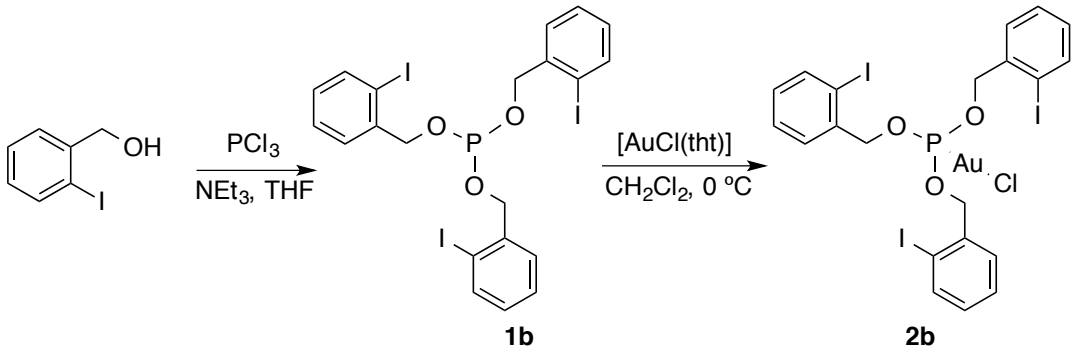


Tris(2-iodophenyl)phosphite (1a). To a solution of 2-iodophenol (2.00 g, 9.1 mmol) and PCl_3 (265 μL, 3.0 mmol) in dry THF (15 mL) in an Schenk flask under strictly inert conditions was added NEt_3 (1.26 mL, 9.1 mmol, 3 equiv) using a syringe pump. The solution was stirred at room temperature for 24 h. After making sure that all PCl_3 had been consumed (^{31}P NMR) the solution was filtered under a flow of Ar over a pad of silica. The filtrate was quickly evaporated on a rotavap connected to the Ar line and the resulting gray oil was dried over night under high vacuum and then transferred into the glove box. The phosphite ligand was used without further purification. ^{1}H NMR (500 MHz, CD_2Cl_2) δ 7.85 (dd, J = 7.9, 1.5 Hz, 1H), 7.39 (m, 1H), 7.34 (m, 1H), 6.91 (m, 1H). ^{31}P NMR (202 MHz, CD_2Cl_2) δ 132.7 (s).

Chloro[tris(2-iodophenyl)phosphite] gold (2a).[1] A dry tube containing chloro(tetrahydrothiophene) gold (205 mg, 0.64 mmol) was transferred into the glove-box. To the tube was added tris(2-iodophenyl)phosphite (**1a**) (1.3 mL, 1.46 M stock solution in CH_2Cl_2). After stirring for 30 min the tube was taken out of the glove box and the solution was concentrated. The complex was then purified by column chromatography (83% CH_2Cl_2 in cyclohexane) to give the pure complex as a snow-white solid (102 mg, 17%). ^{1}H NMR (500 MHz, CD_2Cl_2) δ 7.93 (d, J = 7.7 Hz, 1H), 7.53 (d, J = 8.2 Hz, 1H), 7.44 (t, J = 7.7 Hz, 1H), 7.12 – 7.04 (m, 1H). ^{13}C NMR (126 MHz, CD_2Cl_2) δ 149.94 (s, C), 140.98 (s, CH), 130.48 (s, CH), 128.78 (s, CH), 123.11 (s, CH), 90.17 (s, C). ^{31}P NMR (162 MHz, CD_2Cl_2) δ 116.59 (s). HRMS-ESI: *m/z* calcd for $C_{18}H_{12}AuClI_3O_3P$: 942.6910; found 942.6865 $[M+1]Na^+$. $C_{18}H_{12}AuClI_3O_3P$: calcd C 23.49, H 1.31: found C 23.74, H 1.49.

Synthesis of Gold(I) Complex 2b

(1) A. S. K. Hashmi, A. Loos, A. Littmann, I. Braun, J. Knight, S. Doherty, F. Rominger, *Adv. Synth. Catal.* **2009**, *351*, 576-582.

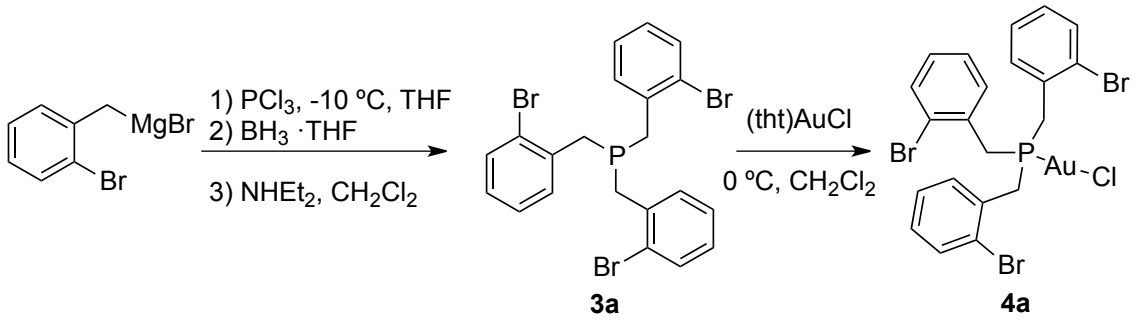


1b **2b**

Tris(2-iodobenzyl)phosphite (1b). To a solution of 2-iodobenzyl alcohol (2.0 g, 8.3 mmol,) and PCl_3 (250 μL, 2.8 mmol) in dry THF (15 mL) in an Schenk flask under strictly inert conditions was added NEt_3 (1.15 mL, 8.3 mmol, 3 equiv) using a syringe pump. The solution was stirred at room temperature for 24 h. After making sure that all PCl_3 had been consumed (^{31}P NMR) the solution was filtered under a flow of Ar over a pad of silica. The filtrate was quickly evaporated on a rotavap connected to the Ar line and the resulting gray oil was dried over night under high vacuum and then transferred into the glove box. The phosphite ligand was used without further purification. ^{1}H NMR (500 MHz, CD_2Cl_2) δ 7.83 (d, J = 7.6 Hz, 1H), 7.46 (d, J = 7.6 Hz, 1H), 7.35 (t, J = 7.6 Hz, 1H), 7.01 (t, J = 7.6 Hz, 1H), 4.95 (d, J = 7.3 Hz, 2H). ^{31}P NMR (202 MHz, CD_2Cl_2) δ 143.10 (s).

Chloro[tris(2-iodobenzyl)phosphite] gold (2b).[1] A dry tube containing the chloro(tetrahydrothiophene) gold (221 mg, 0.69 mmol) was transferred into the glove box and dissolved in 0.5 mL dry CH_2Cl_2. To the tube was added tris(2-iodobenzyl)phosphite (507 mg, 0,69 mmol, 1 equiv) (**1b**) in 0.5 mL CH_2Cl_2. After stirring for 30 min the tube was taken out of the glove-box and the solution was concentrated. The complex was then purified by column chromatography (50% CH_2Cl_2 in cyclohexane) to give the pure complex as a snow-white solid (60 mg, 10%). ^{1}H NMR (400 MHz, CD_2Cl_2) δ 7.86 (d, J = 7.9 Hz, 1H), 7.38 (m, 2H), 7.11–7.02 (t, J = 7.6 Hz 1H), 5.17 (d, J = 9.8 Hz, 2H). ^{13}C NMR (126 MHz, CD_2Cl_2) δ 140.06 (s, CH), 137.39 (s, C), 130.57 (s, CH), 129.86 (s, CH), 128.65 (s, CH), 98.60 (s, C), 73.18 (s, CH2). ^{31}P NMR (162 MHz, CD_2Cl_2) δ 121.91 (s). HRMS-ESI: *m/z* calcd for $C_{21}H_{18}AuClI_3O_3P$: 984.7380; found 984.7311 $[M+1]Na^+$. $C_{21}H_{18}AuClI_3O_3P$: calcd C 26.21, H 1.89: found C 26.80, H 2.04.

Synthesis of Gold (I) Complex 4a



3a **4a**

Tris(2-bromobenzyl)phosphine (3).

To a solution of 2-bromobenzyl magnesium bromide (20 mL, 5.0 mmol, 3.1 eq, 0.25M in THF) in dry THF (20 mL) in an Schenk flask under strictly inert conditions was added PCl_3 (142 µL, 1.6 mmol, 1 equiv) at -10 ºC dropwise. The Schenk flask was carefully closed with parafilm and the key to the Ar line was closed. When at room temperature the ice-bath was removed and the solution was left stirring in this manner over night. After making sure that all PCl_3 had been consumed (^{31}P NMR) the solution was cooled down to 0 ºC and BH_3·THF complex (15 mL, 15 mmol, 1M in THF) was added. The solution was left stirring until reaching room temperature and all phosphine had been protected (^{31}P-NMR), normally 2 h. The solution was carefully quenched by the slow addition of H_2O at 0 ºC. The two organic phases were separated and the aqueous phase washed once with EtOAc. The organic fractions were combined, dried and concentrated onto Florisil. The concentrated product was then purified by column chromatography (3% EtOAc in cyclohexane) and the purified protected phosphine was transferred into a dried flask. Degassed $NHEt_2$ was added and the solution was stirred for 3 h at 50 ºC or until all phosphine had been deprotected. The excess amine was removed by inert evaporation and the resulting oil was dissolved in dry degassed CH_2Cl_2 and transferred into a tarred Schenk and the solution was concentrated. The pure phosphine was then transferred for storage to the glove box (520 mg, 60%).

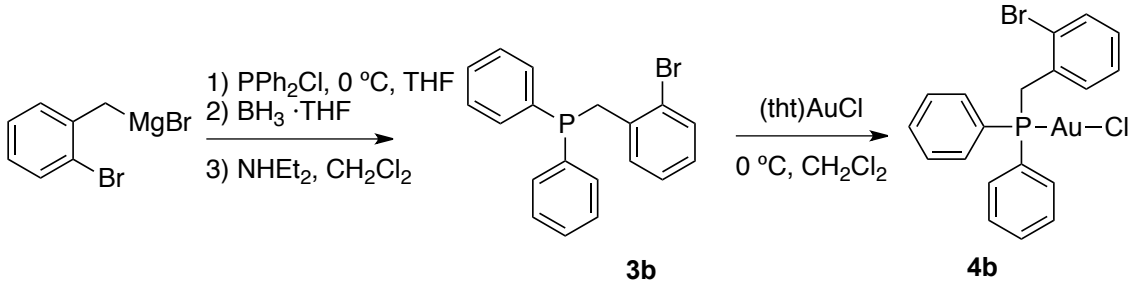
^{1}H NMR (400 MHz, CD_2Cl_2) δ ^{1}H NMR (400 MHz, CD_2Cl_2) δ 7.52 (d, J = 8.0 Hz, 1H), 7.23 – 7.15 (m, 2H), 7.03 (m, 1H), 3.14 (s, 3H). ^{13}C NMR (126 MHz, CD_2Cl_2) δ 138.29 (d, J = 6.9 Hz, C), 133.27 (CH), 131.34 (d, J = 7.4 Hz, CH), 127.98 (d, J = 2.8 Hz, CH), 127.79 (CH), 125.00 (d, J = 4.1 Hz, C), 35.41 (d, J = 21.7 Hz, CH_2). ^{31}P NMR (162 MHz, CD_2Cl_2) δ -6.32 (s).

Chloro[tris(2-bromobenzyl)phosphine] gold (4a).[1]

A dry tube containing the chloro(tetrahydrothiophene) gold (100.0 mg, 0.3 mmol, 1 equi) was transferred into the glove-box and dissolved in 0.5 mL dry CH_2Cl_2. To the tube was added tris(2-bromobenzyl)phosphine (**3a**) (170.0 mg, 0.3 mmol, 1 equiv) in 0.5 mL CH_2Cl_2. After stirring for 30 min the tube was taken out of the glove-box and the solution was concentrated. The complex was then purified by column chromatography (50% CH_2Cl_2 in cyclohexane) to give the pure complex as a snow-white solid (115 mg, 50%).

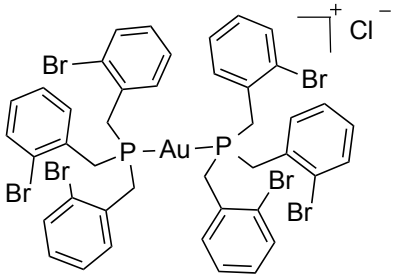
^{1}H NMR (500 MHz, CD_2Cl_2) δ 7.63 (d, J = 8.0 Hz, 1H), 7.46 (dt, J = 7.7, 1.9 Hz, 1H), 7.33 (t, J = 8.0, 1H), 7.21 (tt, J = 8.0, 1.9 Hz, 1H), 3.65 (d, J = 11.4 Hz, 2H). ^{13}C NMR (126 MHz, CD_2Cl_2) δ 133.96 (s, CH), 133.06 (s, C), 132.32 (s, CH), 129.87 (s, CH), 128.61 (s, CH), 125.53 (s, C), 33.60 (s, CH2). ^{31}P NMR (162 MHz, CD_2Cl_2) δ 40.39 (s). HRMS-ESI: *m/z* calcd for $C_{21}H_{18}AuClBr_3P$: 734.8362; found 734.8362 [M+].

Synthesis of Gold(I) complex 4b



(2-Bromobenzyl)diphenylphosphine: To a solution of diphenylphosphine chloride (0.8 mL, 4.5 mmol) in dry THF (15 mL) was added 2-bromobenzyl magnesium bromide (27 mL, 6.80 mmol, 0.25 M in THF) at 0 ºC. When at room temperature the ice-bath was removed and the solution was left stirring until all chlorophosphine had been consumed (^{31}P NMR). The solution was then cooled down to 0 ºC and BH_3·THF complex (15 mL, 15 mmol, 1M in THF) was added. The solution was left stirring until reaching room temperature and all phosphine had been protected (^{31}P-NMR), normally 2 h. The reaction was carefully quenched by the slow addition of H_2O at 0 ºC. The two organic phases were separated and the aqueous phase washed once with EtOAc. The organic fractions were combined, dried and concentrated onto Florisil. The concentrated product was then purified by column chromatography (3% EtOAc in cyclohexane) and the purified protected phosphine was transferred into a dried flask. ^{1}H NMR (400 MHz, CD_2Cl_2) δ 7.67-7.62 (m, 4H), 7.55-7.51 (m, 2H), 7.47-7.42 (m, 5H), 7.23-7.16 (m, 2H), 7.10-7.06 (m, 1H), 3.89 (d, J = 12.0 Hz, 2H). ^{31}P NMR (162 MHz, CD_2Cl_2) δ 21.73 (d,

J = 64.4). ^{11}B NMR (160 MHz, CD_2Cl_2) δ -38.68 (d, J = 54.7 Hz). Degassed $NHEt_2$ was added and the solution was stirred for 3 h at 50 ºC or until all phosphine had been deprotected (^{31}P NMR). The excess amine was removed by inert evaporation and the resulting oil was dissolved in dry degassed CH_2Cl_2 and filtered inertly over a plug of celite into a tarred flask. The solvent was concentrated under the hood and the resulting oil was transferred into the glove box. Phosphine (**3b**) was isolated as a sticky oil in 38% yield (620 mg, 1.75 mmol (including 10% of the oxidized phosphine)). ^{1}H NMR (400 MHz, CD_2Cl_2) δ 7.54-7.53 (m, 1H), 7.45-7.41 (m, 5H), 7.35-7.34 (m, 5H), 7.07-7.01 (m, 2H), 6.84 (dt, J = 7.3 Hz, 1.9 Hz, 1H) 3.58 (s, 2H). ^{13}C NMR (126 MHz, CD_2Cl_2) *δ* 137.9 (C), 137.2 (C), 132.9 (CH), 132.8 (CH), 132.7 (CH), 130.9 (CH), 128.7 (CH), 128.3 (CH), 128.3 (CH), 127.5 (CH), 126.9 (CH), 99.9 (C), 36.1 (CH_2). ^{31}P NMR (162 MHz, CD_2Cl_2) *d* -9.83 (s), 31.09 (s). HRMS-ESI: *m/z* calcd for $C_{19}H_{17}BrP$: 355.0246; found 355.0256. The spectral data is in accordance with previously reported synthesis.[2]



5

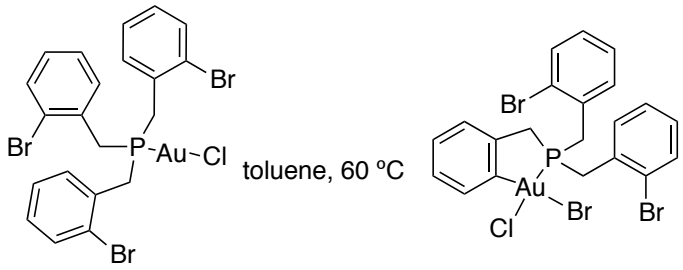
Synthesis of Gold (I) Complex 5.

Cationic bis[tris(2-bromobenzyl)phosphine] gold chloride (**5**) was synthesized using the same method as for complex **4a** but applying two equivalents of phosphine **3b**. The product precipitated as a practically insoluble white powder in 70% yield (276 mg, 0.2 mmol).

^{1}H NMR (400 MHz, CD_2Cl_2) δ 7.47 (d, *J* = 8.3 Hz, 1H), 7.42 (d, *J* = 7.1 Hz, 1H), 7.16 (t, *J* = 7.1 Hz, 1H), 7.01 (bs, 1H), 3.97 (bs, 2H). ^{13}C NMR (126 MHz, CD_2Cl_2) δ 133.7 (CH), 133.3 (CH), 129.8 (CH), 128.6 (CH), 125.2 (C), 33.3 (CH_2). ^{31}P NMR (162 MHz, CD_2Cl_2) δ 45.94 (bs).

Attempted Formation of Gold (III) Complexes by Oxidative Addition.

[2] Morales-Morales, D.; Redón, R.; Zheng, Y.; Dilwort, J. R. *Inorg. Chim. Acta* **2002**, 39-44.



4a

Chloro[tris(2-bromobenzyl)phosphine] gold (**4a**) was dissolved in dry toluene and stirred over night at 23 ºC in the glove box. After monitoring the reaction by NMR the tube was removed from the glove box and stirred under Ar in the fume hood at 60 ºC. The reaction was monitored for several days without the detection of formation of the auracycle nor decomposed Au(0).

Similar negative results were obtained using complex **4b** under these conditions

Cationic bis[tris(2-bromobenzyl)phosphine] gold chloride (**5**) was dissolved in DMSO and stirred at 100 ºC for several days without the detection of formation of the auracycle nor decomposed Au(0).

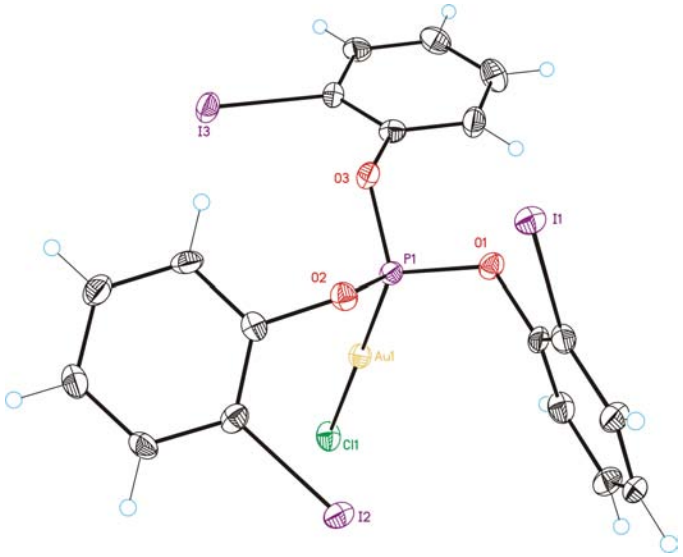


Figure 1. Crystal structure of complex **2a**. Carbon atoms are shown in light gray, hydrogen atoms in white, oxygen atoms in red, gold atom in yellow, phosphorous and iodine atoms in purple and chloride in green.

Table 1. Crystal data and structure refinement for complex **2a**.

