Supporting Information

Gold(I)-Catalyzed Enantioselective [4+2] Cycloaddition of Allene-Dienes

*Ana Z. Gonzalez and F. Dean Toste**

Department of Chemistry, University of California, Berkeley, California, 94720

fdtoste@berkeley.edu

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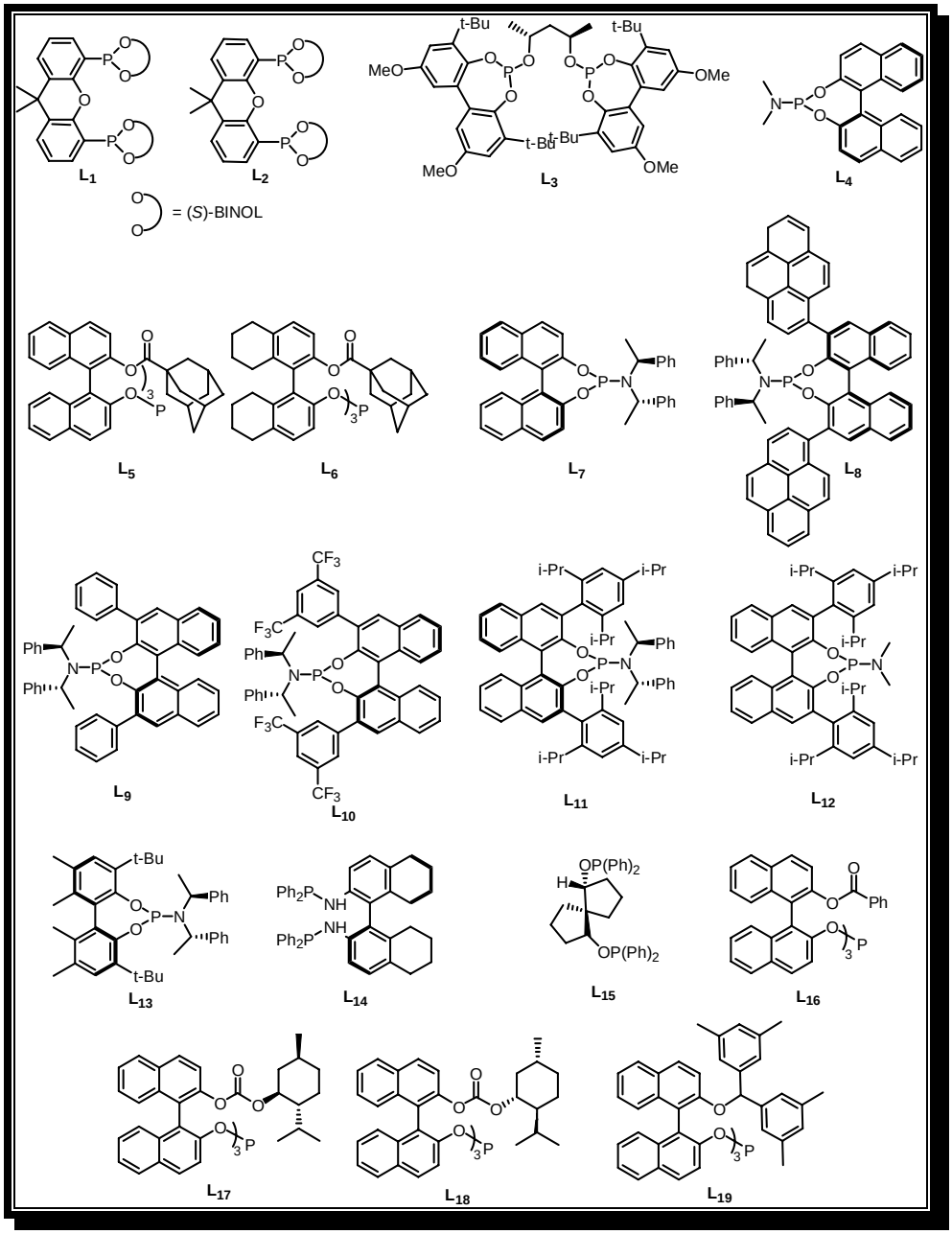
1. General Information

Unless otherwise noted, all reagents were obtained commercially and used without further purification. All reaction mixtures excluding the gold(I)-catalysis mixtures were stirred with a magnetic stir bar in flame-dried glassware under a nitrogen atmosphere. Tetrahydrofuran (THF), diethyl ether (Et_2O) and dichloromethane (CH_2Cl_2) were dried by passing commercially available pre-dried, oxygen-free formulations through activated alumina columns. Triethylamine (Et_3N) was distilled from CaH_2.[1] Dry DMSO and DMF were obtained from Acros. Extracts were dried over $MgSO_4$ or Na_2SO_4 and solvents were removed in a rotary evaporator. TLC analysis of reaction mixtures was performed on Merck silica gel 60 F254 TLC plates. Unless otherwise indicated, chromatography was carried out on ICN SiliTech 32-63 D 60 Å silica gel. ^1H, ^{13}C NMR and ^{31}P NMR spectra were recorded with Bruker AMX-300, AVQ-400, AVB-400, DRX-500 and AV-500 spectrometers and referenced to $CDCl_3$, CD_2Cl_2 or C_6D_6. Structures were confirmed using NOESY, COSY and HSQC experiments. Mass spectra data were obtained at the Micro-Mass/Analytical Facility in the College of Chemistry, University of California, Berkeley.

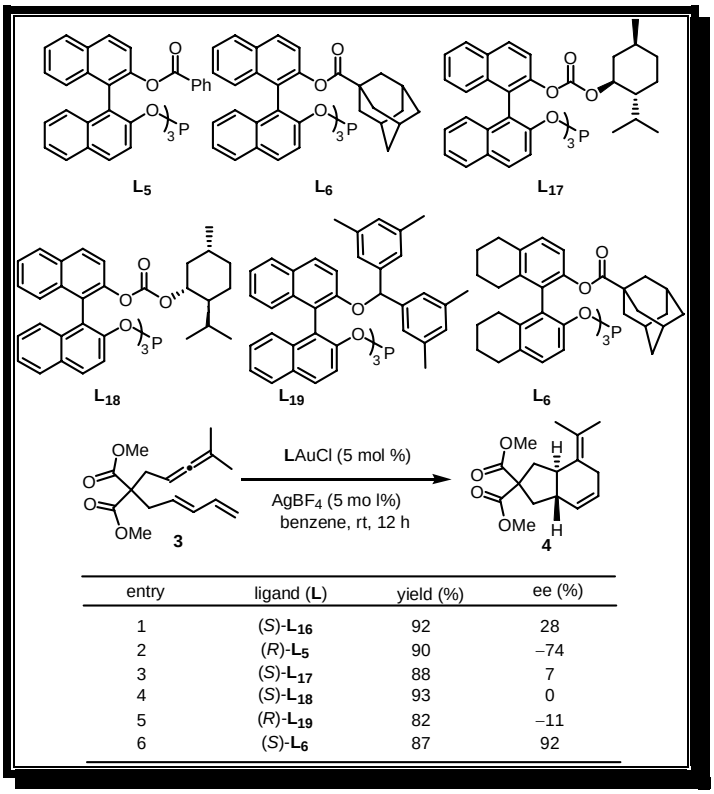
[1] Alaimo, P.J.; Peters, D.W.; Arnold, J.; Bergman, R.G. *J. Chem. Ed.* **2001**, *78*, 64.