Empirical formula	C18 H12 Au Cl I3 O3 P	
Formula weight	920.36	
Temperature	293(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/n	
Unit cell dimensions	a = 11.0595(5) Å	⟨= 90.00 °.
	b = 12.7552(6) Å	® = 105.0190(10) °.
	c = 16.4234(8) Å	© = 90.00 °.
Volume	2237.64(18) Å^3	
Z	4	
Density (calculated)	2.732 Mg/m^3	
Absorption coefficient	10.920 mm^{-1}	
F(000)	1656	
Crystal size	0.25 x 0.10 x 0.03 mm^3	
Theta range for data collection	2.00 to 30.03 °.	
Index ranges	-14 <=h<=15 ,-17 <=k<=15 ,-22 <=l<=21	
Reflections collected	5473	
Independent reflections	4935 [R(int) = 0.0401]	
Completeness to theta =30.03 °	0.837 %	
Absorption correction	Empirical	
Max. and min. transmission	0.98 and 0.81	

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Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	5473 / 0 / 244
Goodness-of-fit on F^2	0.761
Final R indices [I>2sigma(I)]	R1 = 0.0268 , wR2 = 0.0859
R indices (all data)	R1 = 0.0307 , wR2 = 0.0918
Largest diff. peak and hole	1.739 and -1.597 e.Å^{-3}

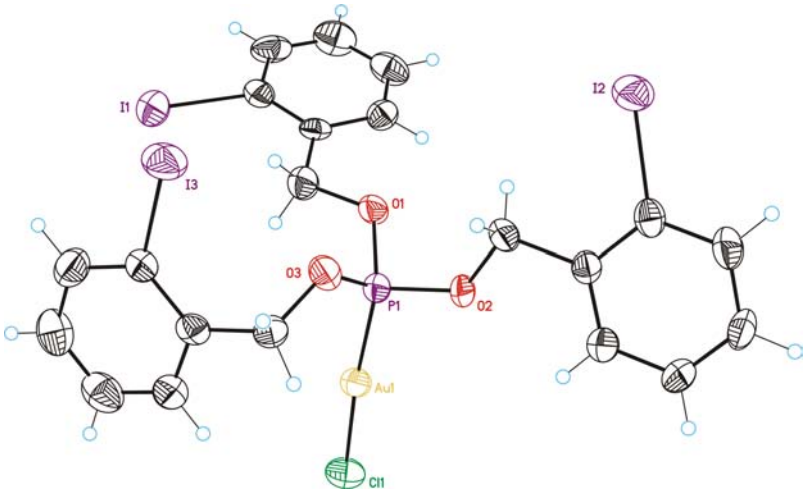

Figure 2. Crystal structure of complex **2b**. Carbon atoms are shown in light gray, hydrogen atoms in white, oxygen atoms in red, gold atom in yellow, phosphorous and iodine atoms in purple and chloride in green.

Table 2. Crystal data and structure refinement for complex **2b**.

Empirical formula	C21 H18 Au Cl I3 O3 P	
Formula weight	962.44	
Temperature	300(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	Pbca	
Unit cell dimensions	a = 18.718(2) Å	⟨= 90°.
	b = 8.0042(12) Å	®= 90°.
	c = 33.333(5) Å	© = 90°.
Volume	4994.0(13) Å^3	
Z	8	
Density (calculated)	2.560 Mg/m^3	
Absorption coefficient	9.792 mm^{-1}	
F(000)	3504	
Crystal size	0.21 x 0.20 x 0.20 mm^3	
Theta range for data collection	1.22 to 25.04°.	
Index ranges	-22<=h<=19, -8<=k<=9, -39<=l<=38	
Reflections collected	29265	
Independent reflections	4402 [R(int) = 0.0705]	
Completeness to theta = 25.04°	99.5 %	
Max. and min. transmission	0.2448 and 0.2329	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4402 / 0 / 271	
Goodness-of-fit on F^2	1.062	

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Final R indices [I>2sigma(I)]	R1 = 0.0340, wR2 = 0.0634
R indices (all data)	R1 = 0.0491, wR2 = 0.0727
Largest diff. peak and hole	0.757 and -0.904 e.Å^{-3}

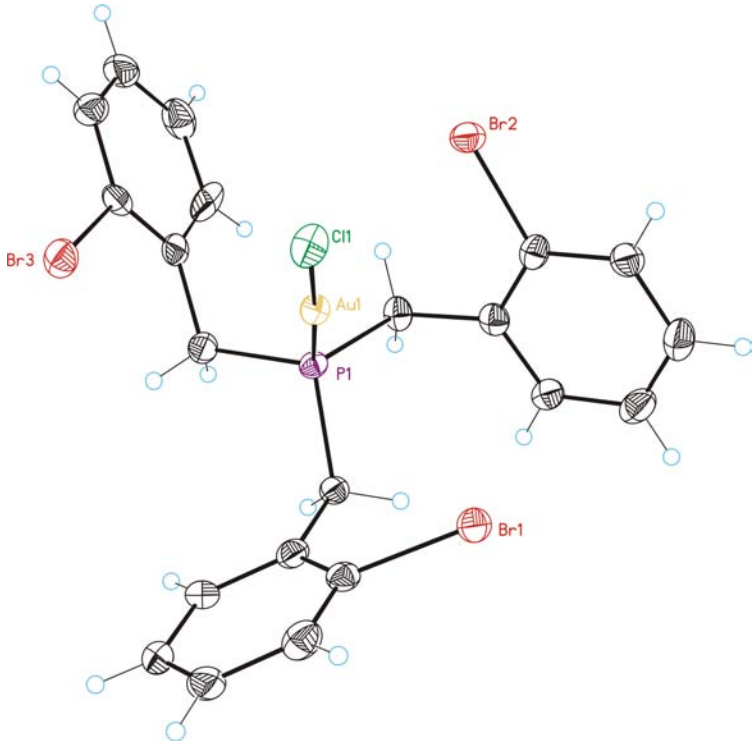

Figure 3. Crystal structure of complex **4a**. Carbon atoms are shown in light gray, hydrogen atoms in white, gold atom in yellow, phosphorous atoms in purple, bromide atoms in red and chloride atom in green.

Table 3. Crystal data and structure refinement for complex **4a**.

Empirical formula	C23 H21 Au Br3 Cl N P	
Formula weight	814.52	
Temperature	293(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	P2(1)2(1)2(1)	
Unit cell dimensions	a = 12.6165(5) Å	⟨= 90.00 °.
	b = 13.1976(4) Å	® = 90.00 °.
	c = 14.9182(5) Å	© = 90.00 °.
Volume	2483.99(15) Å^3	
Z	4	
Density (calculated)	2.178 Mg/m^3	
Absorption coefficient	10.932 mm^{-1}	
F(000)	1528	
Crystal size	0.20 x 0.20 x 0.15 mm^3	
Theta range for data collection	2.06 to 30.03 °.	
Index ranges	-16 <=h<=16 ,-18 <=k<=17 ,-19 <=l<=19	
Reflections collected	17891	

Independent reflections	6257 [R(int) = 0.0445]
Completeness to theta =30.03 °	0.898 %
Absorption correction	Empirical
Max. and min. transmission	0.1983 and 0.1113
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	6257 / 6 / 272
Goodness-of-fit on F^2	1.042
Final R indices [I>2sigma(I)]	R1 = 0.0326 , wR2 = 0.0807
R indices (all data)	R1 = 0.0339 , wR2 = 0.0814
Absolute Structure Flack parameter	x =-0.0008(7)
Largest diff. peak and hole	3.287 and -1.474 e.$Å^{-3}$

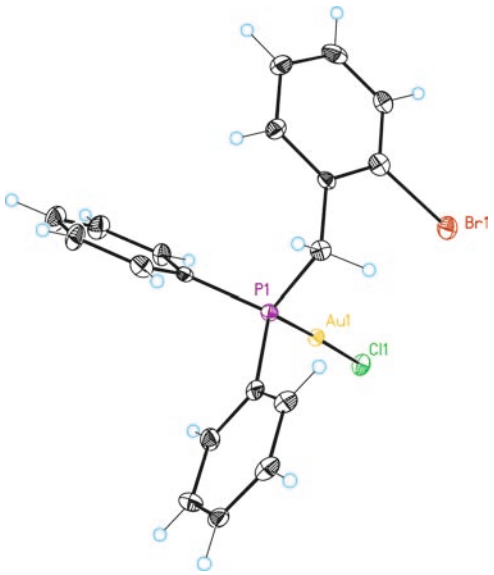

Figure 7. Crystal structure of complex **4b**. Carbon atoms are shown in light gray, hydrogen atoms in white, gold atom in yellow, phosphorous atoms in purple, bromide atoms in red and chloride atom in green.

Table 7. Crystal data and structure refinement for **4b**.

Identification code		mo_MLd84_0m
Empirical formula		C19 H16 Au Br Cl P
Formula weight		587.61
Temperature		100(2)K
Wavelength		0.71073 Å
Crystal system		Monoclinic
Space group		P2(1)/n
Unit cell dimensions	a = 8.4286(9) Å	a= 90.00 °.
	b = 16.0606(18) Å	b = 106.295(4) °.
	c = 13.9197(16) Å	g = 90.00 °.
Volume		1808.6(3) $Å^3$
Z		4
Density (calculated)		2.158 Mg/m^3
Absorption coefficient		10.575 mm^{-1}
F(000)		1104
Crystal size		0.30 x 0.18 x 0.10 mm^3
Theta range for data collection		1.98 to 30.24 °.
Index ranges		-11 <=h<=9 ,-22 <=k<=21 ,-13 <=l<=19
Reflections collected		15740
Independent reflections		4852 [R(int) = 0.0595]
Completeness to theta =30.24 °		0.901 %

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Absorption correction	Empirical
Max. and min. transmission	0.4177 and 0.1436
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4852 / 0 / 208
Goodness-of-fit on F^2	1.052
Final R indices [I>2sigma(I)]	R1 = 0.0404 , wR2 = 0.1082
R indices (all data)	R1 = 0.0525 , wR2 = 0.1185
Largest diff. peak and hole	3.678 and -3.188 e.Å^{-3}

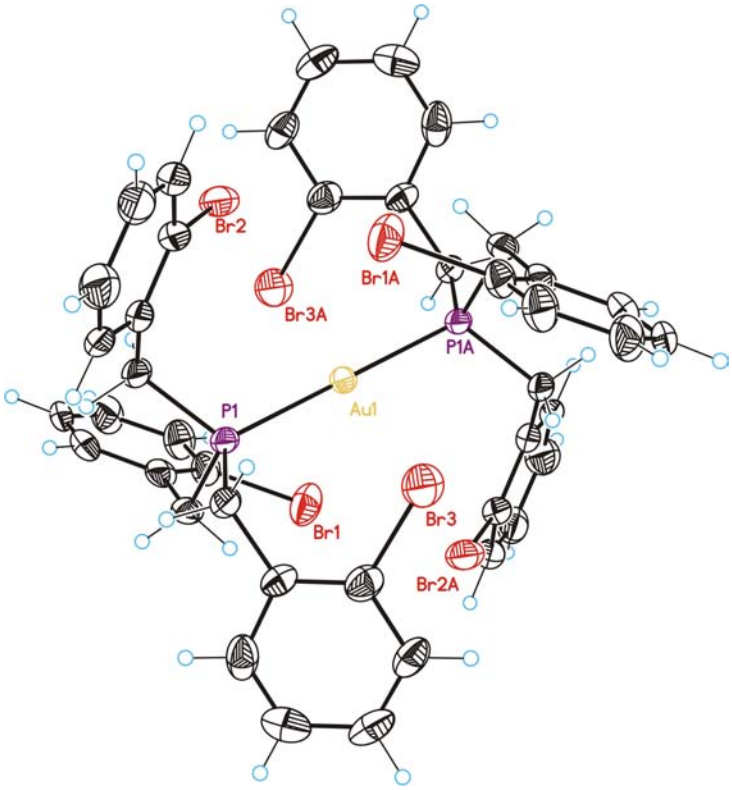

Figure 4. Crystal structure of complex **5**. Carbon atoms are shown in light gray, hydrogen atoms in white, gold atom in yellow, phosphorous atoms in purple, bromide atoms in red and chloride atom in green.

Table 4. Crystal data and structure refinement for complex **5**.

Empirical formula	C46.50 H44 Au Br6 Cl8.50 P2	
Formula weight	1642.51	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	C2/c	
Unit cell dimensions	a = 17.0229(14) Å	⟨= 90.00 °.
	b = 16.1927(14) Å	® = 106.408(3) °.
	c = 20.3819(17) Å	© = 90.00 °.
Volume	5389.4(8) Å^3	
Z	4	
Density (calculated)	2.024 Mg/m^3	
Absorption coefficient	7.693 mm^{-1}	
F(000)	3146	
Crystal size	0.30 x 0.10 x 0.10 mm^3	
Theta range for data collection	1.77 to 30.04 °.	
Index ranges	-22 <=h<=23 ,-22 <=k<=22 ,-28 <=l<=28	

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Reflections collected	51011
Independent reflections	7285 [R(int) = 0.0381]
Completeness to theta =30.04 °	0.923 %
Absorption correction	Empirical
Max. and min. transmission	0.5134 and 0.2062
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	7285 / 112 / 322
Goodness-of-fit on F^2	1.083
Final R indices [I>2sigma(I)]	R1 = 0.0443 , wR2 = 0.1121
R indices (all data)	R1 = 0.0621 , wR2 = 0.1229
Largest diff. peak and hole	1.736 and -1.391 e.$Å^{-3}$

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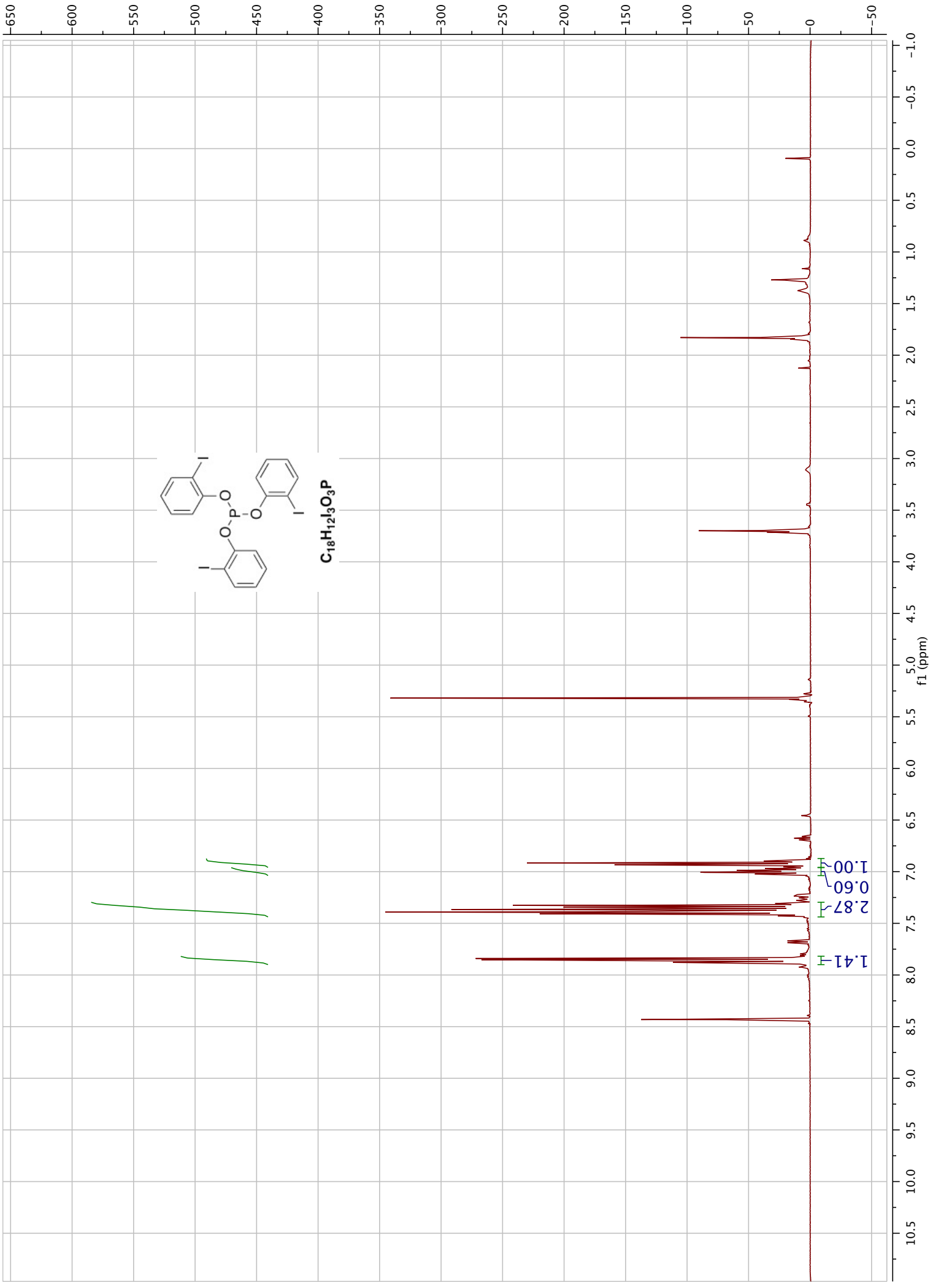

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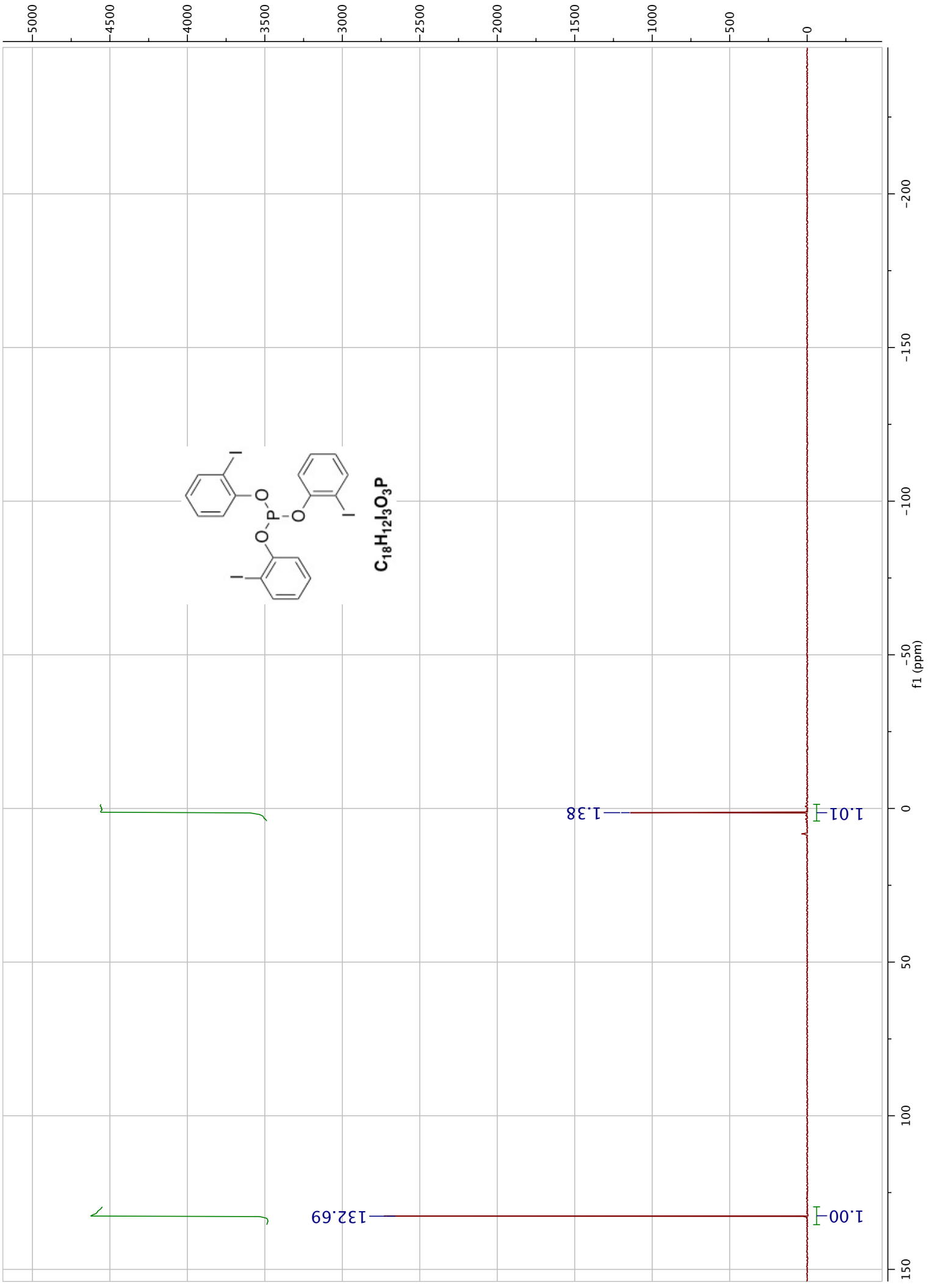