2. Selected Analytical Data and Representative Experimental Procedures.

Ligand Leyend:

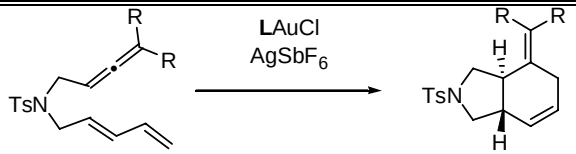


Ligand Optimization with C_3-symmetric phosphites:



entry	ligand (**L**)	yield (%)	ee (%)
1	(*S*)-**L16**	92	28
2	(*R*)-**L5**	90	–74
3	(*S*)-**L17**	88	7
4	(*S*)-**L18**	93	0
5	(*R*)-**L19**	82	–11
6	(*S*)-**L6**	87	92

Ligand Optimization with phosphoramiditesgold(I)-catalysts phosphites:

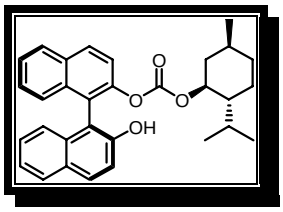


Entry	R	L	solvent	temp (^{o}C)	Product	Yield (%)	ee (%)*
1	Me	(*R*,*R*)-**L$_3$** (10 mol %)	CH_2Cl_2	25	**3**	91	0
2	-$(CH_2)_4$-	(*R*)-**L$_4$** (10 mol %)	CH_2Cl_2	25	**10**	92	0
3	Me	(*R*)-**L$_4$** (10 mol %)	CH_2Cl_2	25	**3**	88	–14
4	Me	(*R*)-**L$_5$** (10 mol %)	CH_2Cl_2	25	**3**	92	16
5	-$(CH_2)_4$-	(*R*)-**L$_6$** (5 mol %)	CH_2Cl_2	25	**10**	77	28
6	Me	(*R*)-**L$_6$** (5 mol %)	CH_2Cl_2	25	**3**	76	24
7	Me	(*S*)-**L$_6$** (5 mol %)	benzene	25	**3**	86	–34
8	-$(CH_2)_4$-	(*S*,*S*,*S*)-**L$_7$** (10 mol %)	CH_2Cl_2	25	**10**	87	0
9	Me	(*S*,*S*,*S*)-**L$_7$** (10 mol %)	CH_2Cl_2	25	**3**	89	21
10	Me	(*R*,*S*,*S*)-**L$_7$** (10 mol %)	CH_2Cl_2	25	**3**	92	0
11	-$(CH_2)_4$-	(*R*,*R*,*R*)-**L$_9$** (10 mol %)	CH_2Cl_2	-30	**10**	89	–69
12	Me	(*R*,*R*,*R*)-**L$_9$** (10 mol %)	CH_2Cl_2	-30	**3**	89	–82
13	-$(CH_2)_4$-	(*R*,*R*,*R*)-**L$_{10}$** (10 mol %)	CH_2Cl_2	-30	**10**	86	–76
14	Me	(*R*,*R*,*R*)-**L$_{10}$** (10 mol %)	CH_2Cl_2	-30	**3**	81	–80
15	-$(CH_2)_4$-	(*S*,*S*,*S*)-**L$_{11}$** (10 mol %)	CH_2Cl_2	-30	**10**	85	74
16	Me	(*S*,*S*,*S*)-**L$_{11}$** (10 mol %)	CH_2Cl_2	25	**3**	83	40
17	Me	(*S*,*S*,*S*)-**L$_{11}$** (10 mol %)	CH_2Cl_2	-30	**3**	83	69
18	-$(CH_2)_4$-	(*S*,*S*,*S*)-**L$_{13}$** (10 mol %)	CH_2Cl_2	25	**10**	90	0
19	Me	(*R*)-**L$_{14}$** (5 mol %)	CH_2Cl_2	25	**3**	88	8
20	Me	(*R*,*R*)-**L$_{15}$** (5 mol %)	CH_2Cl_2	25	**3**	81	0
21	-$(CH_2)_4$-	(*S*,*S*,*S*)-**L$_8$** (10 mol %)	CH_2Cl_2	-15	**10**	91	99
22	Me	(*S*,*S*,*S*)-**L$_8$** (10 mol %)	CH_2Cl_2	-15	**3**	83	99

* The stereochemistry of the product was assigned according to those previosly reported in the literature (Alonso, I.; Trillo, B.; Lopez, F.; Montserrat, S.; Ujaque, G.; Castedo, L.; Lledos, L.; Mascarenas, J. L. *J. Am. Chem. Soc.* **2009**, *131*, 13020). The negative sign in fron of ee value denotes the opposite enantiomer.

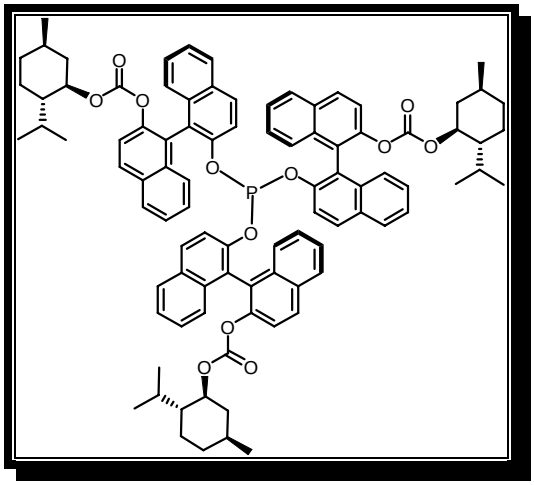
2.1 Preparation of Phosphites

Ligands $\mathbf{L_1}$, $\mathbf{L_2}$, $\mathbf{L_3}$ and $\mathbf{L_{15}}$ where purchased form Sigma-Aldrich and used as such. $\mathbf{L_5}$ and $\mathbf{L_{16}}$ where synthesized as described by Reetz *et al.*[2] All other phosphites ($\mathbf{L_{17}}$, $\mathbf{L_{18}}$, $\mathbf{L_{19}}$) where prepared via a modification of a procedure reported by Reetz.[2] A flamed-dried, cooled under N_2 flask was charged with the corresponding alcohol, THF (0.1 M), and Et_3N (1.2 equiv). This mixture was cooled to 0 °C followed by the dropwise addition of PCl_3 (0.33 equiv). Once the addition was complete, the reaction was left to react at room temperature for 24 hrs. After this period, the reaction was quenched with distilled water, extracted with ethyl acetate and the combined organic phase was dried over $MgSO_4$, fitered, and concentrated. The crude mixture was then purified by flash chromatography (hexanes:EtOAc 95:5) yielding the desired phosphite.