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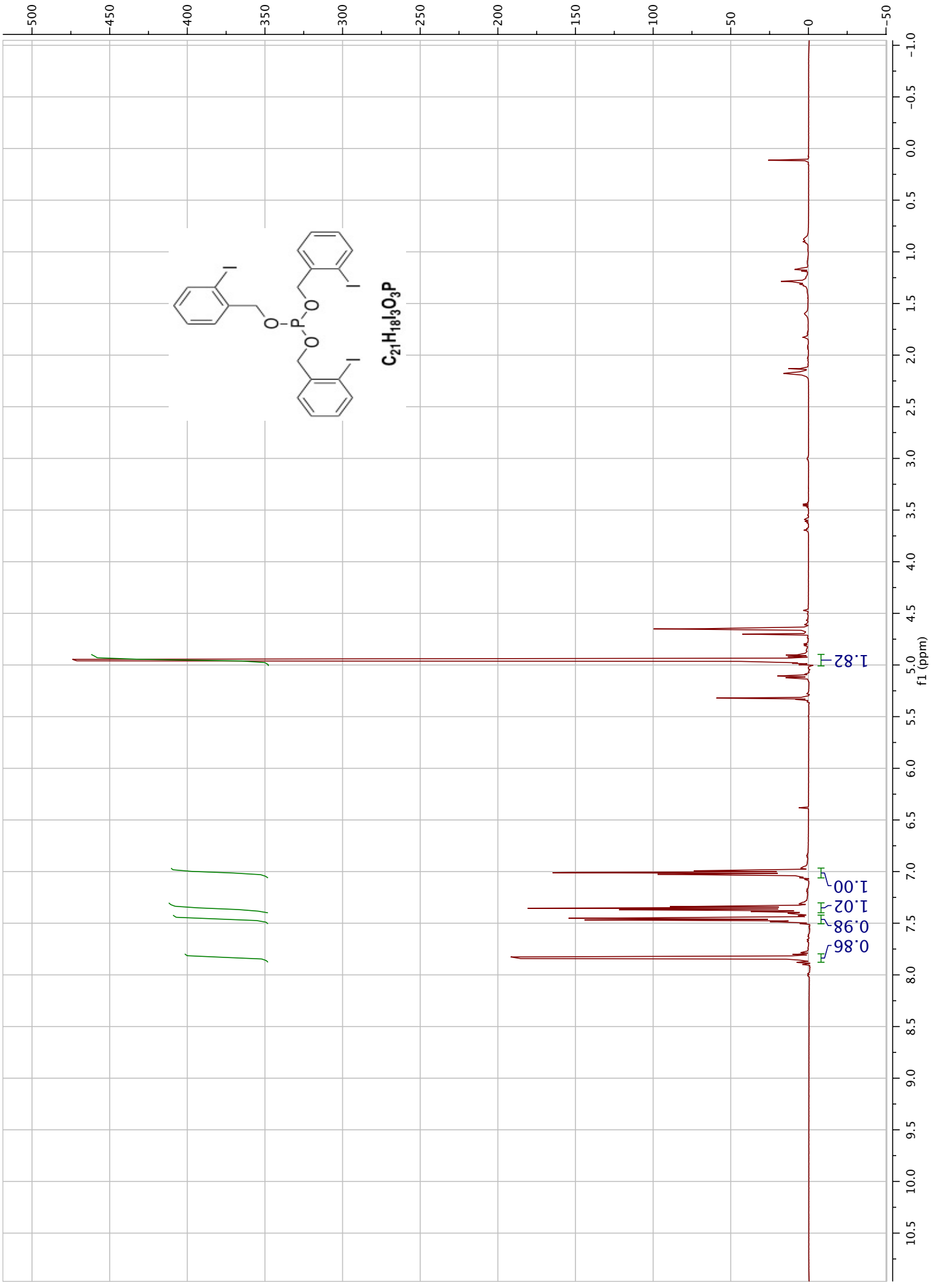

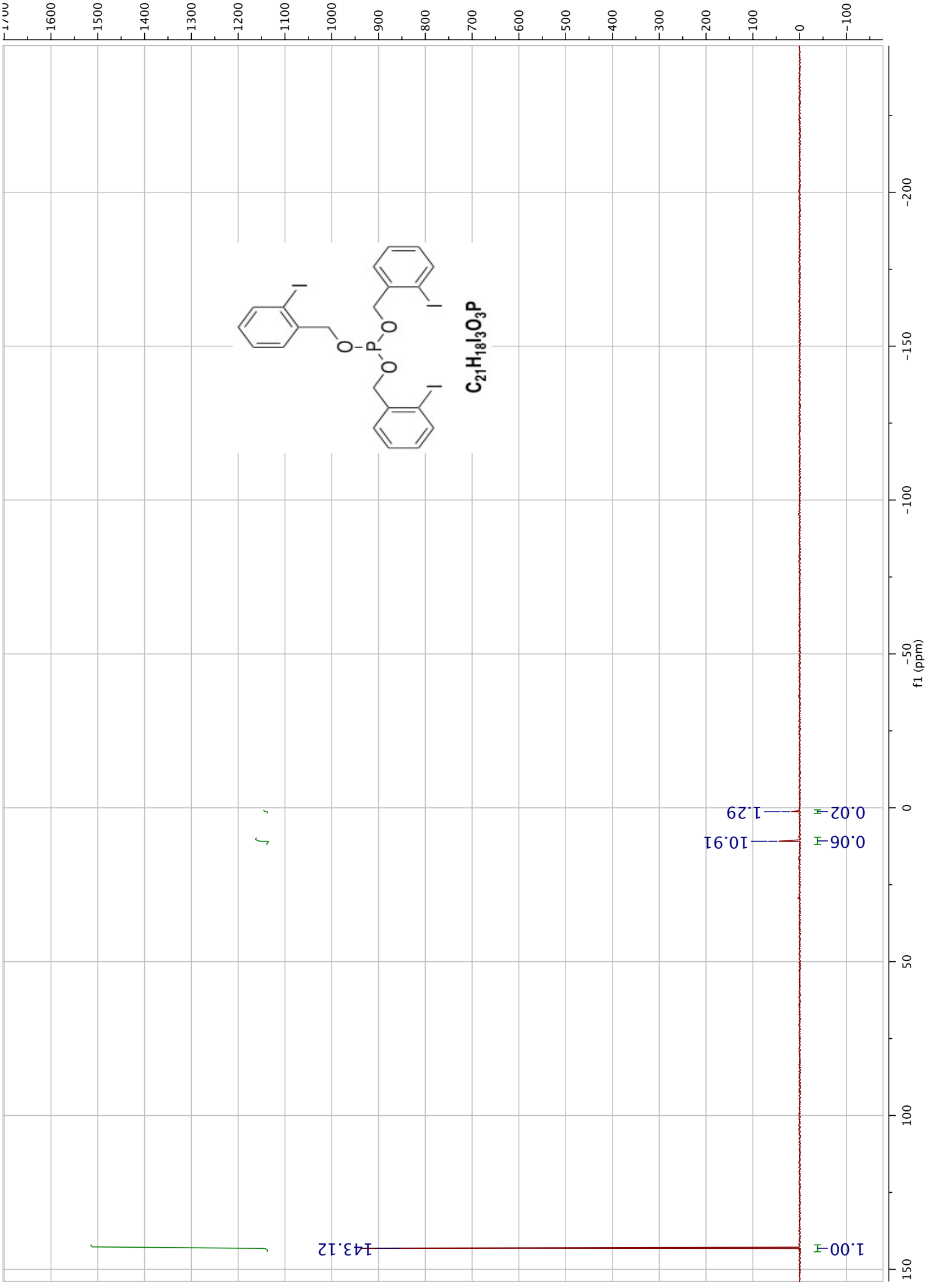
1.00
143.12
0.06
10.91
0.02
1.29
f1 (ppm)
C21H18I3O3P

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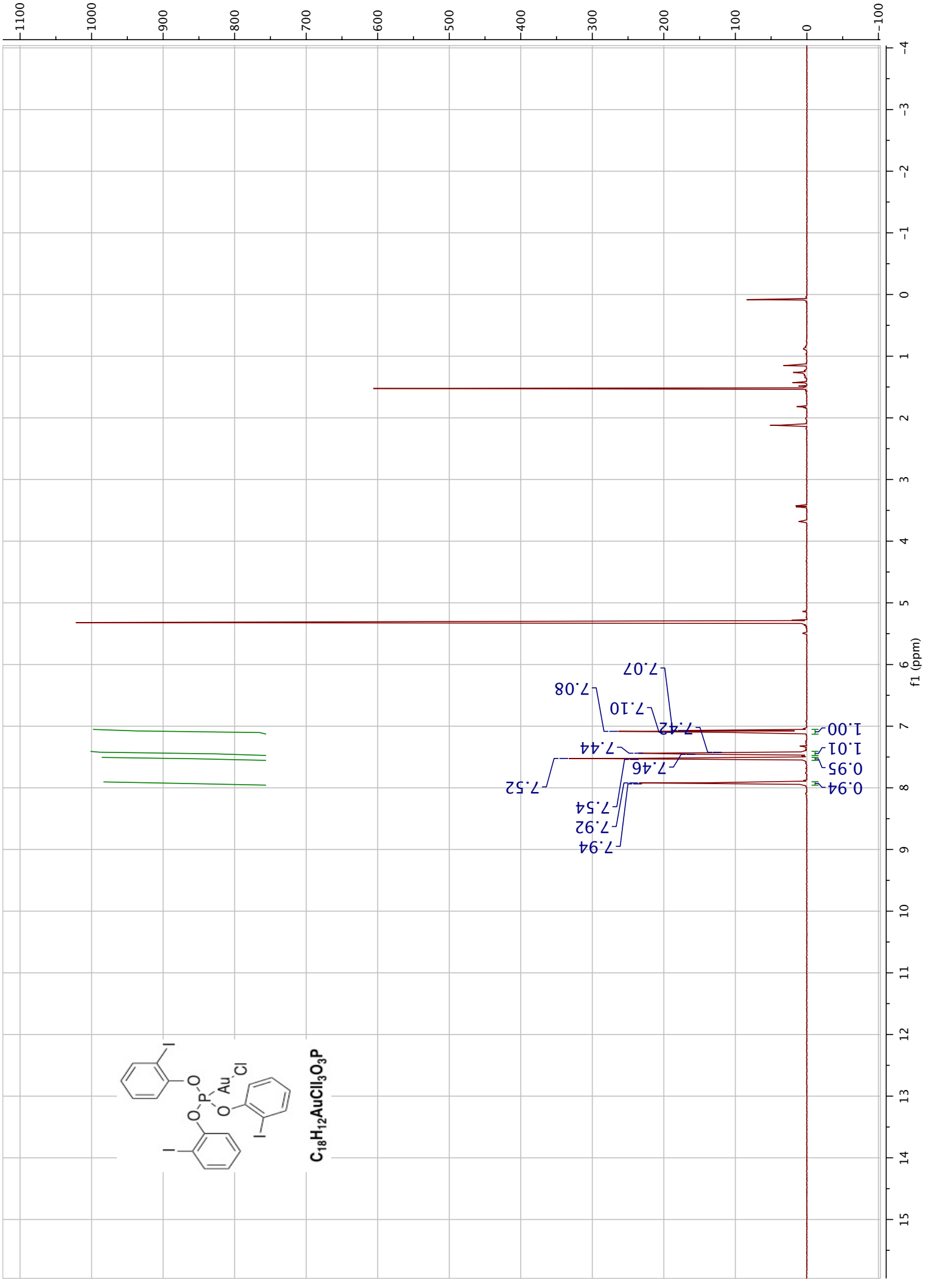

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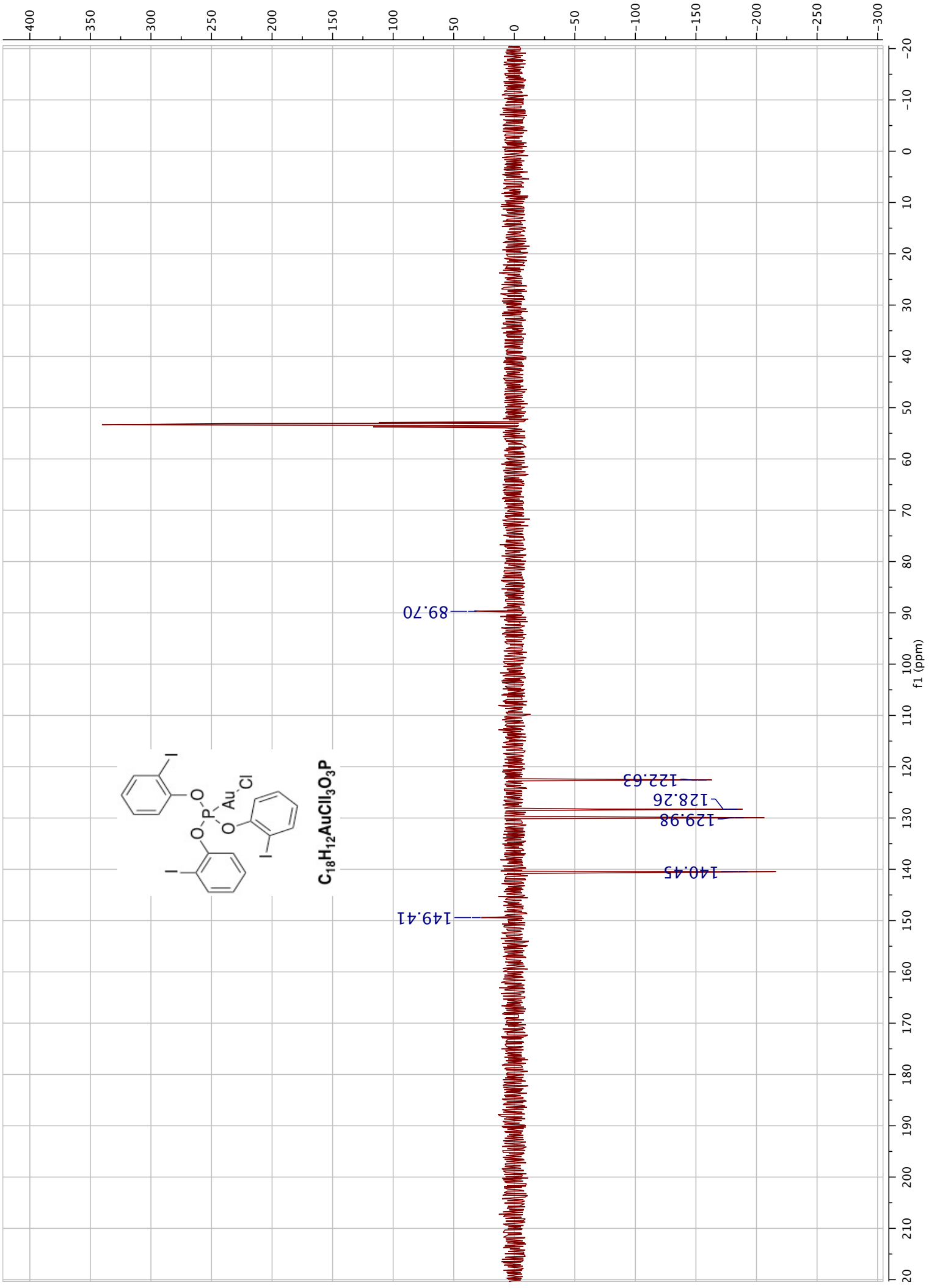

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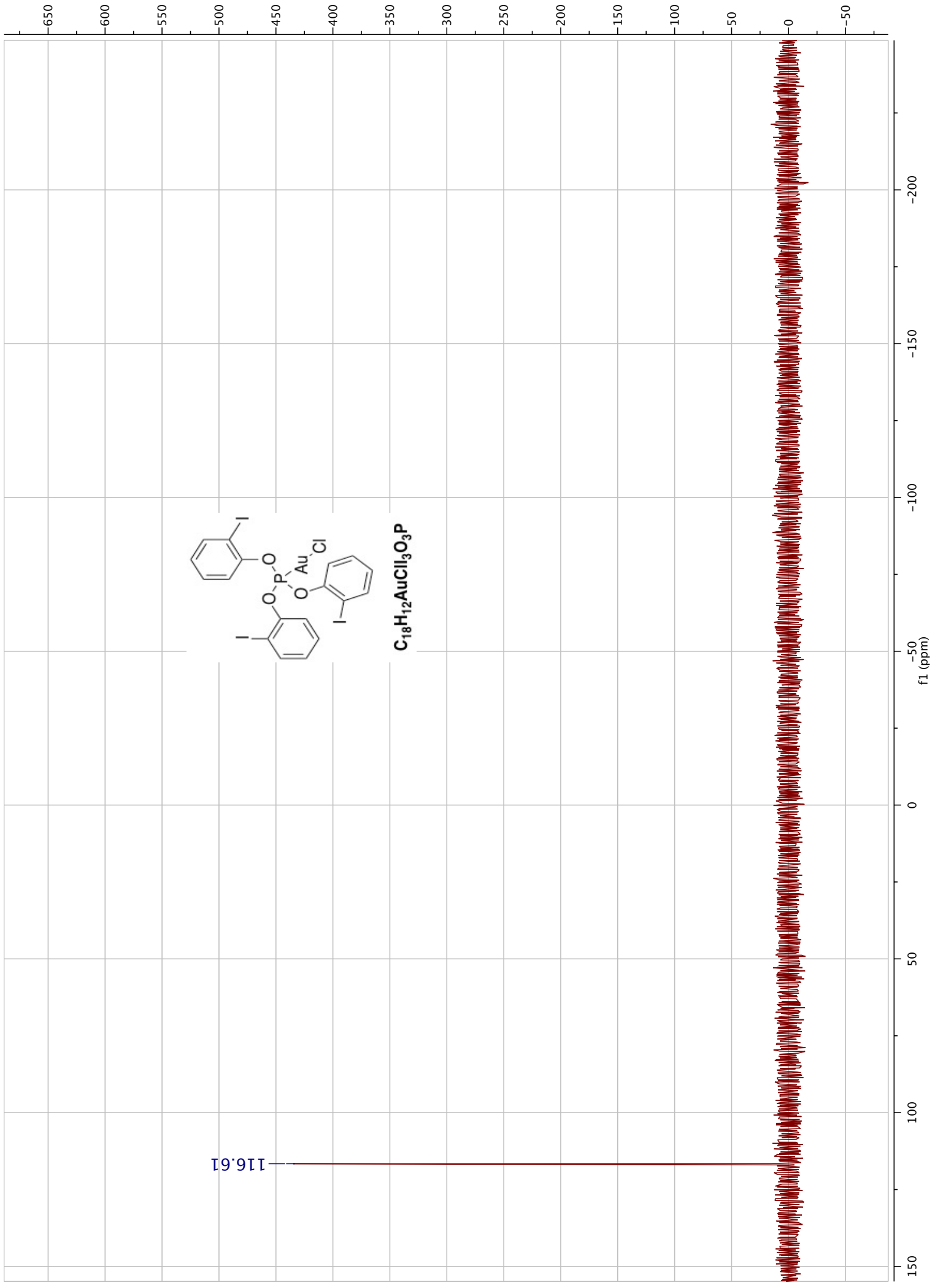

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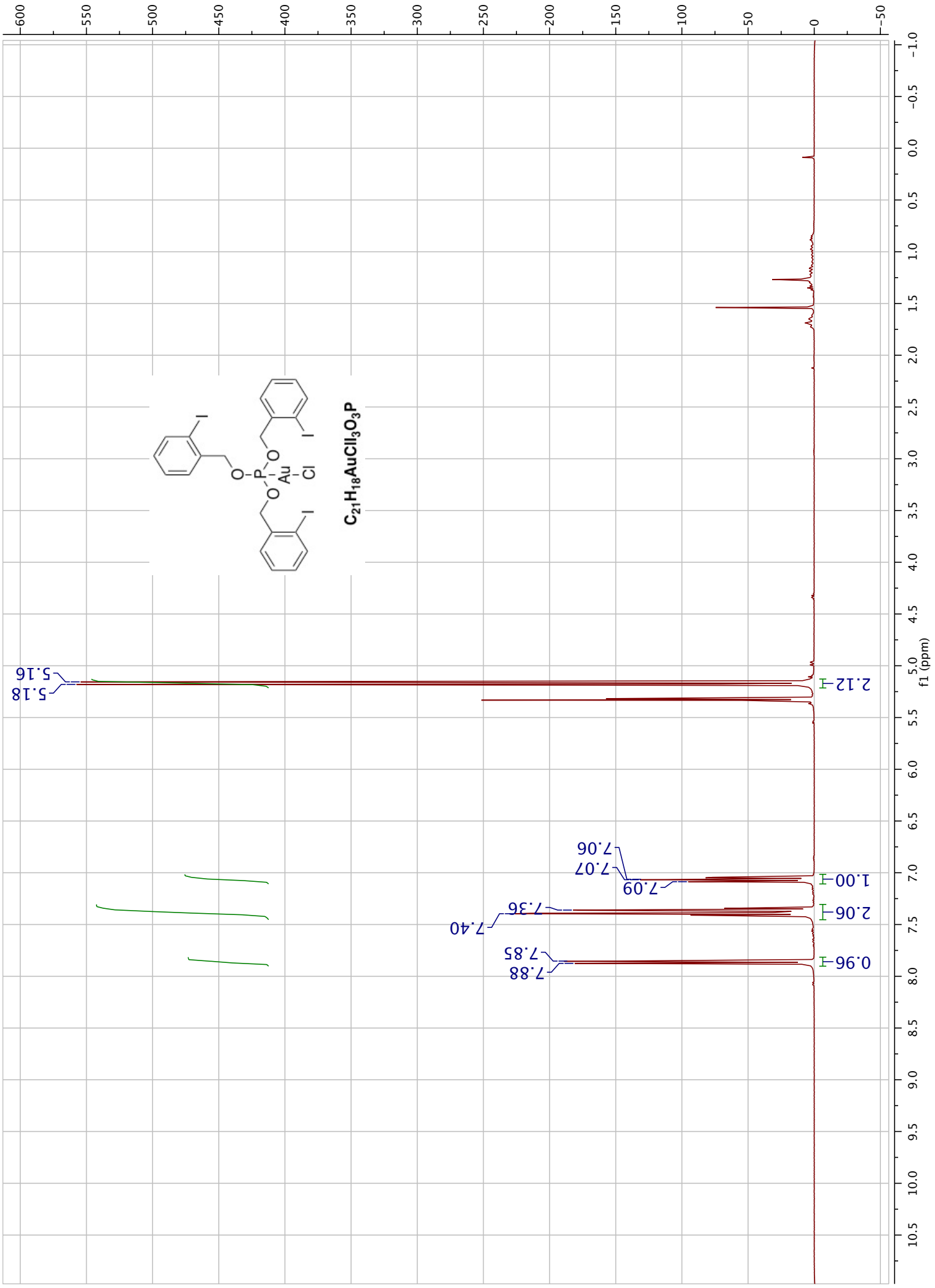

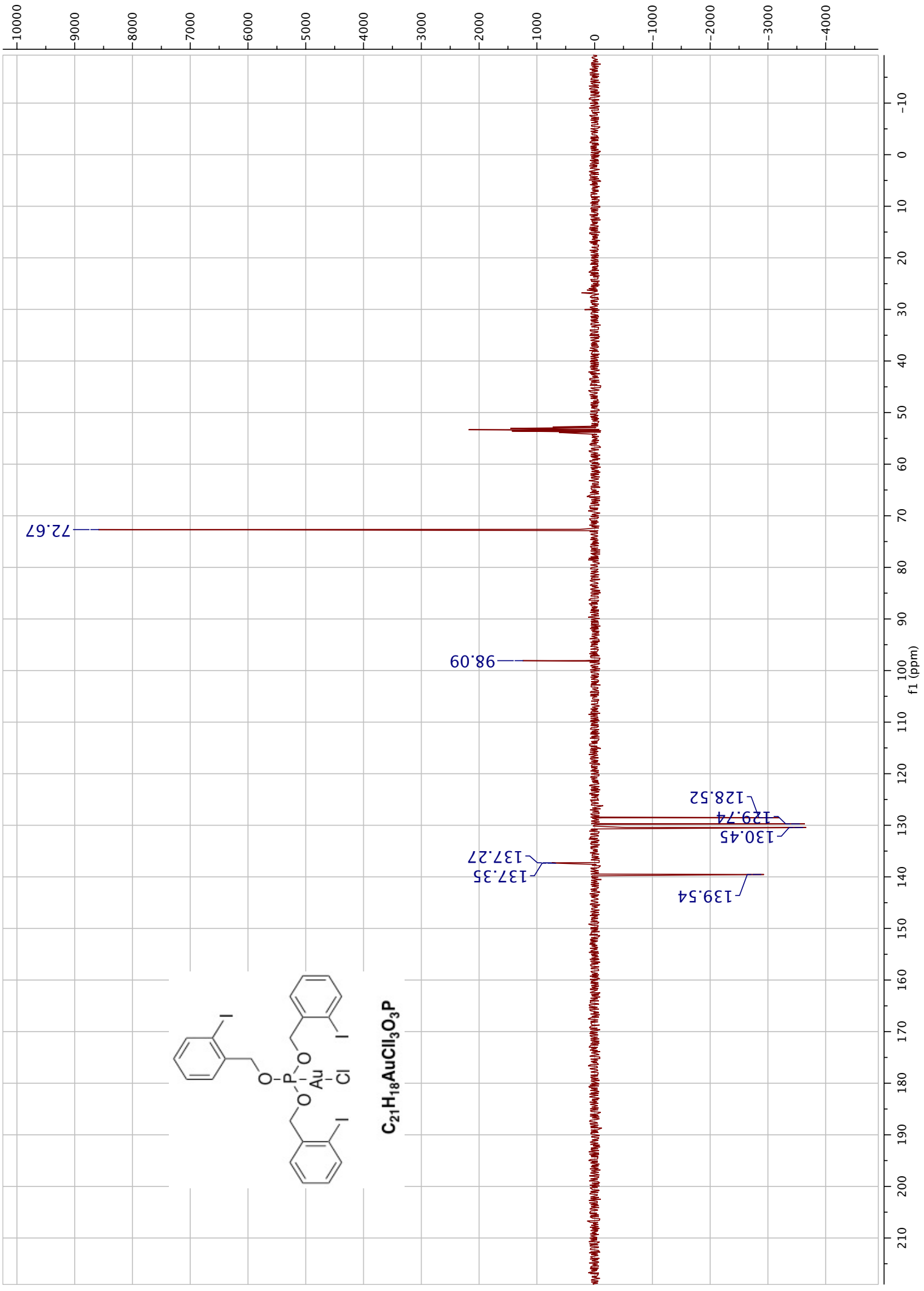
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137.27
137.35
139.54
f1 (ppm)
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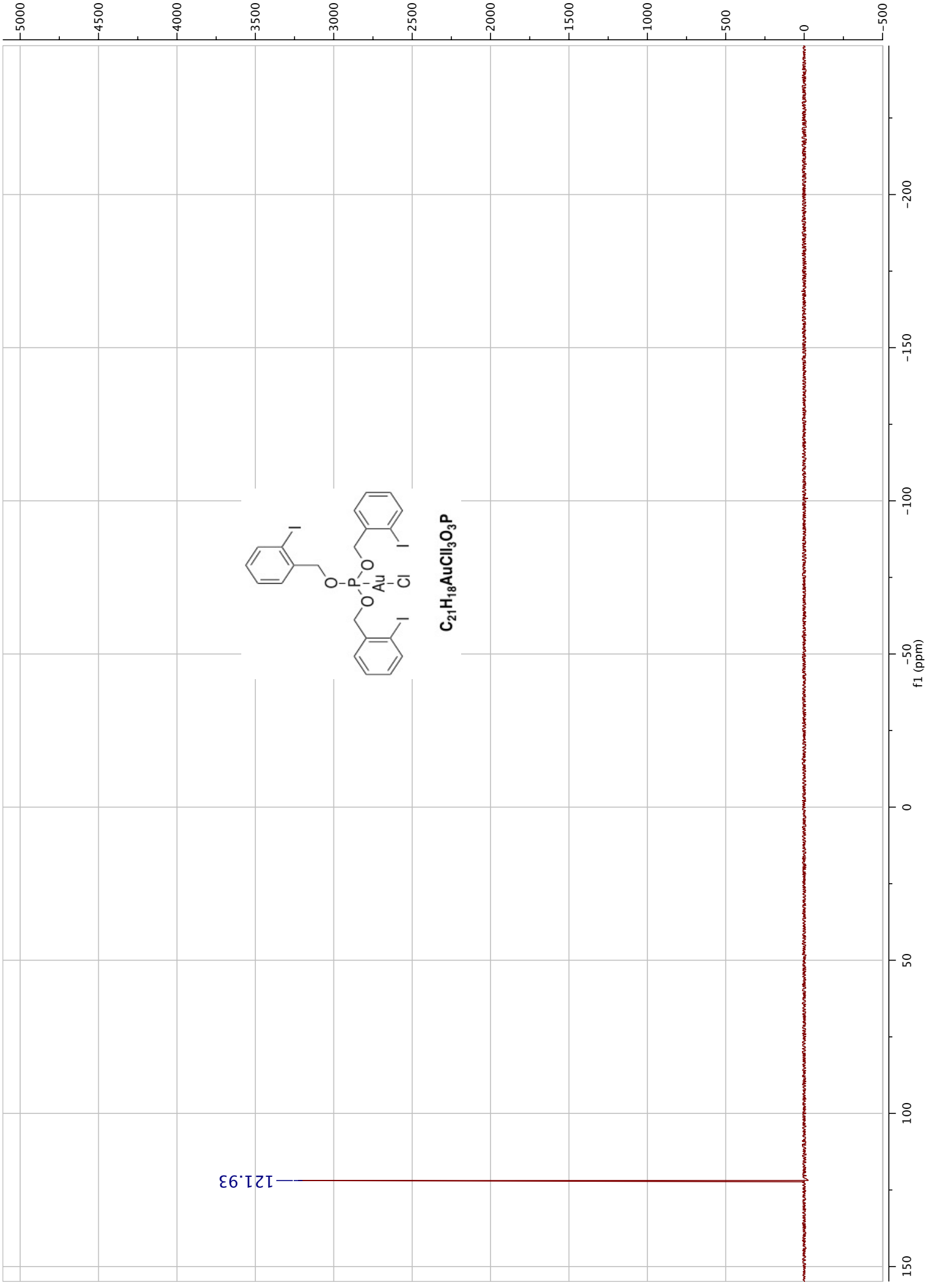
121.93
f1 (ppm)
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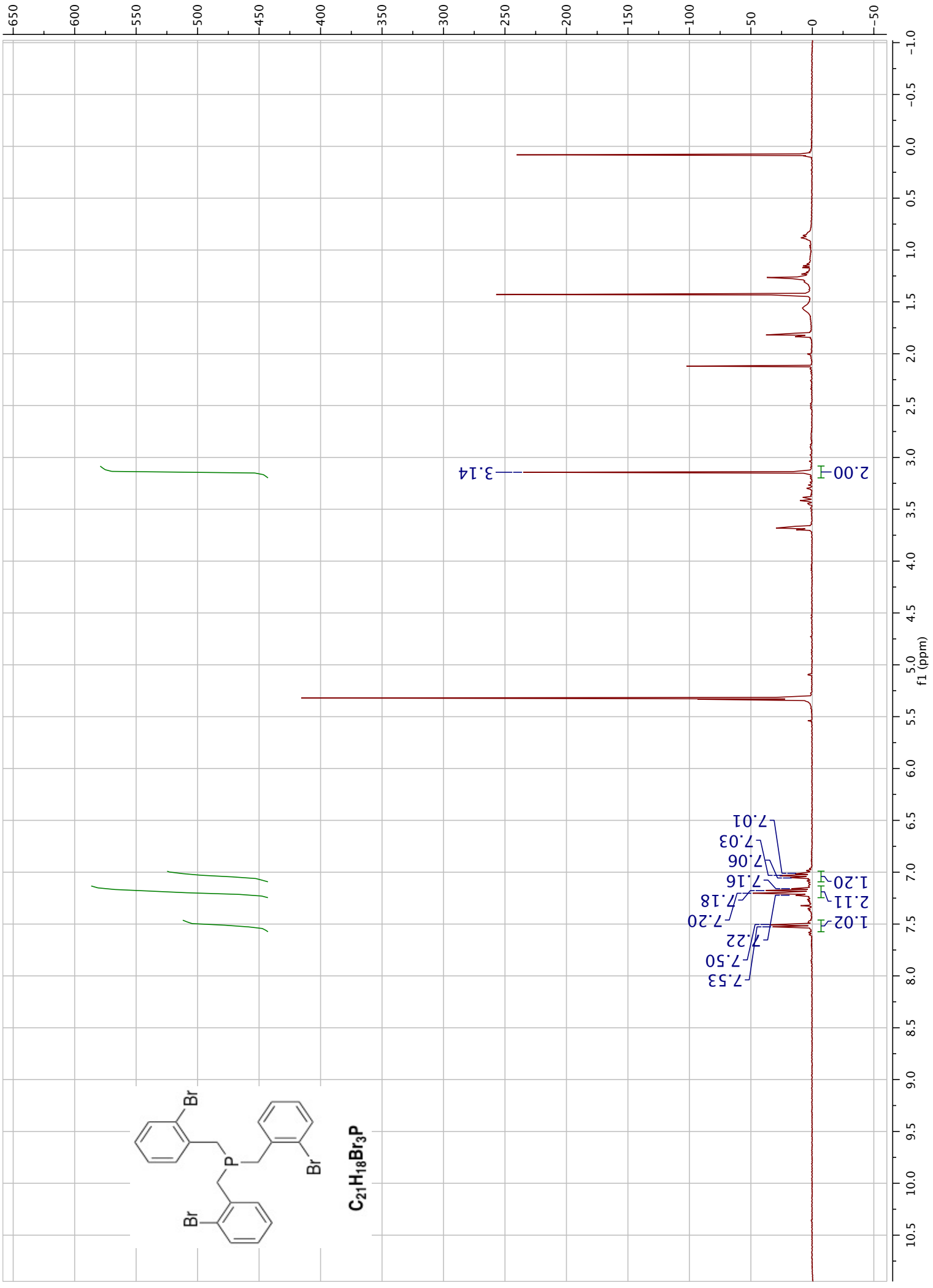

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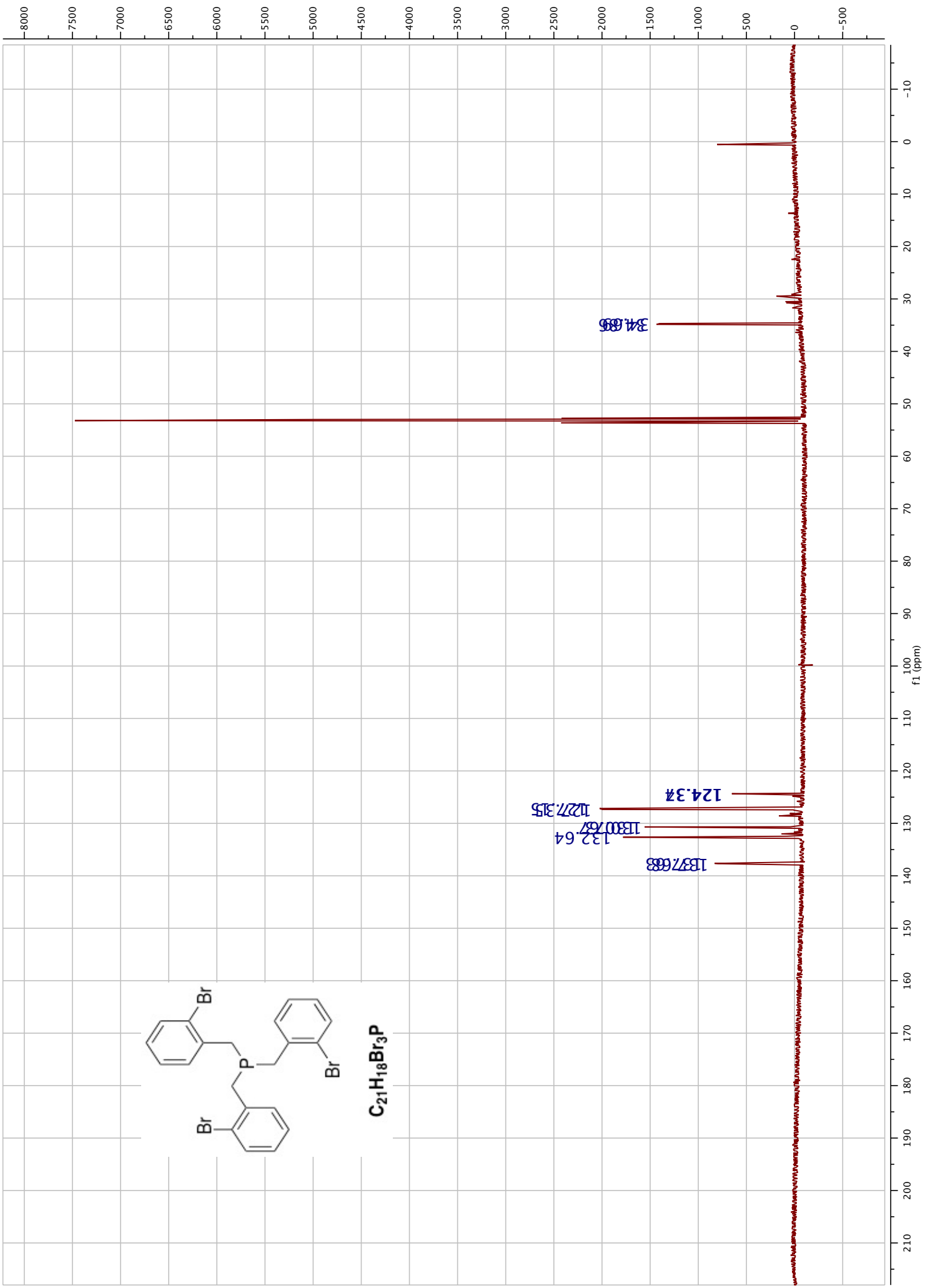

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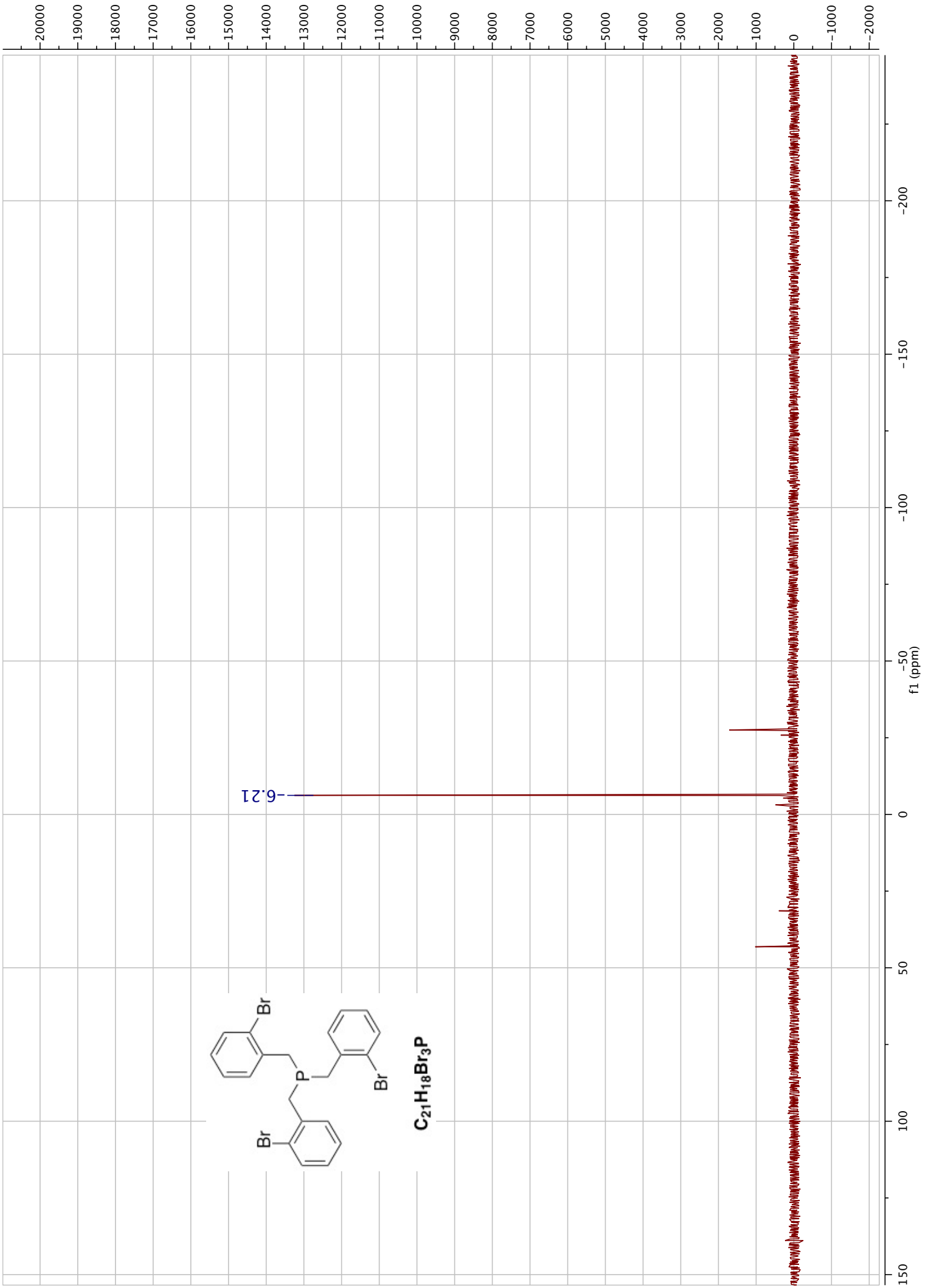