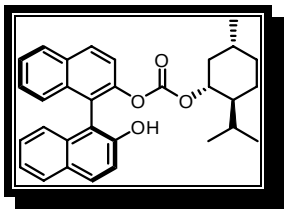


11. Prepared via a modification of a procedure reported by Reetz from (*S*)-BINOL and (+)-menthyl chloroformate.[2] Isolated via silica gel column chromatography (hexanes:EtOAc 90:10, Rf = 0.2) as colorless crystals (81%). ^{1}H NMR (300 MHz, $CDCl_3$): δ 0.54 (d, *J* = 6.9 Hz, 3H), 0.63 (q, *J* = 11.4 Hz, 1H), 0.74 (d, *J* = 7.0 Hz, 3H), 0.87 (d, *J* = 6.5 Hz, 3H), 0.94-0.97 (m, 1H), 1.17-1.34 (m, 2H), 1.55-1.69 (m, 4H), 4.33 (td, *J* = 10.9, 4.4 Hz, 1H), 5.27 (s, 1H), 7.04 (d, *J* = 8.3 Hz, 1H), 7.21-7.38 (m, 5H), 7.49-7.54 (m, 2H), 7.84 (d, *J* = 8.0 Hz, 1H), 7.90 (d, *J* = 8.9 Hz, 1H), 7.97 (d, *J* = 8.2 Hz, 1H), 8.07 (d, *J* = 8.9 Hz, 1H) . ^{13}C NMR (75 MHz, $CDCl_3$): δ 16.0, 20.5, 21.8, 23.1, 25.9, 31.1, 33.8, 39.7, 46.4, 79.6, 113.7, 118.2, 121.4, 123.3, 123.5, 124.6, 125.8, 126.3, 126.8, 127.5, 127.9, 128.3, 129.1, 130.5, 130.9, 132.3, 133.4 (2C), 148.1, 151.7, 153.8. HRMS (EI+): calculated for $C_{31}H_{32}O_4$ 468.2301, found 468.2306.

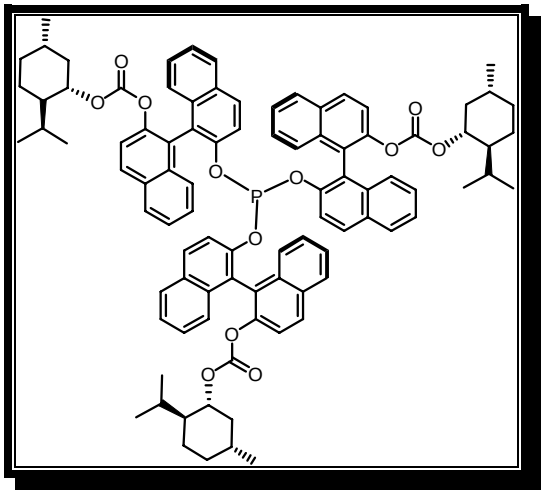
[2] Reetz, M. T.; Guo, H.; Ma, J-A.; Goddard, R.; Mynott, R. J. *J. Am. Chem. Soc.* **2009**, *131*, 4136-4142.



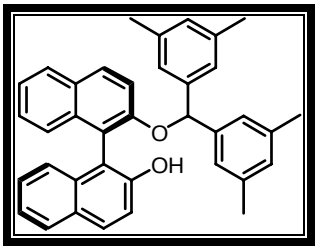
L_{17}. Isolated via silica gel column chromatography (hexanes:EtOAc 85:15, Rf = 0.4) as a white powder (77%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 0.19 (bs, 9H), 0.54 (bs, 9H), 0.75-0.87 (bs, 20H), 1.12 (bs, 3H), 1.29 (bs, 5H), 1.51-1.57 (m, 7H), 1.89 (bs, 3H), 4.24 (bs, 3H), 6.56 (bs, 3H), 6.79 (bs, 3H), 7.04-7.34 (m, 20H), 7.67-7.84 (m, 9H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 15.9, 20.3, 21.9, 23.6, 31.2, 33.2, 40.4, 46.6, 78.5, 120.6, 120.7, 120.8 (2C), 121.6, 124.4, 125.3, 125.7, 126.2 (2C), 126.3, 127.6, 127.7, 129.3, 130.1, 131.6, 133.1, 133.3, 146.9, 147.4, 153.0. ^{31}P NMR (162 MHz, $CDCl_3$): δ 130.5. HRMS (EI+): calculated for $C_{93}H_{93}O_{12}P$ 1433.6438, found 1433.6438.



12. Prepared via a modification of a procedure reported by Reetz from (*S*)-BINOL and (-)-menthyl chloroformate. Isolated via silica gel column chromatography (hexanes:EtOAc 85:15, Rf = 0.3) as a white powder (60%).[2] ^{1}H NMR (300 MHz, $CDCl_3$): δ 0.59 (d, *J* = 6.9 Hz, 3H), 0.62 (q, *J* = 11.4 Hz, 1H), 0.76-1.02 (m, 6H),1.11-1.43 (m, 4H), 1.55-1.82 (m, 3H), 4.39 (td, *J* = 10.9, 4.4 Hz, 1H), 5.37 (s, 1H), 7.09 (d, *J* = 8.3 Hz, 1H), 7.25-7.40 (m, 5H), 7.51-7.54 (m, 2H), 7.86 (d, *J* = 8.0 Hz, 1H), 7.92 (d, *J* = 8.9 Hz, 1H), 7.98 (d, *J* = 8.2 Hz, 1H), 8.09 (d, *J* = 8.9 Hz, 1H) . ^{13}C NMR (75 MHz, $CDCl_3$): δ 16.4, 20.3, 21.8, 23.4, 25.8, 31.1, 33.8, 40.1, 46.5, 79.5, 113.6, 118.3, 121.3, 123.4, 124.4, 125.7, 126.3, 126.7, 127.4, 127.8, 128.2, 129.0, 130.3, 132.2, 133.3, 147.9, 151.7, 153.7.