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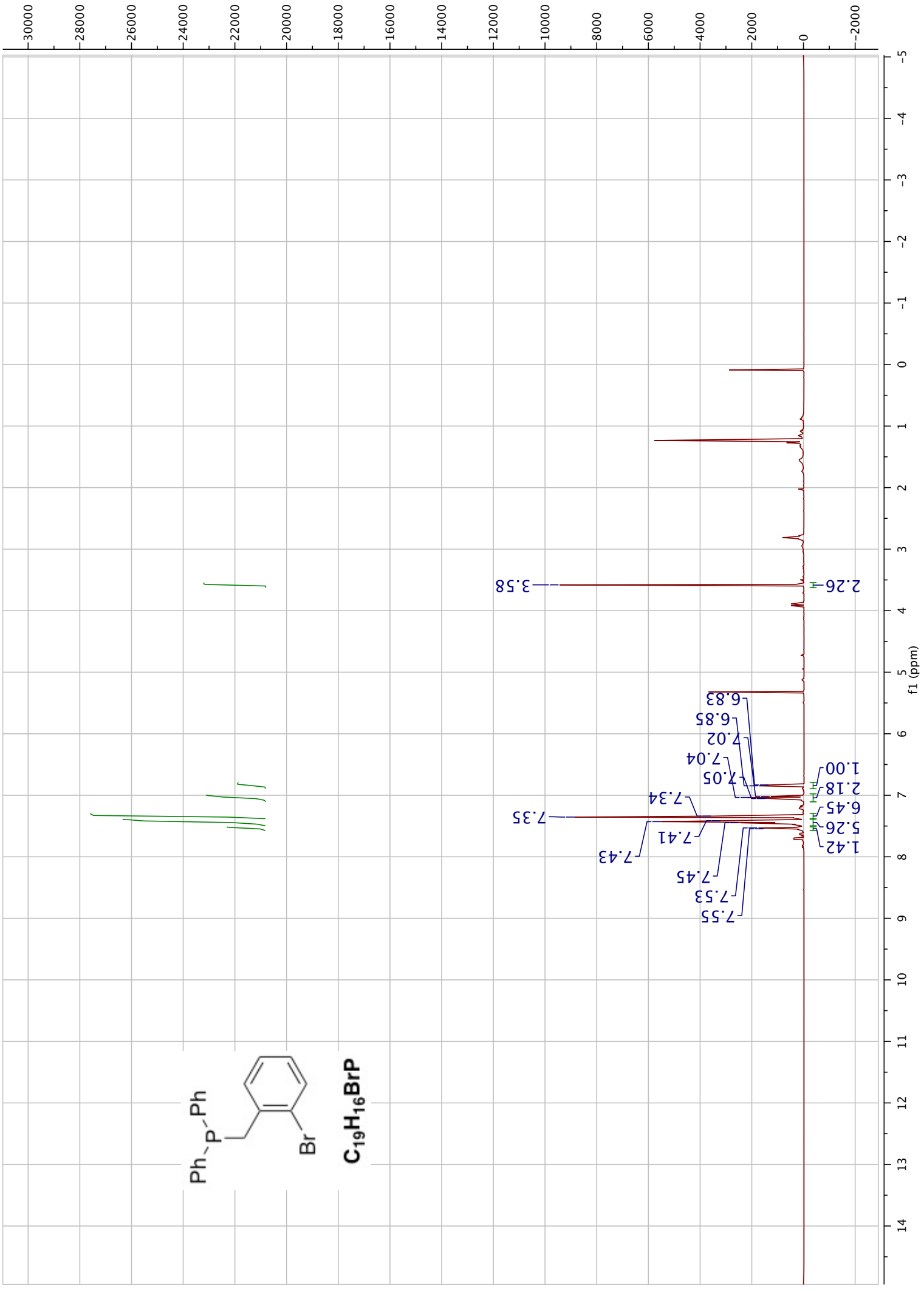

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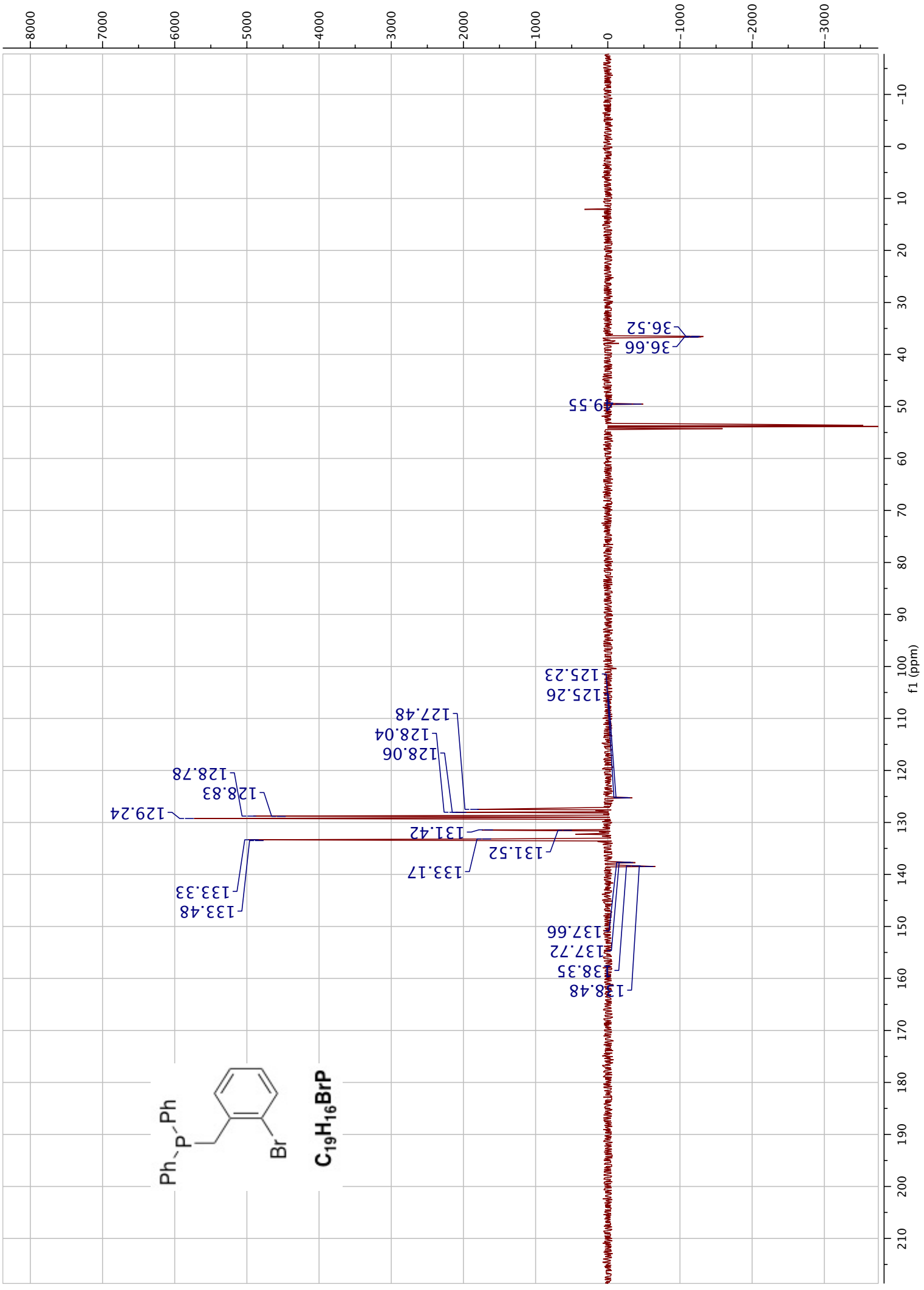

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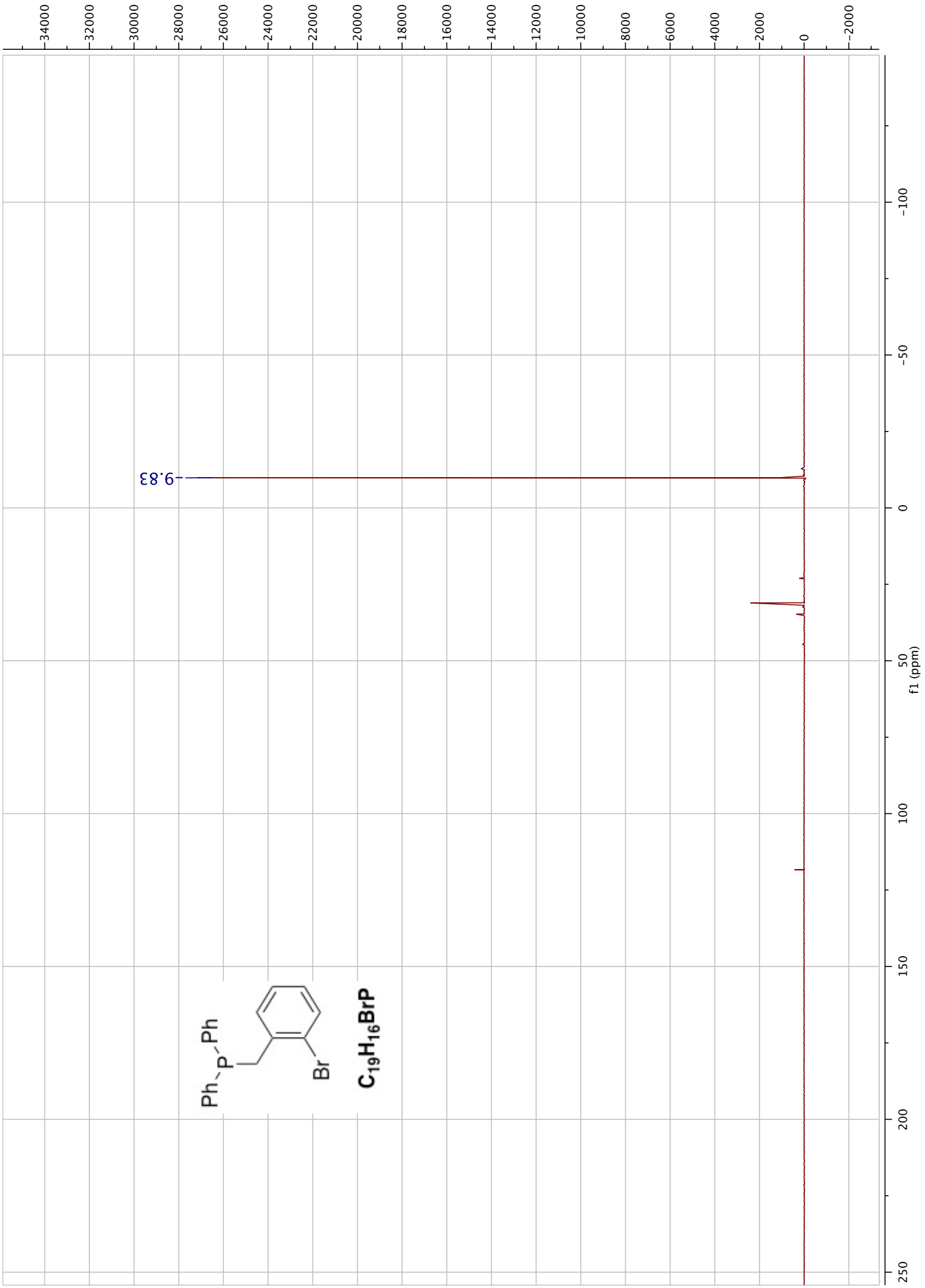

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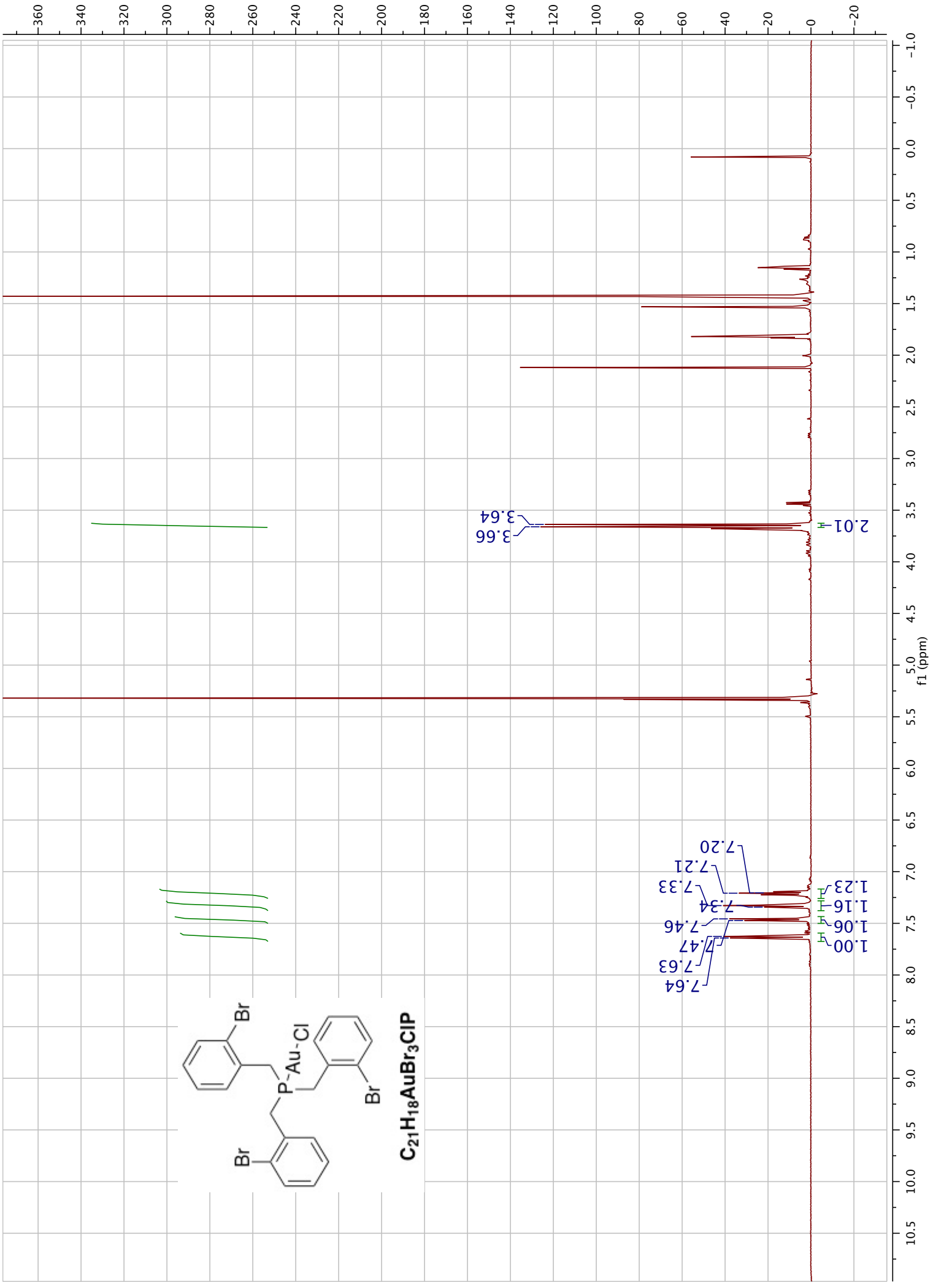

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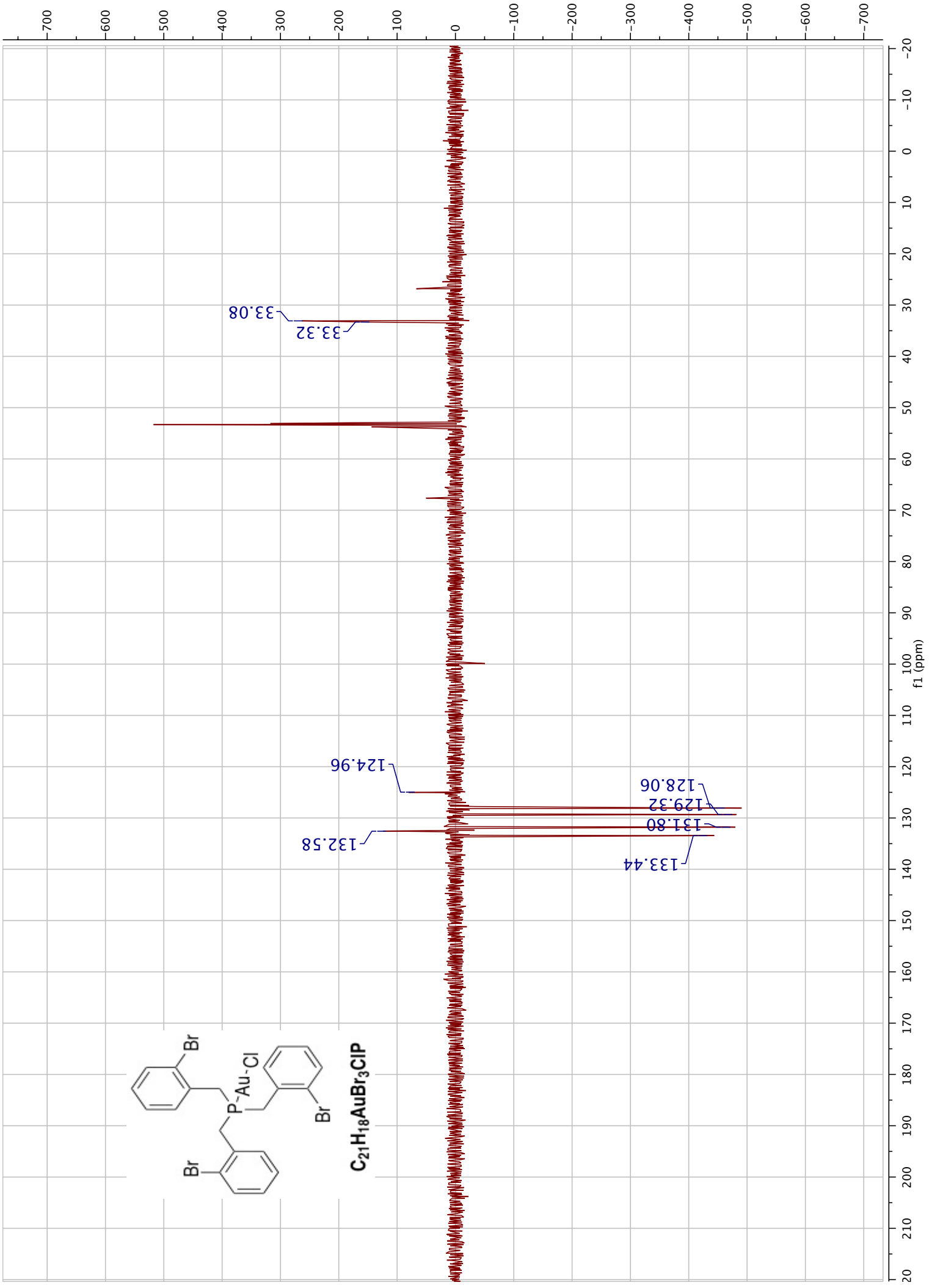

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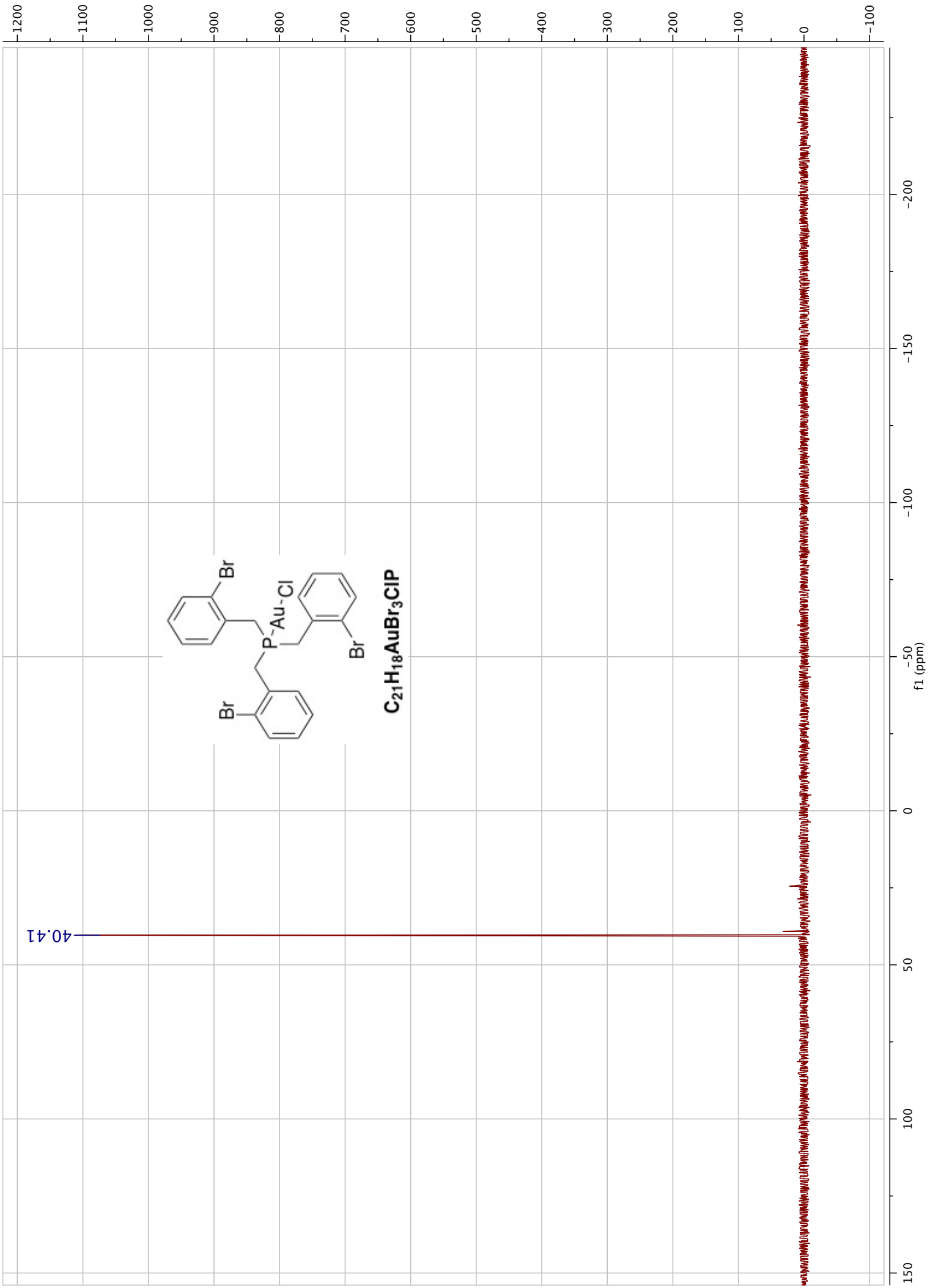

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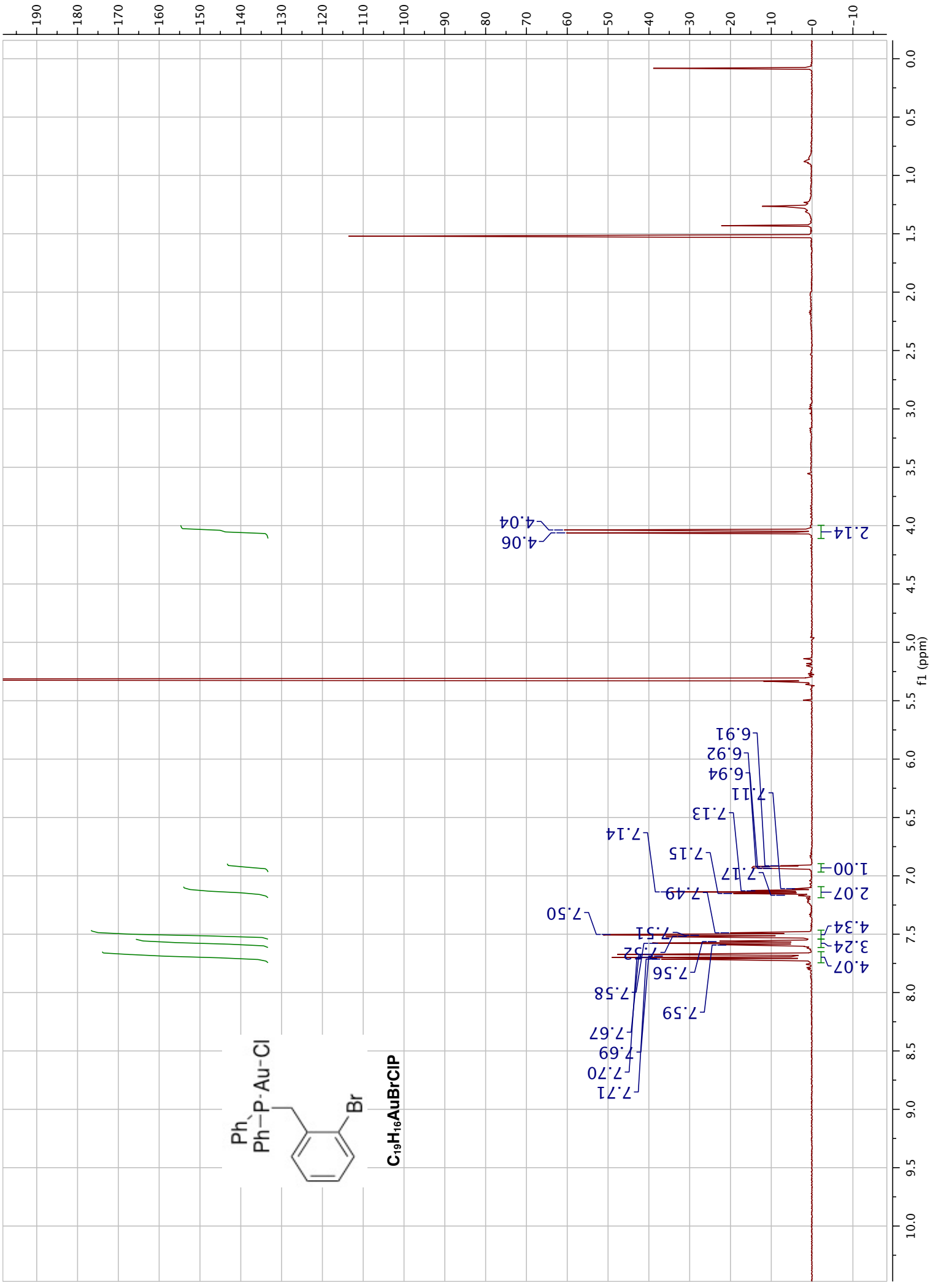

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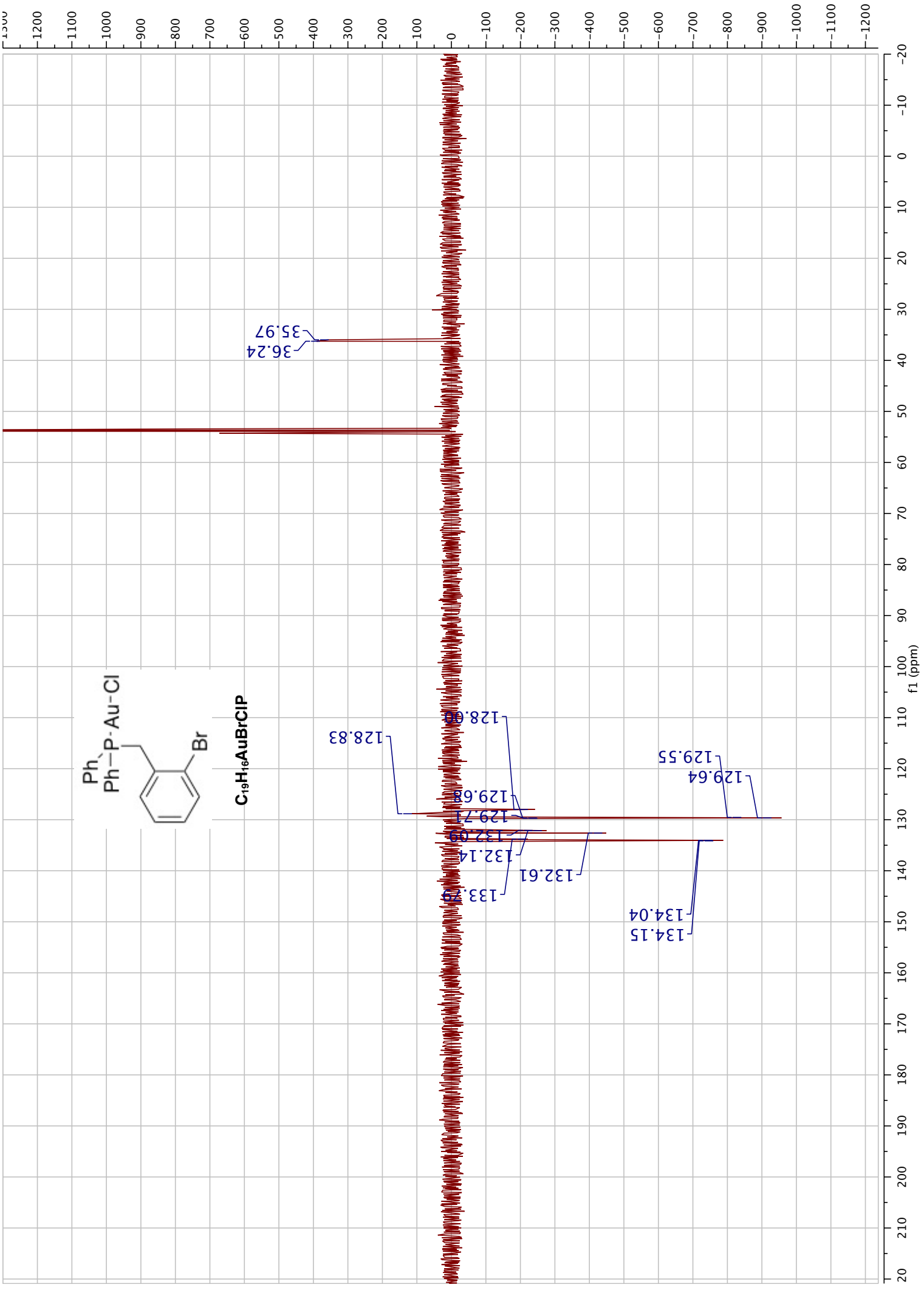

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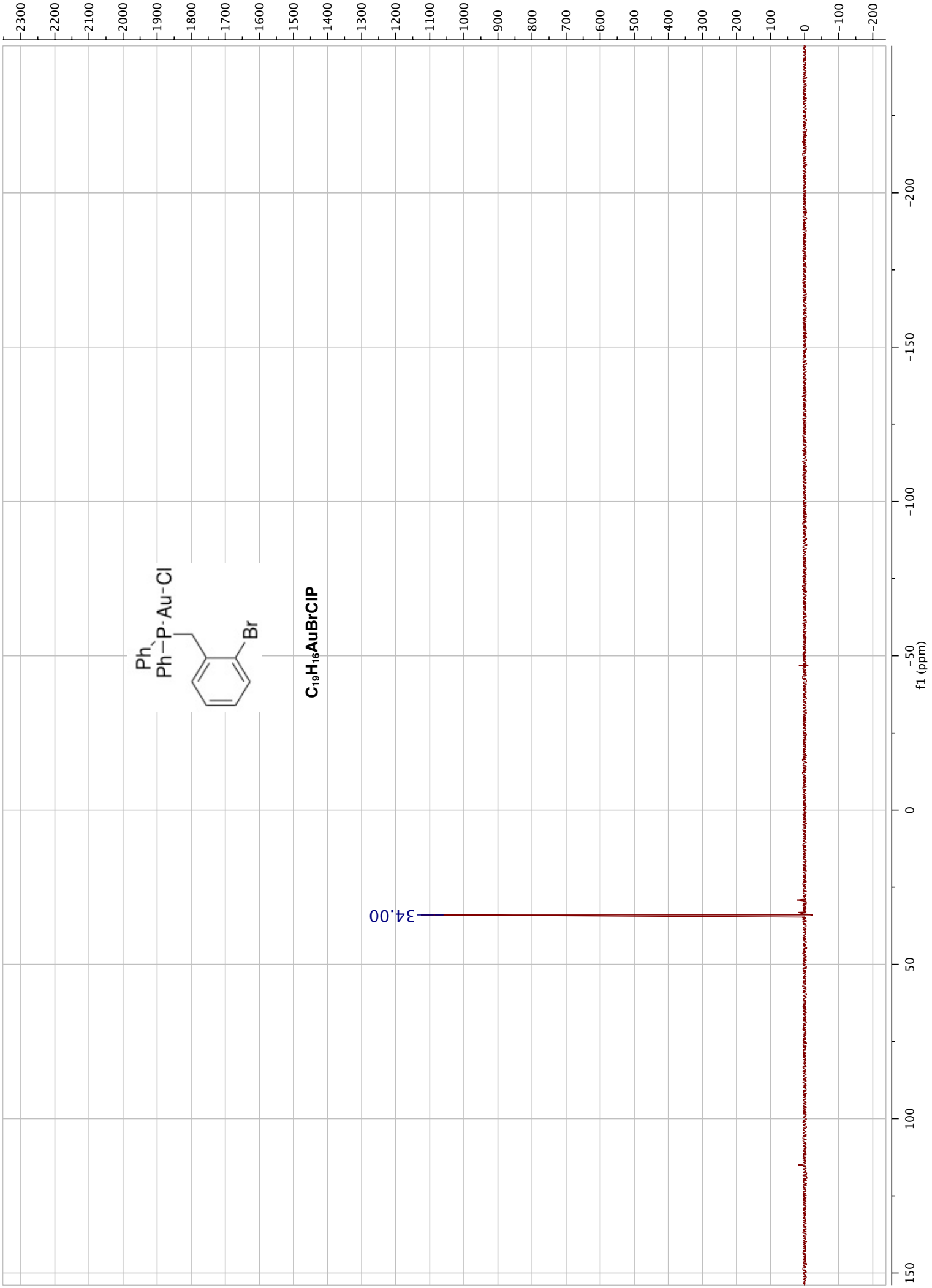

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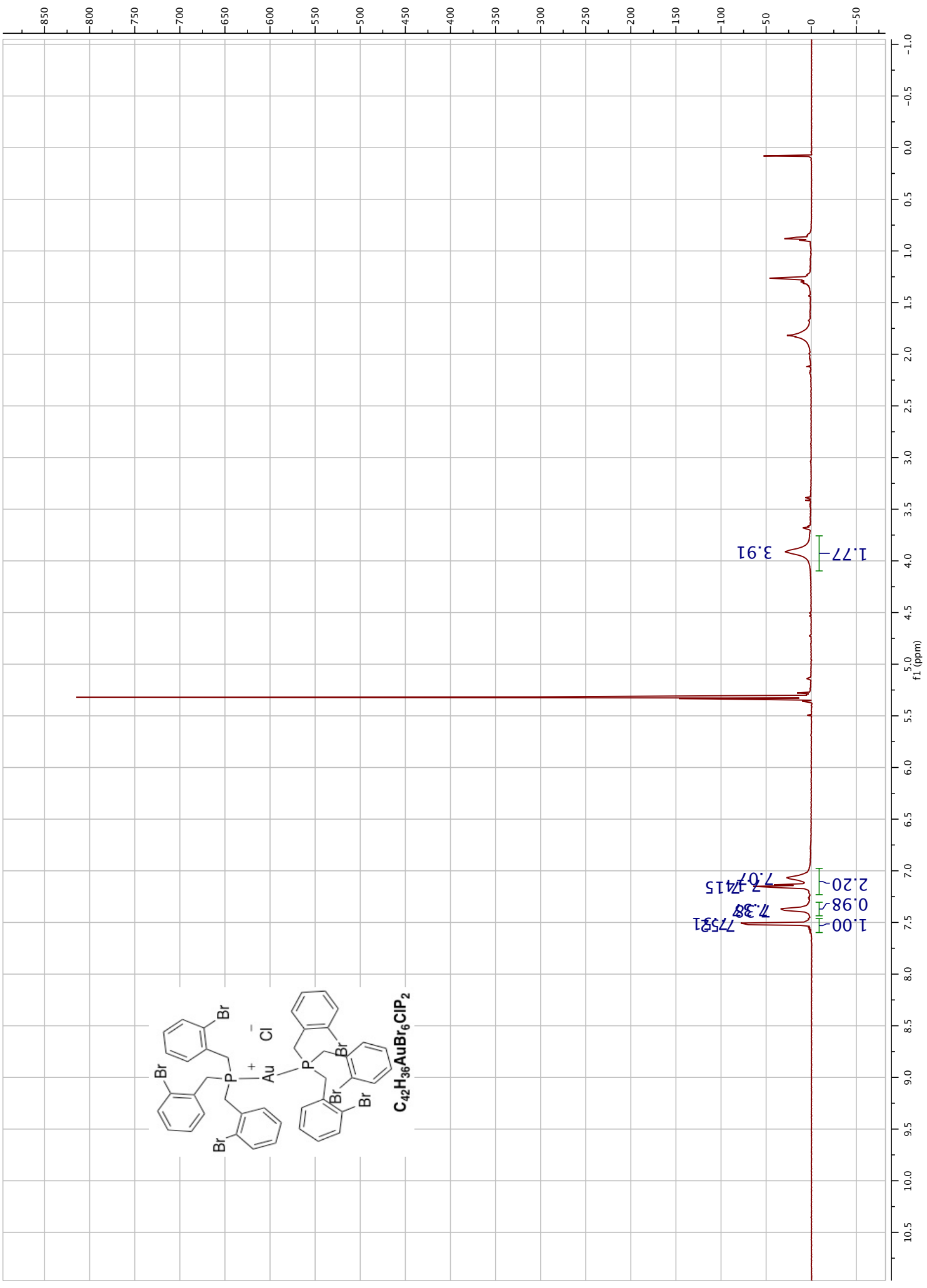

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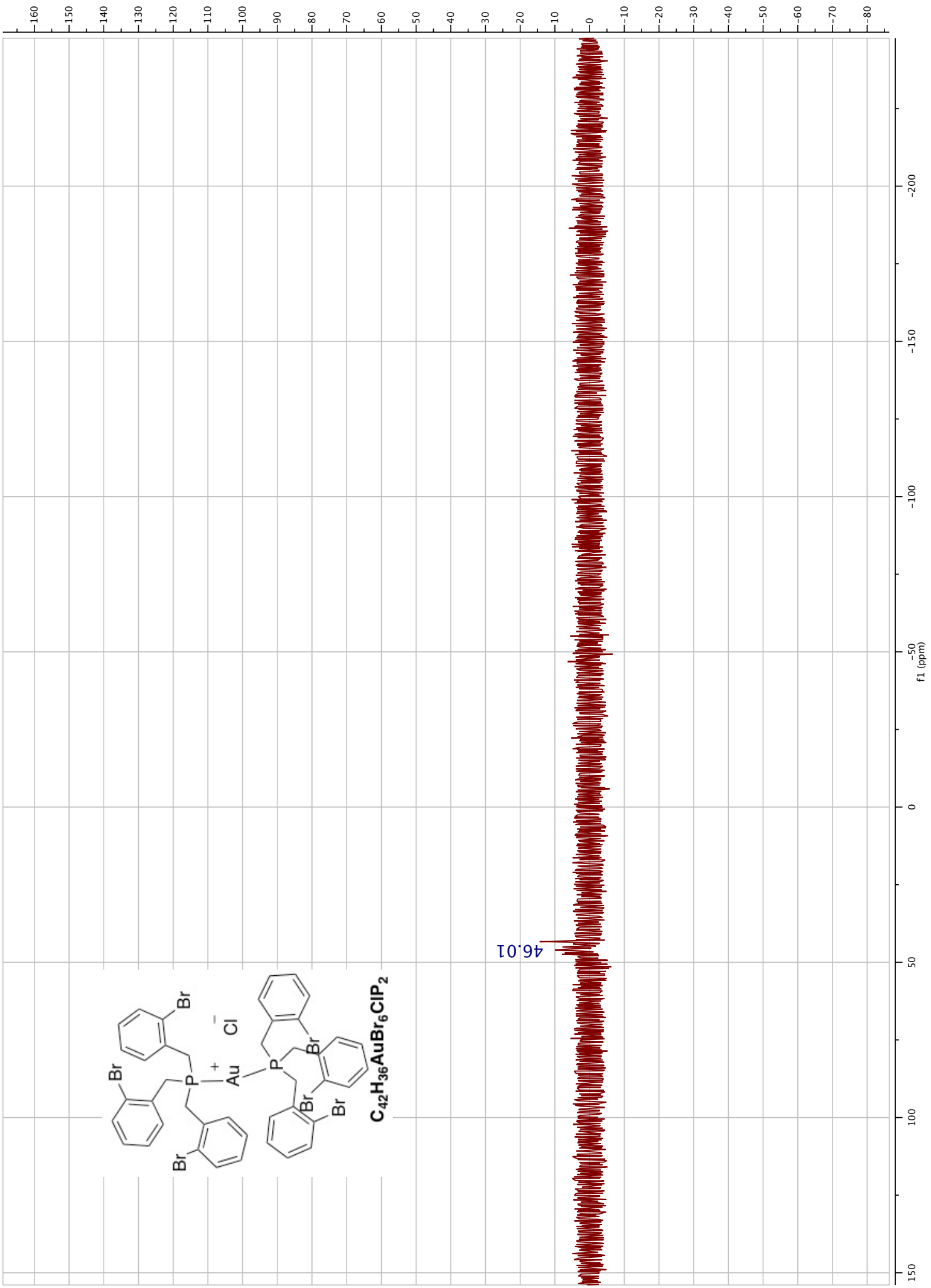

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S.1. Computational details

All reported calculations were performed by the means of the Gaussian 09 suite of programs.[1] Density Functional Theory (DFT) was applied using the Meta-Hybrid Generalised Gradient Approximation (MH-GGA) M06 functional.[2] The SDD basis set and ECP was used to describe Au[3] while 6-31+G(d) was used for all remaining atoms.[4] Full geometry optimizations were performed in water, through an implicit solvent PCM model.[5] Water was chosen as the most polar solvent that should favor most the oxidative addition. The nature of the stationary points as minima or transition states was confirmed by inspection of frequencies. Additionally, Intrinsic Reaction Coordinate (IRC) calculations confirmed connection on the potential energy surface between transition states, reactants and products. All reported energies are free energies in solution, computed at 298 K and 1 atm.

S.2. References

1Gaussian09, Revision B.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2010.

2Y. Zhao and D. G. Truhlar, *Theor. Chem. Acc.*, 2008, **120,** 215-241.