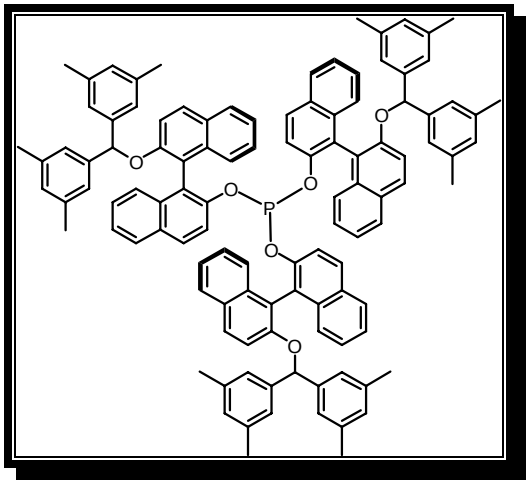
L_{18}. Isolated via silica gel column chromatography (hexanes:EtOAc 85:15, Rf = 0.5) as a white powder (84%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 0.47 (bs, 3H), 0.54-1.16 (m, 32H), 1.24 (bs, 11H), 1.60-1.78 (bs, 10H), 4.26 (bs, 3H), 6.70 (bs, 5H), 7.05 (bs, 5H), 7.09-7.68 (m, 16H), 7.78-7.89 (m, 9H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 16.3, 20.6, 21.8, 23.2, 31.0, 33.9, 39.4, 46.3, 78.8, 120.5, 120.7, 121.6, 121.6, 124.4, 124.7, 125.2, 125.8, 126.0 (2C), 126.2, 126.4, 127.6, 129.4, 130.1, 131.6, 133.0, 133.2, 146.9, 147.2, 153.0. ^{31}P NMR (162 MHz, $CDCl_3$): δ 130.5.



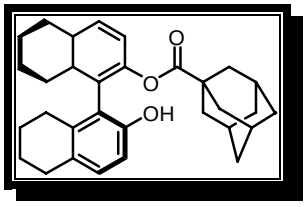
13. Prepared via a modification of a procedure reported by Pericàs from (*R*)-BINOL and bis(3,5-xylyl)bromomethane.[3] An oven-dried, cooled under N_2, round-bottomed flask was charged with (*R*)-BINOL (0.85 mmol, 244 mg) and diluted in dichloromethane (2 mL). To this solution Triethylamine (2.55 mmols, 0.36 mL) and DMAP (0.43 mmol, 52 mg) where added follwed by the addition of bis(3,5-xylyl)bromomethane (0.83 mmol, 258 mg). The reaction mixture was allowed to react at 25 °C for 2 hrs and then refluxed overnight. The crude product was extracted form Brine (20 mL) with diethyl ether (3 × 20 mL). The combined organic phase was then dried over $MgSO_4$, filtered and concentrated. The crude oil was purified via silica gel column

[3] Cattoën, X; Pericàs, M. A. *J. Org. Chem.* **2007**, *72*, 3253-3258.

chromatography (hexanes:EtOAc, 95:5, Rf = 0.2) to yield the desired product in 43% as a white solid. To a ^{1}H NMR (300 MHz, $CDCl_3$): δ 2.08 (s, 6H), 2.21 (s, 6H), 4.96 (s, 1H), 6.18 (s, 1H), 6.57 (s, 2H), 6.72-6.80 (m, 4H), 7.19-7.45 (m, 8H), 7.85 (m, 4H). ^{13}C NMR (75 MHz, $CDCl_3$): δ 21.1, 21.2, 81.5, 115.5, 116.4, 117.0, 117.6, 123.2, 123.9, 124.1, 124.2, 124.9, 125.3, 126.3, 127.2, 128.0, 128.1, 128.9, 129.1, 129.2, 129.4, 129.7, 130.5, 133.9, 134.0, 137.6, 137.8, 141.2, 141.3, 151.4, 153.9.



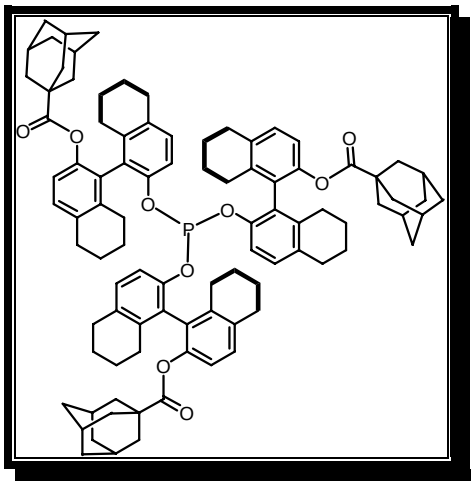
L_{19}. Isolated via silica gel column chromatography (hexanes:diethyl ether 70:30, Rf = 0.2) as a white powder (66%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 2.01 (s, 18H), 2.02 (s, 18H), 5.91 (s, 3H), 6.21 (d, *J* = 9.0 Hz, 3H), 6.47 (s, 6H), 6.57 (bs, 9H), 6.62 (d, *J* = 8.4 Hz, 3H), 6.67 (s, 3H), 6.86 (d, *J* = 9.0 Hz, 3H), 6.96-7.00 (m, 3H), 7.02-7.05 (m, 6H), 7.13-7.17 (m, 6H), 7.31-7.35 (m, 3H), 7.50 (d, *J* = 8.0 Hz, 3H), 7.62 (d, *J* = 9.0 Hz, 3H), 7.71 (d, *J* = 8.1 Hz, 3H). ^{31}P NMR (162 MHz, $CDCl_3$): δ 134.1.



14. Prepared via a modification of a procedure reported by Reetz from (*S*)-H_8-BINOL[4] and 1-adamantane carbonyl chloride. (98% yield).[2] ^{1}H NMR (400 MHz, $CDCl_3$): δ 1.57-1.77 (m, 20H),

[4] H_8-BINOL was synthesized as described by: McDougal, N. T.; Trevellini, W. L.; Rodgen, S. A.; Kliman, L. T.; Schaus, S. E. *Adv. Synth. Catal.* **2004**, *346*, 1231.

1.91 (s, 3H), 2.03-2.08 (m, 1H), 2.15-2.21 (m, 1H), 2.35-2.50 (m, 2H), 2.66-2.84 (m, 4H), 6.78 (d, *J* = 8.3 Hz, 1H), 6.88 (d, *J* = 8.2 Hz, 1H), 6.98 (d, *J* = 8.3 Hz, 1H), 7.17 (d, *J* = 8.2 Hz, 1H) . ^{13}C NMR (100 MHz, $CDCl_3$): δ 22.6, 22.8, 23.1, 23.2, 26.8, 27.2, 27.7, 29.3, 29.6, 36.3, 38.1, 40.5, 114.0, 119.3, 122.5, 127.9, 129.4, 129.6, 130.2, 135.7, 135.8, 138.2, 147.1, 150.7, 177.2. HRMS (EI+): calculated for [M – 1] $C_{31}H_{37}O_3$ 458.2743, found 458.2753.



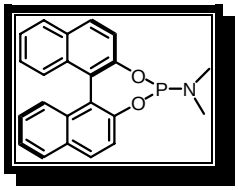
L_6. Isolated via silica gel column chromatography (hexanes:EtOAc 95:5, Rf = 0.5) as a white powder (88%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 1.52-1.69 (m, 60H), 1.85 (bs, 9H), 1.97-2.09 (m, 6H), 2.17-2.21 (m, 6H), 2.57-2.76 (m, 13H), 6.14 (d, *J* = 8.3 Hz, 3H), 6.55 (d, *J* = 8.3 Hz, 3H), 6.91 (d, *J* = 8.2 Hz, 3H), 7.06 (d, *J* = 8.3 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 22.5, 22.7, 23.1, 23.2, 26.9, 27.5, 27.6, 27.8, 29.5, 29.6, 36.4, 38.2, 40.6, 118.7, 118.8, 119.8, 127.2, 128.9, 129.4, 132.3, 134.5, 136.3, 136.7, 146.2, 146.4, 175.9. ^{31}P NMR (162 MHz, $CDCl_3$): δ 133.2. HRMS (EI+): calculated for $C_{93}H_{105}O_9P$ 1397.7529, found 1397.7587.

2.2. Preparation of Phosphoramidites

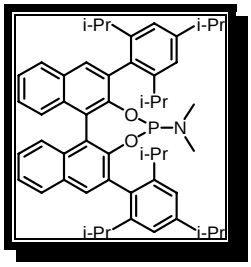
L_7 and **L_{14}** where purchased from Sigma-Aldrich and used without further purification. **L_{13}** was synthezised as reported by Ojima *et al.*[5] All spectroscopic data were in complete agreement with the reported literature values. All other phosphoramidites, except **L_4** and **L_7**, where prepared via a modification of a procedure reported by Ojima (see Ref. 5): A flamed-dried, cooled under N_2 flask was charged with NEt_3 (5.0 equiv) and cooled to 0 °C. To this compound PCl_3 (1.0 equiv)

[5] Chapsal, B. D.; Hua, Z.; Ojima, I. *Tetrahedron: Asym.* **2006**, *17*, 642.

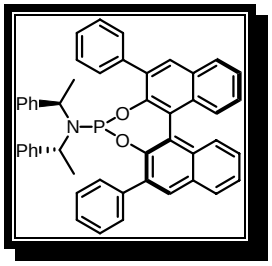
was added dropwise. To this mixture, a solution of amine (1.0 equiv) in THF (0.5 M) was added and allowed to stir at 25 °C until ^{31}P NMR analysis of the reaction mixture showed a sole peak corresponding to the newly formed aminophosphorous dichloride (3 hrs, δ 165 approximately). At this point a solution of the diol (1.0 equiv) in THF (0.5 M) where added to the reaction mixture, then stirred at 25 °C for 12 hrs. After addition of ether (0.5 M with respect to the diol), the resulting solid was filtered through a silica gel plug and washed with diethyl ether. The combined solution was concentrated in vacuo to give a crude product which was then purified via silica gel column chromatography (see bellow for detailed conditions for each ligand) to give the desired product.



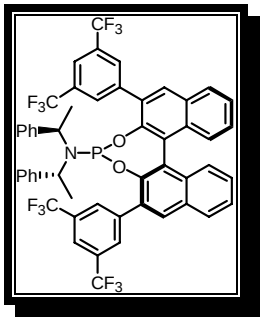
L_4. An oven-dried, cooled under N_2, round bottomed flask equipped with a reflux condenser was charged with (*R*)-BINOL (1.7 mmols, 0.5 g) and flushed with N_2. To this solid toluene was added (10 mL) followed by $P(NMe_2)_3$ (1.7 mmols, 0.31 mL). The reaction mixture was then refluxed for 2 hrs. ^{31}P NMR analysis of the cooled reaction mixture showed the sole formation of the desired phosphoramidite product (δ 148.8). The crude reaction mixture was concentrated and purified via silica gel column chromatography (hexanes:EtOAc, 90:10, Rf = 0.5). The product was isolated as a white powder (95%). ^1H NMR (400 MHz, $CDCl_3$): δ 2.59 (s, 3H), 2.61 (s, 3H), 7.29 (dd, *J* = 7.3, 9.0 Hz, 2H), 7.40-7.48 (m, 5H), 7.56 (d, *J* = 8.7 Hz, 1H), 7.93-7.96 (m, 3H), 8.01 (d, *J* = 8.6 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 35.8, 36.0, 121.9, 122.0, 122.7 (2C), 123.8, 123.9, 126.0 (2C), 126.8, 126.9, 128.2, 130.0, 130.2, 130.7, 131.3, 132.5, 132.7, 149.4 (2C), 149.9, 150.0. ^{31}P NMR (162 MHz, $CDCl_3$): δ 148.8. HRMS (EI+): calculated for $C_{22}H_{18}NO_2P$ 359.1072, found 359.1069.



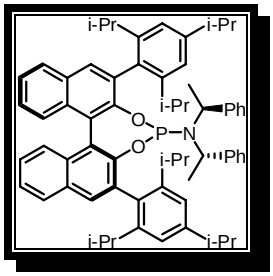
L_{12}. Synthesized as described above for **L_4**. The crude reaction mixture was concentrated and purified via silica gel column chromatography (hexanes:EtOAc 95:5, Rf = 0.6). The product was isolated as a white powder (91%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 0.87 (d, *J* = 6.76 Hz, 2H), 1.10-1.39 (m, 32H), 1.45 (d, *J* = 6.6 Hz,2H), 2.21 (s, 3H), 2.23 (s, 3H), 2.79-2.83 (m, 3H), 2.98-3.05 (m, 3H), 7.11-7.12 (m, 3H), 7.20-7.24 (m, 3H), 7.26-7.37 (m, 3H), 7.41-7.43 (m, 1H), 7.46-7.49 (m, 2H), 7.84-7.86 (m, 1H), 7.91-7.95 (m, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 23.1, 23.2, 23.3, 23.6, 23.8, 24.0, 24.1, 24.2, 24.3, 24.6, 25.2, 25.9, 27.5, 30.5, 30.8, 30.8, 30.8, 31.0, 34.2, 34.2, 34.4, 35.2, 35.4, 120.2, 120.7, 120.8, 121.2, 121.2, 122.1, 122.4, 124.3, 124.5, 124.6, 125.3, 125.5, 125.5, 126.5, 127.0, 127.1, 128.0, 128.2, 128.2 129.0, 129.6, 130.4, 130.7, 131.0, 131.7, 132.1, 132.3, 132.7, 132.8, 133.4, 133.8, 146.3, 147.7, 147.9, 148.0, 148.5, 149.0, 149.1, 150.6. ^{31}P NMR (162 MHz, $CDCl_3$): δ 145.6.



L_9. Purified via silica gel column chromatography (hexanes:EtOAc, 90:10, Rf = 0.55). The product was isolated as a white powder (98%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 1.14 (s, 3H), 1.16 (s, 3H), 4.14-4.18 (m, 2H), 6.64-6.66 (m, 4H), 6.92-6.96 (m, 4H), 6.92-6.96 (m, 4H), 7.01-7.04 (m, 2H), 7.25-7.31 (m, 3H), 7.40-7.50 (m, 9H), 7.66 (d, *J* = 6.8 HZ, 2H), 7.78 (d, *J* = 8.1 Hz, 2H), 7.93 (d, *J* = 7.9 Hz, 1H), 7.96 (d, *J* = 8.1 Hz, 1H), 8.00 (s, 1H), 8.05 (s, 1H). ^{31}P NMR (162 MHz, $CDCl_3$): δ 148.9. HRMS (EI+): calculated for [M + 1] $C_{48}H_{39}NO_2P$ 692.2718, found 692.2720.