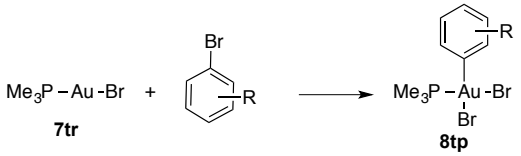
3D. Andrae, U. Haussermann, M. Dolg, H. Stoll, H. Preuss, *Theor. Chim. Acta*, 1990, **77**, 123-141.

4(a) W. J. Hehre, R. Ditchfield, J. A. Pople, J. Chem. Phys. 1972, 56, 2257-2258. (b) M. M. Francl, W. J. Pietro, W. J. Hehre, J. S. Binkley, M. S. Gordon, D. J. Defrees and J. A. Pople, *J. Chem. Phys.*, 1982, **77**, 3654-3665. (c) T. Clark, J. Chandrasekhar, G. W. Spitznagel, and P. v. R. Schleyer, *J. Comput. Chem.*, 1983, **4,** 294-301.

5S. Miertus, E. Scrocco and J. Tomasi, *Chem. Phys.* 1981, **55**, 117-129.

S.3.

Effects of substitutional patterns on aryl bromide in the oxidative addition Computed M06 Relative Energies (kcal·mol-1) of transition states.



Substitution	CN	NH_2	NO_2	H
none				42.4
ortho	40.3	40.8	36.9	
ortho-ortho	39.0	41.1	31.9	
meta	42.7	41.8	45.2	
meta-meta	42.8	41.6	43.5	
para	41.4	41.7	40.6	
all positions	34.2	40.1	31.7	
ortho-ortho-para	35.8	40.6	28.0	

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S.4 Cartesian coordinates and potential energies for optimized structures

1tr

SCF E(RM06) = -9461.59093257

Au 10.140042 13.633157 7.595724

Cl 10.158912 15.158593 9.418307

P 10.052480 12.161927 5.805515

Br 7.302861 11.600855 8.513025

Br 13.150551 11.827758 8.144196

Br 10.283792 15.989104 4.998095

C 8.349045 11.503498 5.485412

C 7.322793 12.549452 5.788807

C 6.812525 12.759939 7.076528

C 5.938622 13.803687 7.361144

C 5.552908 14.671206 6.342403

C 6.029617 14.477090 5.048626

C 6.900362 13.425784 4.782067

C 11.104687 10.647988 5.960112

C 11.011218 10.064153 7.335681

C 11.787405 10.516498 8.411019

C 11.625832 10.017019 9.698591

C 10.672321 9.030757 9.937432

C 9.901641 8.543934 8.884862

C 10.074541 9.058896 7.604566

C 10.559920 12.892644 4.180238

C 11.838672 13.660026 4.305589

C 11.890635 14.999692 4.711297

C 13.096330 15.667681 4.898041

C 14.294469 14.996858 4.669117

C 14.275671 13.672530 4.239946

C 13.060546 13.019566 4.063451

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H 8.303211 11.184313 4.434491

H 12.133258 10.940208 5.710126
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H 9.732441 13.529039 3.838508
H 10.662163 12.064593 3.463997
H 5.564029 13.936659 8.374166
H 4.873475 15.491918 6.564093
H 5.724951 15.143930 4.244376
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1ts

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C 6.837161 12.108624 6.987772
C 6.692972 12.506797 8.323418
C 5.762121 13.465662 8.708222
C 4.934032 14.041836 7.748351
C 5.030282 13.640423 6.418582
C 5.971951 12.684914 6.050607
C 10.841506 10.854378 6.284250

C 11.148622 10.765426 7.743510
C 11.282202 11.922144 8.513314
C 11.559784 11.951099 9.865770
C 11.608779 10.720693 10.527467
C 11.429326 9.533504 9.822598
C 11.201433 9.558754 8.447927
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C 11.168749 16.001963 4.154571
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C 12.422665 14.305319 2.988604
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H 11.043501 17.029696 4.488806

1tp

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phenyl bromide

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C -3.720105 6.906278 0.112502
C -3.858970 5.553820 -0.195100
H -2.835961 3.716312 -0.702269
H -2.337136 8.539809 0.391482
H -4.600673 7.510091 0.323823
H -4.846639 5.097110 -0.228205
Br 0.063060 4.310883 -0.771738
H -0.326498 7.159585 -0.082826

2t1r

SCF E(RM06) = -1056.99890691
Au 2.021376 9.579074 0.248653
P 4.151858 10.455424 0.193821

C 4.332813 12.019430 1.110209
H 5.367273 12.379646 1.034069
H 3.654933 12.773889 0.695523
H 4.080952 11.862098 2.164805
C 4.753559 10.834867 -1.483106
H 4.086648 11.560231 -1.962100
H 5.766699 11.254715 -1.428560
H 4.771746 9.921201 -2.087504
C 5.424401 9.358727 0.897852
H 6.409087 9.840245 0.833273
H 5.193760 9.144347 1.947376
H 5.446934 8.414443 0.342438
Cl -0.182039 8.680964 0.296672

2t1ts

SCF E(RM06) = -3859.66385545
C 0.175956 5.720777 -0.816912
C 0.086926 6.608065 0.254097
C -0.890580 7.598169 0.329809
C -1.846025 7.655276 -0.683718
C -1.806154 6.758700 -1.751787
C -0.795891 5.797730 -1.813178
H 0.973398 4.981378 -0.865758
H -2.626500 8.412885 -0.629680
H -2.553124 6.816876 -2.540830
H -0.753080 5.098007 -2.646592
Au 0.478745 5.612233 2.259389
P -1.444204 4.212363 2.422354
C -1.803824 3.545062 4.076691
H -2.713674 2.931310 4.044468
H -0.962416 2.928699 4.413241
H -1.943140 4.365515 4.789714
C -1.302810 2.750104 1.343637

H -0.441614 2.144883 1.648700
H -2.215321 2.142777 1.408027
H -1.157018 3.071831 0.305065
C -2.978119 5.031337 1.881995
H -3.818835 4.327355 1.939655
H -3.186573 5.898633 2.519049
H -2.866339 5.377698 0.846670
Br 2.080229 7.264288 1.076904
Cl 1.778002 5.155952 4.469899
H -0.912480 8.298505 1.162542

2t1p

SCF E(RM06) = -3859.67546325
C -1.601723 6.328571 -0.867905
C -0.554267 6.066726 0.009457
C 0.399072 7.042856 0.288339
C 0.282326 8.305434 -0.295485
C -0.777338 8.585407 -1.155269
C -1.712181 7.594128 -1.446270
H -2.326877 5.552341 -1.114446
H 1.030879 9.068034 -0.082423
H -0.866836 9.570750 -1.610193
H -2.530151 7.799290 -2.136310
Au -0.424136 4.262798 0.980797
P -1.673219 5.135031 2.791587
C -3.028836 4.044625 3.315525
H -3.527289 4.467824 4.198292
H -3.756819 3.941972 2.502401
H -2.619528 3.054522 3.545742
C -2.449865 6.762123 2.534261
H -3.199499 6.696721 1.736663
H -2.938056 7.087959 3.462980
H -1.701066 7.504514 2.231433

C -0.583735 5.334808 4.232470
H -1.158049 5.680167 5.102685
H -0.111934 4.369982 4.453723
H 0.199406 6.067874 4.001964
Br 0.891129 3.428337 -0.944116
Cl -0.255869 2.235533 2.315981
H 1.241492 6.825083 0.946779

2t2r

SCF E(RM06) = -1631.75982752
Au 2.709212 12.661803 -0.235338
P 4.944848 13.249382 -0.248296
C 6.024227 11.928083 0.390181
C 5.615236 11.239717 1.538355
C 7.254918 11.626337 -0.199479
C 6.436064 10.266366 2.098151
H 4.650839 11.468461 1.995652
C 8.070815 10.644404 0.359846
H 7.582306 12.157652 -1.093371
C 7.664186 9.967450 1.507400
H 6.114932 9.734730 2.992085
H 9.027819 10.411260 -0.103692
H 8.304516 9.201612 1.941763
C 5.579849 13.641987 -1.909542
C 6.468978 14.698434 -2.127798
C 5.198418 12.822685 -2.978602
C 6.974843 14.928909 -3.405695
H 6.771846 15.343212 -1.302310
C 5.711656 13.051588 -4.251098
H 4.497796 12.001981 -2.814064
C 6.599756 14.106126 -4.465256
H 7.666348 15.753251 -3.570869
H 5.413451 12.410642 -5.078860

H 6.997609 14.287451 -5.462313
C 5.308763 14.712144 0.773250
C 6.464928 14.795772 1.554615
C 4.424532 15.795724 0.720352
C 6.735075 15.958711 2.273404
H 7.158773 13.956057 1.603528
C 4.701879 16.957613 1.433421
H 3.517257 15.729877 0.117142
C 5.857126 17.038559 2.211237
H 7.635078 16.018233 2.882921
H 4.012645 17.798842 1.387594
H 6.071502 17.945565 2.774019
Cl 0.419102 12.045925 -0.213974

2t2ts

SCF E(RM06) = -4434.42553294
C 0.114781 4.793438 -3.162022
C 0.100368 4.717644 -1.770984
C -1.042192 4.980225 -1.015753
C -2.184671 5.418748 -1.683899
C -2.185633 5.555123 -3.071630
C -1.038690 5.241765 -3.802767
H 1.008292 4.537737 -3.731084
H -3.079057 5.649980 -1.106940
H -3.083712 5.891264 -3.586143
H -1.034195 5.339987 -4.887647
Au 2.015857 5.416189 -0.816973
Br 1.242525 2.953832 -0.867855
H -1.036517 4.859821 0.065786
H -2.255069 9.085103 -1.303655
C -1.236831 9.387224 -1.545454
C -0.211020 8.444994 -1.512988
C -0.955474 10.709505 -1.880769

C 1.097038 8.821303 -1.823517
H -0.433628 7.412345 -1.245440
C 0.352208 11.092023 -2.184169
H -1.755599 11.447389 -1.904804
P 2.409915 7.564097 -1.867637
C 1.378053 10.152828 -2.156441
H 0.573404 12.125667 -2.444616
C 2.675203 7.174061 -3.626909
C 3.894325 8.426691 -1.267007
H 2.397626 10.454437 -2.400830
C 3.655400 6.226575 -3.958605
C 1.854785 7.697980 -4.629420
C 3.913864 8.794807 0.084014
C 4.980887 8.737749 -2.087267
C 3.821867 5.826027 -5.278931
H 4.289612 5.795405 -3.180599
C 2.019694 7.286447 -5.951624
H 1.074893 8.418927 -4.383055
C 5.008164 9.473377 0.606547
H 3.070042 8.544633 0.729579
C 6.081732 9.409736 -1.556402
H 4.973172 8.465168 -3.142449
C 2.999899 6.353199 -6.277050
H 4.587989 5.094299 -5.528829
H 1.372975 7.694700 -6.726376
C 6.096125 9.777540 -0.213590
H 5.016611 9.759883 1.656731
H 6.927126 9.650508 -2.198688
H 3.123523 6.029928 -7.309229
H 6.956539 10.302510 0.198058
Cl 4.049445 5.202427 0.752107

2t2p

SCF E(RM06) = -4434.45970911

C -1.639355 -1.333857 -1.739080

C -1.757646 -0.941267 -0.410689

C -3.009176 -0.746906 0.168926

C -4.155381 -0.911648 -0.609640

C -4.049205 -1.282852 -1.949694

C -2.793627 -1.499687 -2.510003

H -0.663426 -1.515032 -2.190482

H -5.134517 -0.756124 -0.158129

H -4.946568 -1.411199 -2.552773

H -2.699015 -1.801629 -3.552627

Au -0.043579 -0.812906 0.741478

Br -0.675440 -3.064847 1.692148

H -3.107509 -0.486195 1.222372

H -3.622241 3.301719 1.639580

C -2.809646 3.422488 0.925955

C -1.890858 2.390547 0.747433

C -2.682438 4.602003 0.197613

C -0.845321 2.538016 -0.165457

H -1.984600 1.476360 1.330737

C -1.624809 4.762531 -0.698541

H -3.404595 5.404837 0.334514

P 0.439780 1.269966 -0.341699

C -0.699630 3.740224 -0.872916

H -1.515369 5.690102 -1.257103

C 0.701150 0.888927 -2.092842

C 1.928362 2.084870 0.306804

H 0.138714 3.883365 -1.555972

C 1.729672 -0.006981 -2.421410

C -0.161139 1.355482 -3.088449

C 1.884546 2.531740 1.633496

C 3.069631 2.302574 -0.467401

C 1.905856 -0.407439 -3.740544

H 2.384431 -0.406929 -1.644576
C 0.019420 0.947537 -4.407956
H -0.987437 2.020111 -2.838909
C 2.978988 3.186714 2.181394
H 0.996389 2.358452 2.243199
C 4.167272 2.957018 0.090290
H 3.109097 1.978378 -1.505851
C 1.050416 0.070282 -4.734285
H 2.706494 -1.100283 -3.991418
H -0.656389 1.311469 -5.179479
C 4.124497 3.394791 1.410706
H 2.942388 3.531045 3.213154
H 5.054788 3.129018 -0.515771
H 1.185193 -0.250659 -5.765611
H 4.983967 3.904247 1.843027
Cl 2.054426 -0.799804 2.029798

3t1r

SCF E(RM06) = -636.638166449
Au 1.843013 9.508271 0.238462
P 4.051398 10.413286 0.192968
C 4.276218 11.963412 1.136796
H 5.314079 12.313926 1.057457
H 3.604208 12.736219 0.745795
H 4.033334 11.793513 2.192135
C 4.678156 10.844397 -1.470100
H 4.016097 11.583593 -1.935787
H 5.691940 11.261205 -1.400628
H 4.698967 9.949109 -2.102225
C 5.360541 9.324253 0.859662
H 6.339367 9.818255 0.793971
H 5.147878 9.084722 1.908066
H 5.390625 8.389198 0.288219

C -0.095216 8.721758 0.279199
H -0.091928 7.646642 0.045730
H -0.554313 8.847798 1.270936
H -0.742914 9.222170 -0.455821

3t1ts

SCF E(RM06) = -3439.29360400
C -0.645213 6.159375 -2.071816
C -0.279096 5.906321 -0.749694
C -0.901260 6.552787 0.318614
C -1.859881 7.526784 0.043228
C -2.217093 7.825558 -1.272200
C -1.606931 7.135149 -2.321858
H -0.170555 5.620510 -2.890728
H -2.335270 8.049175 0.873159
H -2.972750 8.581574 -1.477442
H -1.880333 7.353878 -3.353976
Au 2.020269 5.657473 -0.390948
P 3.690132 4.062950 0.526324
Br 0.034976 3.691723 -0.323524
H -0.631203 6.311449 1.345870
C 2.169636 7.652370 -1.118550
H 3.163546 8.084994 -0.953048
H 1.951404 7.619316 -2.195233
H 1.404781 8.259801 -0.615388
C 3.899608 2.558186 -0.493249
H 2.929722 2.060100 -0.616335
H 4.279740 2.829931 -1.484911
H 4.602949 1.862656 -0.015385
C 3.254177 3.387805 2.170284
H 3.206387 4.198651 2.906436
H 2.269150 2.907967 2.115796
H 3.998307 2.648034 2.495579

C 5.405144 4.656854 0.752389
H 5.809690 4.993650 -0.209175
H 5.416564 5.503047 1.448873
H 6.041389 3.854379 1.149519

3t1p

SCF E(RM06) = -3439.36641932
C -0.872748 6.218172 -1.256183
C -0.578345 6.162388 0.109379
C -0.322723 7.352600 0.796060
C -0.334936 8.576922 0.123343
C -0.625593 8.625542 -1.239077
C -0.899362 7.443464 -1.926050
H -1.075215 5.301903 -1.812932
H -0.121322 9.495547 0.670027
H -0.642032 9.580628 -1.762846
H -1.132677 7.471182 -2.990536
Au -0.481847 4.329292 1.076897
P -0.366143 2.178522 2.239394
C 1.191046 1.975285 3.165523
H 1.226683 0.982480 3.633106
H 2.037736 2.086760 2.478275
H 1.264264 2.744294 3.943104
C -0.417562 0.753661 1.102541
H 0.410198 0.829059 0.388222
H -0.330529 -0.183515 1.667819
H -1.362898 0.754641 0.547892
C -1.666069 1.815572 3.465194
H -1.476199 0.837376 3.926073
H -1.676485 2.581871 4.248727
H -2.648894 1.794176 2.980650
Br 1.642192 3.624568 -0.257650
H -0.110838 7.335470 1.866638

C -2.173285 4.914002 2.146400
H -2.946492 4.153932 1.989769
H -1.881402 4.952345 3.202363
H -2.525697 5.891412 1.811055

3t2r

SCF E(RM06) = -1211.40146337
Au 2.584691 12.655784 -0.256390
P 4.833773 13.490455 -0.259338
C 6.063332 12.301843 0.381176
C 5.723965 11.573303 1.527923
C 7.320034 12.120794 -0.203032
C 6.635008 10.684403 2.089903
H 4.740641 11.706500 1.983702
C 8.228336 11.223986 0.357561
H 7.596598 12.681502 -1.096660
C 7.888392 10.508066 1.503556
H 6.364406 10.122779 2.982543
H 9.205487 11.087177 -0.103116
H 8.599591 9.807592 1.938407
C 5.451630 13.955741 -1.914096
C 6.232887 15.093830 -2.135994
C 5.136768 13.114927 -2.988677
C 6.696651 15.383762 -3.418075
H 6.482493 15.758600 -1.308213
C 5.607646 13.402308 -4.266252
H 4.519532 12.229937 -2.821931
C 6.386631 14.539331 -4.482101
H 7.302270 16.273085 -3.584715
H 5.359414 12.743140 -5.096428
H 6.748903 14.768755 -5.482903
C 5.070328 14.987657 0.758195
C 6.226137 15.211662 1.512520

C 4.061531 15.958006 0.735784
C 6.372123 16.397204 2.230546
H 7.018052 14.462351 1.539055
C 4.212859 17.144474 1.447556
H 3.152989 15.780525 0.156808
C 5.369117 17.364087 2.196291
H 7.274061 16.566229 2.816538
H 3.425048 17.895455 1.422822
H 5.485726 18.289757 2.757569
C 0.630322 11.922859 -0.248512
H 0.164352 12.056389 0.738430
H 0.009749 12.445518 -0.990513
H 0.614452 10.849846 -0.488554

3t2ts

SCF E(RM06) = -4014.06087783
C -0.844758 5.333089 -1.785746
C -0.535861 5.543565 -0.441608
C -1.328869 6.348685 0.375593
C -2.402869 7.024769 -0.197474
C -2.703851 6.872370 -1.553074
C -1.922869 6.024297 -2.338007
H -0.242226 4.662078 -2.397042
H -3.012284 7.675222 0.429551
H -3.548679 7.401075 -1.990544
H -2.153783 5.884468 -3.393717
Au 1.760409 5.749084 -0.165440
Br 0.144830 3.630481 0.590363
H -1.094486 6.465900 1.432580
H 3.184093 3.671502 4.916487
C 3.378523 3.188431 3.960164
C 3.532753 3.960028 2.814522
C 3.463315 1.796812 3.880992

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C 3.792145 3.350791 1.578808
H 3.447941 5.047123 2.878850
C 3.707117 1.184978 2.654578
H 3.334063 1.191723 4.776817
P 3.872586 4.428052 0.109357
C 3.873782 1.958064 1.504583
H 3.770604 0.100069 2.587252
C 5.393010 5.415553 0.317095
C 4.231972 3.309053 -1.289867
H 4.065997 1.469543 0.548753
C 5.518937 6.576169 -0.455075
C 6.432753 5.041601 1.174600
C 3.156842 2.806719 -2.031882
C 5.536042 2.923734 -1.619923
C 6.675330 7.347599 -0.380513
H 4.703564 6.874921 -1.116786
C 7.584879 5.821124 1.255216
H 6.348333 4.137479 1.778618
C 3.381825 1.922821 -3.084225
H 2.137167 3.108648 -1.783680
C 5.759131 2.044335 -2.676838
H 6.383383 3.310866 -1.052648
C 7.708066 6.971655 0.477882
H 6.765928 8.247677 -0.986238
H 8.390779 5.525368 1.925046
C 4.683307 1.542509 -3.408097
H 2.539574 1.536540 -3.655795
H 6.776891 1.751448 -2.929842
H 8.610017 7.578163 0.542006
H 4.860154 0.856115 -4.234569
C 1.514537 7.819685 -0.587328
H 2.469516 8.334401 -0.748395
H 0.882364 7.907163 -1.481753