L_{10} Purified via silica gel column chromatography (hexanes:EtOAc, 95:5). The product was isolated as a white powder (77%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 1.22 (s, 3H), 1.24 (s, 3H), 4.18 (bs, 2H), 6.56 (d, *J* = 7.7 Hz, 4H), 6.88 (d, *J* = 7.6 Hz, 2H), 6.90 (d, *J* = 7.7 Hz, 2H), 7.01 (d, *J* = 7.4 Hz, 1H), 7.04 (d, *J* = 7.3 Hz, 1H0, 7.23 (d, *J* = 8.4 Hz, 1H), 7.33-7.39 (m 2H), 7.45-7.53 (m, 4H), 7.84 (s, 1H), 7.93 (s, 1H), 7.96 (s, 1H), 7.98 (s, 1H), 8.04 (d, *J* = 8.1 Hz, 1H), 8.08 (s, 2H), 8.13 (s, 1H), 8.23 (s, 2H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 29.7 (2C), 54.4, 54.5, 121.2, 121.3, 122.0, 122.1, 122.6 (2C), 124.7, 124.8, 125.5, 125.9, 126.6, 126.8, 127.0, 127.1, 127.2, 127.6, 128.4, 128.7, 129.7, 130.0, 130.4, 131.0, 131.3, 131.4, 131.6, 131.7, 131.9, 132.2, 133.1, 133.2, 140.0, 142.1, 146.7, 147.4, 149.9. ^{31}P NMR (162 MHz, $CDCl_3$): δ 151.4. HRMS (EI+): calculated for [M + 1] $C_{52}H_{35}F_{12}NO_2P$ 964.2214, found 964.2223.

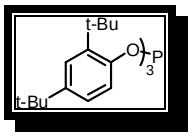


L_{11}. Purified via silica gel column chromatography (hexanes:CH_2Cl_2 4:1, Rf = 0.65). The product was isolated as a white powder (88%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 0.86 (d, *J* = 6.7 Hz, 3H), 0.99 (d, *J* = 6.8 Hz, 3H), 1.05 (d, *J* = 7.0 Hz, 6H), 1.12-1.17 (m, 7H), 1.20 (d, *J* = 6.8 Hz, 3H), 1.29 (d, *J* = 6.7 Hz, 4H), 1.40-1.46 (m, 19H), 2.91-3.23 (m, 6H), 4.07 (dq, *J* = 7.6 Hz, 2H), 6.61 (d, *J* = 7.5 Hz, 4H), 6.83 (d, *J* = 7.4 Hz, 2H), 6.85 (d, *J* = 7.6 Hz, 2H), 6.91-6.95 (m, 2H), 7.08 (s, 1H), 7.16-7.29 (m, 8H), 7.39-7.43 (m, 1H), 7.49 (t, *J* = 7.3 Hz, 1H), 7.86 (s, 1H), 7.89 (d, *J* = 8.1 Hz, 1H), 7.97 (s, 1H), 7.98 (d, *J* =7.3 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 22.6, 22.7, 23.0, 23.1, 23.4, 23.6, 24.0, 24.1, 24.1, 24.6, 25.1, 25.3, 26.6, 27.2, 30.6 (2C), 30.8, 30.8, 31.0 (2C), 34.1, 34.6, 56.9, 57.0, 120.0, 120.7, 121.0, 121.0, 122.2, 124.0, 124.8, 125.3, 125.6, 125.7, 127.1,

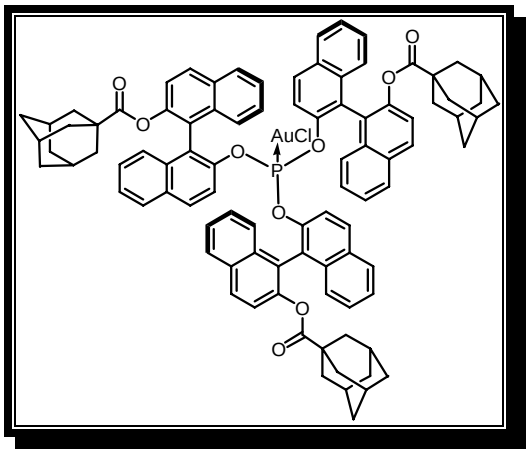
127.5, 127.6, 128.0, 129.0, 130.7, 132.0, 132.6, 133.1, 133.4, 133.6, 133.8, 143.5, 143.5, 146.6, 147.1, 147.5, 147.8, 148.3, 148.4, 148.8, 151.1, 151.2. ^{31}P NMR (162 MHz, $CDCl_3$): δ 145.0. HRMS (EI+): calculated for [M+1] $C_{66}H_{75}NO_2P$ 944.5535, found 944.5556.

2.3. Preparation of Au(I) catalysts

All Phosphoramidites- and phosphite-Au(I) complexes were synthesized via a modification of a procedure reported by Puddephat.[6] In a 20 mL screw-top vial was dissolved (SMe_2)AuCl (1 equiv) in CH_2Cl_2, and the resulting solution was cooled in an ice bath. A solution of the desired ligand (1.0 equiv) in CH_2Cl_2 was added dropwise, and the resulting solution was allowed to warm to room temperature and stirred for two hours. After TLC indicated complete consumption of the starting material, the reaction solution was concentrated in a rotary evaporator to yield the desired Au(I) complexes in nearly quantitative yield.

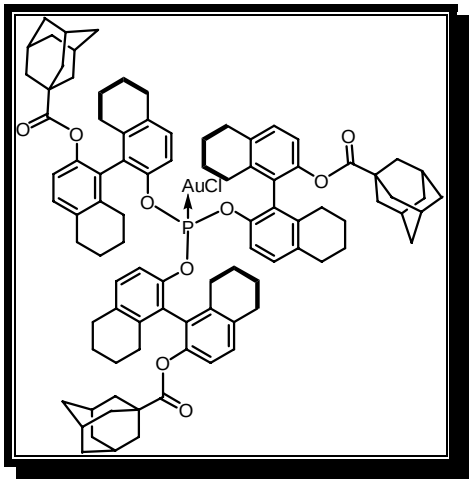


Tris(2,4-di-*t*-butylphenyl)phosphiteAuCl.[9] ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.42 (s, 1H), 7.41 (m, 1H), 7.13 (dd, 1H, *J* = 8.4, 2.4 Hz), 1.45 (s, 9H), 1.29 (s, 9H). ^{31}P NMR (166 MHz, $CDCl_3$): δ 100.5.

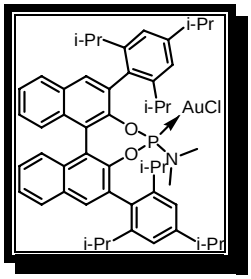


[6] Brandys, M.-C.; Jennings, M. C.; Puddephat, R. J. *Dalton* **2000**, 4601.

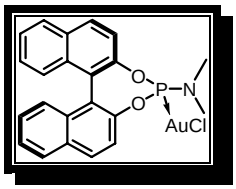
L_5AuCl. ^{1}H NMR (400 MHz, $CDCl_3$): δ 1.29 (bs, 15H), 1.43-1.46 (m, 12H), 1.56-1.59 (m, 12H), 1.76 (bs, 9H), 6.38 (d, *J* = 9.0 Hz, 3H), 6.93-6.95 (d, *J* = 8.4 Hz, 6H), 7.17-7.25 (m, 9H), 7.41-7.45 (m, 9H), 7.80 (d, *J* = 8.2 Hz, 3H), 7.92 (d, *J* = 8.2 Hz, 3H), 8.08 (d, *J* = 8.9 Hz, 3H). ^{31}P NMR (162 MHz, $CDCl_3$): δ 109.7.



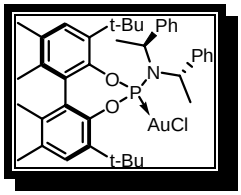
L_6AuCl. ^{1}H NMR (400 MHz, $CDCl_3$): δ 1.44-1.73 (m, 63H), 1.86 (bs, 9H), 2.08-2.31 (m, 9H), 2.53-2.75 (m, 9H), 2.85-2.89 (m, 5H), 5.96 (d, *J* = 8.5 Hz, 3H), 6.52 (d, *J* = 8.5 Hz, 3H), 6.90 (d, *J* = 8.2 Hz, 3H), 7.21 (d, *J* = 8.3 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 22.5, 22.6, 22.7, 22.8, 27.0, 27.8, 28.5, 29.6, 29.8, 36.3, 38.2, 40.5, 116.9, 119.8, 126.8, 126.9, 128.6, 129.8, 129.9, 134.9, 135.3, 137.7, 138.2, 145.3, 146.3, 175.6. ^{31}P NMR (162 MHz, $CDCl_3$): δ 103.8.



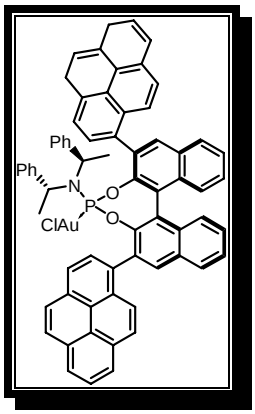
L_{12}AuCl. ^{1}H NMR (400 MHz, $CDCl_3$): δ 0.91 (d, *J* = 6.8 Hz, 3H), 0.94 (d, *J* = 6.8 Hz, 3H), 1.10-1.14 (m, 6H), 1.30-139 (m, 18H), 1.48 (t, *J* = 6.3 Hz, 6H), 2.40 (s, 3H), 2.43 (s, 3H), 2.65-2.74 (m, 1H), 2.88-3.05 (m, 4H), 3.11-3.16 (m, 1H), 7.07-7.21 (m, 6H), 7.21-7.27 (m, 1H), 7.29-7.34 (m, 3H), 7.54 (t, *J* = 7.3 Hz, 2H), 7.96-7.98 (m, 3H), 8.01 (s, 1H). ^{31}P NMR (162 MHz, $CDCl_3$): δ 124.9.



L$_4$AuCl. ^{1}H NMR (400 MHz, $CDCl_3$): δ 2.78 (s, 3H), 2.81 (s, 3H), 7.32-7.33 (m, 2H), 7.36 (d, *J* = 7.2 Hz, 1H), 7.44 (d, *J* = 8.5 Hz, 2H), 7.50-7.54 (m, 2H), 7.59 (d, *J* = 8.9 Hz, 1H), 7.96 (d, *J* = 7.5 Hz, 1H), 7.99 (d, *J* = 7.8 Hz, 1H), 8.02 (d, *J* = 9.0 Hz, 1H), 8.08 (d, *J* = 8.8 Hz, 1H). ^{31}P NMR (162 MHz, $CDCl_3$): δ 128.2.

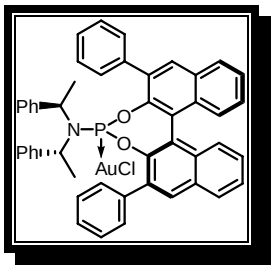


L$_{13}$AuCl. ^{1}H NMR (400 MHz, $CDCl_3$): δ 1.27 (s, 9H), 1.46 (s, 9H), 1.57 (s, 3H), 1.58 (s, 3H), 1.64 (s, 3H), 1.90 (s, 3H), 2.24 (s, 3H), 2.31 (s, 3H), 4.99-5.05 (m, 2H), 6.98 (d, *J* = 7.0 Hz, 4H), 7.13-7.23 (m, 8H). ^{31}P NMR (162 MHz, $CDCl_3$): δ 122.3.

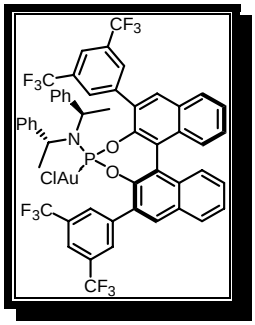


L$_8$AuCl. Isolated as a mixture of three rotomers as visible on ^{1}H and ^{31}P NMR analysis in a 6.3:0.7:3.0. ^{1}H NMR (400 MHz, $CDCl_3$): δ 0.22 (d, *J* = 7.0 Hz), 0.29 (d, *J* = 7.0 Hz), 0.58 (d, *J* = 7.0 Hz) (6H, for the last 3 signals combined), 3.69-3.98 (m, 2H), 5.64-5.81 (m, 4H), 6.03-6.14 (m, 4H), 6.27 (t, *J* = 7.6 Hz), 6.49 (t, *J* = 7.6 Hz) (2H for the last 2 signals combined), 7.43-7.70

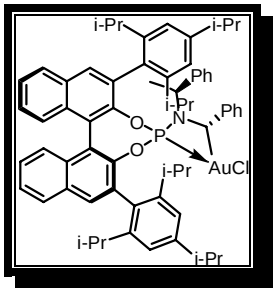
(m, 7H), 7.87-8.46 (m, 21H), 8.62-8.65 (m, 1H). ^{31}P NMR (162 MHz, $CDCl_3$): δ 128.2 (63%), 127.7 (7%), 126.7 (30%).