H 0.988508 8.263538 0.269296

3t2p

SCF E(RM06) = -4014.12780717

C 0.123611 0.768563 0.225529

C -0.003314 0.002887 1.385907

C 1.090665 -0.729115 1.851904

C 2.308098 -0.679928 1.169371

C 2.439419 0.098747 0.019941

C 1.345512 0.823932 -0.449392

H -0.727945 1.330409 -0.161078

H 3.157532 -1.253044 1.540885

H 3.390551 0.137531 -0.509565

H 1.436866 1.432932 -1.348638

Au -1.789273 -0.009940 2.428547

P -3.959829 0.000266 3.632946

Br -0.753297 1.408865 4.361406

C -5.254444 -1.080558 2.932687

C -5.733189 -0.773440 1.651543

C -5.761582 -2.193169 3.607447

C -6.710186 -1.565353 1.059686

H -5.343614 0.094747 1.116211

C -6.738942 -2.988370 3.008741

H -5.405668 -2.441455 4.606814

C -7.214271 -2.676013 1.738352

H -7.079371 -1.315955 0.066354

H -7.132691 -3.850754 3.543994

H -7.979129 -3.296281 1.274203

C -3.712229 -0.550698 5.350978

C -4.134874 0.204337 6.446878

C -2.997213 -1.737284 5.561875

C -3.850073 -0.226897 7.742017

H -4.678278 1.137145 6.298103

C -2.721617 -2.168264 6.854792
H -2.645379 -2.323687 4.710127
C -3.144681 -1.409734 7.947069
H -4.176614 0.369507 8.592271
H -2.167989 -3.092537 7.010717
H -2.919338 -1.741196 8.959325
C -4.772395 1.631931 3.700144
C -4.060836 2.791199 3.377986
C -6.122722 1.727642 4.063854
C -4.692843 4.033021 3.419359
H -3.009597 2.725708 3.097546
C -6.747417 2.969188 4.111804
H -6.688976 0.828703 4.312199
C -6.032901 4.122828 3.787034
H -4.133806 4.930785 3.161247
H -7.795178 3.035836 4.399606
H -6.524791 5.093650 3.819190
H 1.006343 -1.334107 2.755589
C -2.478502 -1.200520 0.858173
H -3.231406 -1.886403 1.261147
H -2.926140 -0.517856 0.125715
H -1.650421 -1.751189 0.406514

4t1r

SCF E(RM06) = -597.357222226
Au 1.885626 9.518660 0.249391
P 4.090347 10.439154 0.197727
C 4.312079 12.008075 1.108301
H 5.352457 12.350446 1.027621
H 3.647243 12.775418 0.695361
H 4.062075 11.862330 2.165344
C 4.718782 10.824359 -1.474340
H 4.062096 11.555630 -1.959258

H 5.734846 11.236614 -1.413098
H 4.735288 9.913329 -2.083487
C 5.383552 9.353067 0.895948
H 6.367185 9.836117 0.823249
H 5.163552 9.139450 1.948301
H 5.406718 8.405427 0.345523
H 0.358152 8.861222 0.276841

4t1ts

SCF E(RM06) = -3400.01125612
C -1.435466 5.563000 -1.489660
C -0.487200 6.138222 -0.645040
C -0.557666 7.474551 -0.255744
C -1.557193 8.274355 -0.808025
C -2.488544 7.737747 -1.697090
C -2.425695 6.381459 -2.026043
H -1.382213 4.506587 -1.746857
H -1.604562 9.327109 -0.531776
H -3.270348 8.367480 -2.117371
H -3.154385 5.950471 -2.711852
Au 1.728178 5.502414 -1.071161
P 3.811462 4.444038 -0.166700
Br 0.173559 4.775857 1.017163
H 0.167482 7.887424 0.443803
H 1.732313 6.236872 -2.584722
C 4.196884 4.889467 1.566228
H 3.339831 4.642113 2.205163
H 5.079664 4.339518 1.920070
H 4.388296 5.966084 1.641359
C 5.383599 4.762035 -1.045319
H 6.213723 4.235798 -0.554591
H 5.304057 4.419299 -2.083565
H 5.593408 5.837981 -1.049979

C 3.719115 2.617075 -0.104994
H 4.632342 2.197598 0.338753
H 2.855154 2.313794 0.499821
H 3.593460 2.214076 -1.116672

4t1p

SCF E(RM06) = -3400.08347162
C -0.848967 6.137919 -1.362572
C -0.496015 6.081125 -0.011822
C -0.193582 7.265230 0.664850
C -0.222824 8.489441 -0.007602
C -0.564231 8.540828 -1.358217
C -0.878842 7.362432 -2.033760
H -1.095406 5.224719 -1.906502
H 0.021891 9.405702 0.529786
H -0.588680 9.495935 -1.881529
H -1.149524 7.392516 -3.089191
Au -0.330998 4.245202 0.945653
P -0.305367 2.123428 2.129993
C 0.952251 2.057494 3.446178
H 0.916493 1.081531 3.947844
H 1.947356 2.206968 3.011202
H 0.765123 2.848422 4.181086
C 0.065469 0.695139 1.061752
H 1.042962 0.838050 0.586563
H 0.081409 -0.224793 1.661037
H -0.697966 0.603861 0.281011
C -1.869617 1.691553 2.958527
H -1.776068 0.725694 3.471679
H -2.126385 2.466926 3.689437
H -2.674276 1.629927 2.216867
Br 2.098673 3.881860 0.140473
H -1.822932 4.546047 1.405768

H 0.073830 7.243124 1.722199

4t2r

SCF E(RM06) = -1172.12000679

Au 2.586929 12.676967 -0.252381

P 4.842429 13.501296 -0.258498

C 6.061183 12.304992 0.384781

C 5.715053 11.575977 1.529074

C 7.319755 12.122949 -0.195163

C 6.622224 10.684463 2.093120

H 4.730430 11.710083 1.981623

C 8.223869 11.223769 0.368004

H 7.600920 12.684436 -1.086804

C 7.877571 10.506889 1.511513

H 6.347032 10.121886 2.983681

H 9.202625 11.085806 -0.088782

H 8.585726 9.804511 1.948179

C 5.453597 13.958388 -1.916677

C 6.238507 15.093328 -2.141724

C 5.133621 13.115741 -2.988222

C 6.701078 15.378447 -3.425179

H 6.491836 15.759043 -1.315878

C 5.603250 13.398983 -4.267136

H 4.513937 12.232924 -2.819198

C 6.385932 14.532721 -4.486640

H 7.309655 16.265093 -3.594932

H 5.351189 12.738999 -5.095433

H 6.747243 14.758629 -5.488551

C 5.075755 14.998591 0.757258

C 6.232039 15.222116 1.510935

C 4.066814 15.968642 0.733570

C 6.378034 16.408122 2.227978

H 7.023665 14.472551 1.537964

C 4.218401 17.155218 1.444924
H 3.158179 15.791363 0.154710
C 5.374843 17.374800 2.193332
H 7.279964 16.577541 2.813763
H 3.430598 17.906120 1.420133
H 5.491488 18.300605 2.754314
H 1.033394 12.100884 -0.245728

4t2ts

SCF E(RM06) = -3974.77842871
C -1.069533 5.154837 -1.490545
C -0.671995 5.683303 -0.263704
C -1.363250 6.724387 0.353220
C -2.422796 7.310866 -0.333317
C -2.809875 6.838199 -1.589898
C -2.133335 5.760178 -2.159196
H -0.545579 4.305720 -1.927712
H -2.950552 8.146570 0.124878
H -3.644214 7.300587 -2.113880
H -2.436706 5.372941 -3.131144
Au 1.657338 5.776656 -0.149082
Br 0.062242 4.109017 1.163946
H -1.058126 7.089576 1.332185
H 1.864035 7.218842 -0.973980
H 2.922035 3.322449 4.904911
C 3.265748 2.932311 3.948188
C 3.325346 3.770854 2.839673
C 3.635184 1.592204 3.828405
C 3.767674 3.280348 1.603764
H 3.023719 4.816424 2.931883
C 4.065943 1.095780 2.599825
H 3.584197 0.934106 4.694331
P 3.814018 4.449063 0.203515

C 4.132264 1.935465 1.488915
H 4.356644 0.050769 2.504140
C 5.344829 5.411652 0.441480
C 4.147224 3.406445 -1.259707
H 4.478348 1.541214 0.532829
C 5.484952 6.598246 -0.288331
C 6.381384 4.991650 1.281365
C 3.061021 2.742427 -1.844805
C 5.424697 3.245243 -1.804180
C 6.653873 7.347940 -0.191539
H 4.672535 6.932892 -0.936320
C 7.545419 5.750577 1.385276
H 6.284686 4.067332 1.852048
C 3.252674 1.918294 -2.949198
H 2.057979 2.868167 -1.429842
C 5.612906 2.425841 -2.916344
H 6.278895 3.758258 -1.360842
C 7.684288 6.925313 0.647905
H 6.757024 8.267335 -0.765540
H 8.348750 5.419225 2.041489
C 4.529896 1.761762 -3.488347
H 2.403026 1.404432 -3.395909
H 6.610580 2.306569 -3.336136
H 8.596508 7.514201 0.729012
H 4.679445 1.123500 -4.357588

4t2p

SCF E(RM06) = -3974.84498415
C -1.172666 6.521751 -1.242853
C -1.743805 6.076686 -0.048534
C -2.726933 6.849664 0.574255
C -3.151013 8.045643 -0.007702
C -2.595004 8.478620 -1.211136

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C -1.606827 7.713608 -1.827711
H -0.388040 5.942154 -1.729602
H -3.923112 8.638026 0.482939
H -2.928782 9.411495 -1.663666
H -1.162191 8.047301 -2.765145
Au -1.176339 4.264016 0.785137
P -0.294564 2.203912 1.799721
Br -3.490226 3.169462 0.377157
C 1.241699 2.430491 2.757809
C 2.294094 3.135903 2.162032
C 1.415679 1.871805 4.026679
C 3.508402 3.274771 2.825341
H 2.167245 3.572714 1.169657
C 2.630956 2.022289 4.693724
H 0.606887 1.313815 4.498408
C 3.676554 2.719700 4.094475
H 4.323641 3.819688 2.352636
H 2.759263 1.586977 5.683392
H 4.625693 2.833186 4.615640
C -1.480285 1.454036 2.957626
C -1.849880 0.110020 2.879560
C -2.042468 2.275586 3.942956
C -2.769144 -0.411925 3.789315
H -1.424544 -0.534804 2.110178
C -2.954094 1.750223 4.851179
H -1.766464 3.330636 3.999505
C -3.318589 0.404826 4.774263
H -3.055055 -1.460395 3.725629
H -3.385791 2.392053 5.617173
H -4.036539 -0.004465 5.483116
C 0.118997 0.922531 0.570384
C -0.613856 0.849872 -0.619599
C 1.135347 -0.008465 0.816335

C -0.333847 -0.146788 -1.550944
H -1.408631 1.570507 -0.815867
C 1.410103 -1.003887 -0.117319
H 1.715579 0.040149 1.738604
C 0.676170 -1.073733 -1.300687
H -0.906331 -0.196416 -2.475566
H 2.200420 -1.726156 0.079764
H 0.894055 -1.850889 -2.031362
H 0.184455 5.057766 1.001187
H -3.178736 6.519246 1.510319

5tr

SCF E(RM06) = -595.950863319
Au 2.981318 12.808750 -0.252856
Cl 0.790332 11.986917 -0.234412

5tts

SCF E(RM06) = -3398.66253982
C -1.437796 5.769163 -1.759995
C -0.704149 6.266400 -0.696616
C -0.770375 7.560342 -0.208820
C -1.586858 8.447150 -0.913473
C -2.315858 8.012886 -2.019465
C -2.242783 6.685744 -2.439557
H -1.384340 4.725788 -2.060234
H -1.650022 9.481265 -0.580194
H -2.959520 8.711588 -2.549643
H -2.819187 6.345451 -3.297730
Au 1.209165 5.320391 -0.437816
Br -0.552251 4.630357 1.144287
H -0.208130 7.875631 0.666794
Cl 3.203240 5.609575 -1.646469

5tp

SCF E(RM06) = -3398.67382582

C -4.128448 4.903047 -0.170241

C -2.888980 5.493748 -0.302979

C -2.635651 6.849482 -0.320292

C -3.748978 7.687514 -0.192080

C -5.027150 7.151838 -0.055378

C -5.217693 5.772355 -0.044977

H -4.265263 3.824398 -0.166342

H -3.598072 8.765444 -0.198659

H -5.883682 7.815610 0.043191

H -6.215310 5.349410 0.059195

Br -0.831741 4.278742 1.826494

H -1.633294 7.257869 -0.424236

Cl -1.635073 4.129595 -2.884356

6t1r

SCF E(RM06) = -596.599707584

Au -2.028652 0.068749 -0.000741

P 0.252562 0.070116 0.000090

C 0.948558 1.745532 -0.058682

H 0.615457 2.318491 0.813235

H 2.044783 1.682729 -0.055385

H 0.616168 2.255352 -0.969162

C 0.950878 -0.715345 1.480284

H 0.624616 -1.759102 1.536817

H 2.046792 -0.678014 1.423950

H 0.614316 -0.186518 2.378460

C 0.948395 -0.819296 -1.421029

H 0.625616 -0.342742 -2.352782

H 2.044500 -0.797667 -1.360313

H 0.604769 -1.859137 -1.414742

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6t1ts

SCF E(RM06) = -3399.29724574

C -0.907873 5.845767 -2.035330

C -0.494745 5.488352 -0.767153

C -0.911577 6.057632 0.420332

C -1.780482 7.145987 0.302968

C -2.208997 7.581583 -0.949695

C -1.779385 6.936153 -2.107772

H -0.570386 5.323260 -2.926652

H -2.119258 7.644378 1.209378

H -2.893739 8.423651 -1.023088

H -2.120836 7.269163 -3.086198

Au 1.586933 4.729905 -0.674938

Br -0.217748 3.024924 -0.596954

H -0.571642 5.698620 1.388525

C 3.322223 7.207799 1.003048

P 3.066525 6.567895 -0.678164

C 2.355693 7.949155 -1.620033

C 4.716310 6.265596 -1.375992

H 3.926553 8.123310 0.968047

H 2.349118 7.432368 1.456103

H 3.832949 6.457384 1.615838

H 3.049550 8.799481 -1.612365

H 2.166751 7.642088 -2.654782

H 1.407626 8.257186 -1.161502

H 5.309892 7.187614 -1.324266

H 5.222341 5.476297 -0.810128

H 4.626022 5.951623 -2.421294

Au -1.285900 4.244377 -0.570105

6t1p

SCF E(RM06) = -3399.31367151

C -1.312373 6.060837 -1.541818

C -1.599895 6.133509 -0.191741
C -2.294211 7.159958 0.421553
C -2.717759 8.207883 -0.401380
C -2.446333 8.190332 -1.767609
C -1.752003 7.125621 -2.335548
H -0.778343 5.220288 -1.980456
H -3.265384 9.036284 0.044277
H -2.780791 9.013669 -2.395433
H -1.544115 7.105047 -3.403706
Au -1.083423 4.526561 0.982293
P 1.028190 5.555118 1.233840
Br -3.236300 3.307196 0.774899
C 0.969824 7.272851 1.798445
C 1.918032 4.592776 2.485539
C 1.993286 5.511505 -0.296187
H -2.506506 7.164999 1.488629
H 0.564363 7.919079 1.012183
H 0.345842 7.353760 2.695160
H 1.991576 7.596508 2.036082
H 3.005260 5.882283 -0.088958
H 2.051570 4.485303 -0.674253
H 1.525785 6.151402 -1.052949
H 1.382641 4.638369 3.439691
H 2.003763 3.548665 2.166603
H 2.922137 5.018736 2.611603

6t2r

SCF E(RM06) = -1171.35821210
Au -1.783140 -0.968346 0.696747
P 0.273172 -0.129837 0.132583
C 0.692247 1.342089 1.107341
C 0.420376 1.342139 2.480421
C 1.332799 2.436897 0.519381

C 0.797575 2.428378 3.262296
H -0.086510 0.491083 2.938460
C 1.702309 3.524888 1.307585
H 1.546914 2.445549 -0.549384
C 1.437215 3.520309 2.675040
H 0.585477 2.426045 4.329702
H 2.198810 4.377571 0.848166
H 1.725563 4.373681 3.286330
C 0.351784 0.352140 -1.614102
C 1.501280 0.124579 -2.377418
C -0.738832 1.027894 -2.173114
C 1.554525 0.573299 -3.695323
H 2.356839 -0.397349 -1.948545
C -0.676699 1.478652 -3.486928
H -1.637090 1.202177 -1.578438
C 0.469393 1.249121 -4.248739
H 2.448360 0.391771 -4.289152
H -1.526055 2.003434 -3.920079
H 0.513973 1.595658 -5.279668
C 1.595754 -1.341969 0.409898
C 2.768024 -0.993179 1.085994
C 1.438510 -2.636229 -0.101099
C 3.779230 -1.938891 1.248128
H 2.898394 0.011781 1.487021
C 2.454485 -3.571639 0.056563
H 0.522113 -2.911902 -0.625957
C 3.623902 -3.223476 0.734390
H 4.689624 -1.667121 1.779052
H 2.331591 -4.575827 -0.344753
H 4.414292 -3.960590 0.864706

6t2ts

SCF E(RM06) = -3974.05936873

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C -1.231600 6.786603 -1.826347
C -0.504886 6.544120 -0.677853
C -0.884582 6.844154 0.613928
C -2.087717 7.543712 0.744345
C -2.848686 7.866154 -0.377177
C -2.425595 7.491275 -1.651313
H -0.896867 6.464760 -2.809052
H -2.420718 7.827705 1.741224
H -3.787557 8.402261 -0.255926
H -3.023275 7.733429 -2.528170
Au 1.691446 6.532248 -0.977105
Br 0.623810 4.306283 -0.777897
H -0.284668 6.572399 1.478981
P 2.469721 8.769768 -1.142337
C 1.258265 9.864123 -0.345566
C 1.070556 9.760832 1.039452
C 0.476773 10.750984 -1.091045
C 0.133634 10.566386 1.675487
H 1.663539 9.054959 1.624159
C -0.472099 11.545475 -0.448773
H 0.606528 10.827765 -2.170566
C -0.637916 11.460157 0.931108
H -0.000616 10.490946 2.753022
H -1.078529 12.236044 -1.031949
H -1.374686 12.087289 1.429960
C 2.654820 9.340369 -2.856872
C 2.057278 8.639697 -3.908321
C 3.360475 10.521933 -3.117921
C 2.154581 9.123747 -5.211052
H 1.520881 7.709639 -3.719293
C 3.456272 10.999686 -4.420107
H 3.835658 11.072006 -2.304795
C 2.851118 10.302544 -5.466072

H 1.687188 8.575380 -6.026656
H 4.005538 11.917913 -4.619614
H 2.928141 10.678803 -6.484600
C 4.071538 9.047099 -0.328686
C 5.067179 8.075061 -0.483026
C 4.346020 10.218392 0.385190
C 6.326825 8.274025 0.072692
H 4.861782 7.160727 -1.042130
C 5.607210 10.409304 0.944035
H 3.580534 10.984506 0.509193
C 6.595662 9.439384 0.789541
H 7.097272 7.515130 -0.049907
H 5.816981 11.320643 1.500982
H 7.579522 9.591046 1.230190

6t2p

SCF E(RM06) = -3974.07293445
C -1.656732 4.278221 -0.730278
C -1.555163 5.255613 0.239767
C -1.745241 6.609522 0.041263
C -2.065038 7.009406 -1.259504
C -2.173040 6.068902 -2.281705
C -1.968997 4.716089 -2.022567
H -1.502219 3.222344 -0.515249
H -2.224052 8.067701 -1.459955
H -2.419427 6.393750 -3.290700
H -2.057190 3.979214 -2.818975
Au -1.187637 4.648349 2.173164
P 1.134934 5.042230 1.812378
Br -3.564955 4.223618 2.727808
H -1.645667 7.339303 0.843077
C 1.527896 6.287034 0.560520
C 1.709561 7.631979 0.897107

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C 1.562376 5.889252 -0.782886
C 1.921594 8.572396 -0.107529
H 1.697241 7.953426 1.937273
C 1.782337 6.832839 -1.778646
H 1.421084 4.842856 -1.053216
C 1.954524 8.175559 -1.442400
H 2.067739 9.617670 0.157260
H 1.813665 6.519273 -2.820425
H 2.120005 8.914614 -2.224190
C 1.983483 3.517594 1.341086
C 3.319481 3.582238 0.919037
C 1.338951 2.280759 1.441010
C 4.000388 2.412111 0.605549
H 3.827225 4.543931 0.837735
C 2.026953 1.113271 1.121583
H 0.298897 2.219780 1.761545
C 3.354284 1.179470 0.706037
H 5.037434 2.462446 0.280181
H 1.522037 0.152326 1.195629
H 3.890280 0.266025 0.454992
C 1.730481 5.582323 3.437946
C 2.805001 4.932383 4.056351
C 1.084377 6.644032 4.091017
C 3.246292 5.362057 5.304326
H 3.300949 4.093519 3.570167
C 1.536282 7.069068 5.334763
H 0.226149 7.142689 3.636780
C 2.616825 6.429182 5.941171
H 4.083890 4.856597 5.780874
H 1.036482 7.895983 5.835102
H 2.964982 6.760836 6.917574