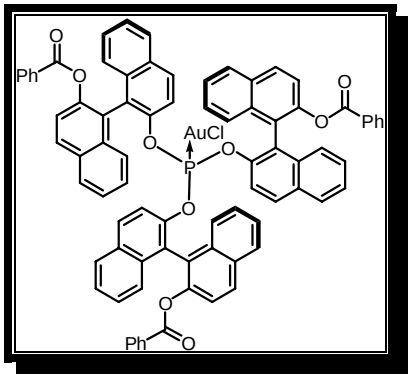
L$_9$AuCl. ^{1}H NMR (400 MHz, $CDCl_3$): δ 0.91 (s, 3H), 0.93 (s, 3H0, 4.62-4.69 (m, 2H), 6.57 (d, *J* = 7.4 Hz, 4H0, 7.06-7.60 (m, 20H), 7.81 (s, 1H), 7.83 (s, 1H), 7.99 (d, *J* = 8.0 Hz, 1H), 8.04 (d, *J* = 8.1 Hz, 1H), 8.10 (s, 1H), 8.16 (s, 1H). ^{31}P NMR (162 MHz, $CDCl_3$): δ 122.4.



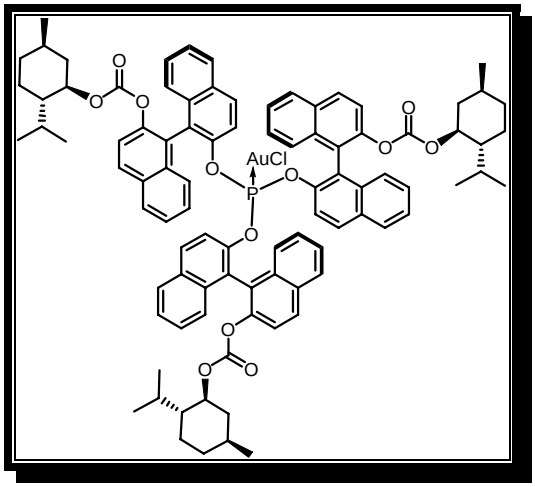
L$_{10}$AuCl. ^{1}H NMR (400 MHz, $CDCl_3$): δ 1.31 (s, 3H), 1.32 (s, 3H), 4.36 (q, *J* = 6.9 Hz, 1H), 4.42 (q, *J* = 7.1 Hz, 1H), 6.68 (d, *J* = 7.7 Hz, 4H), 7.02 (d, *J* = 7.5 Hz, 2H), 7.04 (d, *J* = 7.9 Hz, 2H), 7.13 (d, *J* = 7.4 Hz, 1H), 7.15 (d, *J* = 7.4 Hz, 1H), 7.22 (d, *J* = 8.6 Hz, 1H), 7.37-7.46 (m 3H), 7.59-7.65 (m, 2H), 8.03 (s, 2H), 8.08 (t, *J* = 7.7 Hz, 2H), 8.14 (s, 1H), 8.18 (s, 1H). 8.20 (s, 1H), 8.29 (s, 2H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 21.4, 21.4, 55.1, 55.2, 121.7, 121.8, 121.9, 122.2, 124.5, 124.6, 126.8, 126.9, 127.0, 127.1, 127.4, 127.8, 128.0, 128.0, 128.2, 128.6, 129.1, 129.9, 130.0, 130.7, 131.2, 131.7, 131.8, 131.8, 131.9, 132.2, 132.3, 132.3. 132.6, 132.7, 132.7, 132.8, 132.9, 138.7, 139.1, 139.4, 139.5, 144.4, 144.5, 145.9, 146.1, 149.9. ^{31}P NMR (162 MHz, $CDCl_3$): δ 130.4.



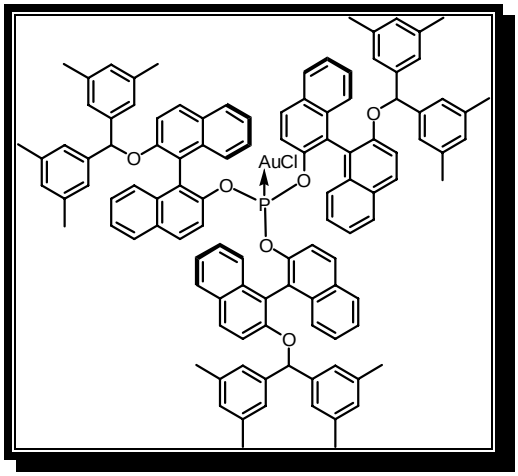
L_{11}AuCl. ^{1}H NMR (400 MHz, $CDCl_3$): δ 0.78 (d, *J* = 6.7 Hz, 4H), 0.99-1.03 (m, 10H), 1.20-1.24 (m, 3H), 1.34-1.49 (m, 23H), 1.57 (s, 3H), 2.68-2.71 (m, 1H) 2.94-3.09 (m, 3H), 3.46-3.61 (m , 2H), 4.74 (dq, *J* = 7.6 Hz, 2H), 6.57 (ad, *J* = 7.6 Hz, 2H), 6.72 (at, *J* = 7.8 Hz, 4H), 6.84 (t, *J* = 7.0 Hz, 3H), 7.00-7.03 (m, 2H), 7.11 (s, 1H), 7.18 (t, *J* = 8.4 Hz, 1H), 7.24-7.31 (m, 4H), 7.47 (m, 1H), 7.89-7.92 (m, 3H). ^{31}P NMR (162 MHz, $CDCl_3$): δ 122.1.



L_{16}AuCl. ^{1}H NMR (400 MHz, $CDCl_3$): δ 6.25 (d, *J* = 9.0 Hz, 3H), 7.99 (d, *J* = 8.3 Hz, 3H), 7.06 (d, *J* = 9.0 Hz, 3H), 7.11-7.15 (m, 9H), 7.21-7.29 (m, 9H), 7.36-7.39 (m, 9H), 7.46-7.49 (m, 3H), 7.57 (d, *J* = 7.3 Hz, 6H), 7.69 (d, *J* = 8.0 Hz, 3H), 7.92 (d, *J* = 8.1 Hz, 3H), 7.98 (d, *J* = 8.9 Hz, 3H). ^{31}P NMR (166 MHz, $CDCl_3$): δ 108.4.



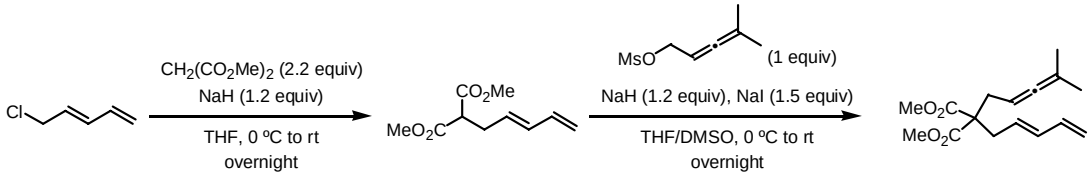
L_{17}AuCl. ^{1}H NMR (400 MHz, $CDCl_3$): δ 0.10 (s, 6H), 0.54 (s, 6H), 0.73-0.89 (m, 22H), 1.09-1.59 (m , 17H), 1.88 (ad, *J* = 11.9 Hz, 3H), 6.33 (d, *J* = 9.0 Hz, 3H), 6.87 (d, *J* = 8.4 Hz, 3H), 7.00 (d, *J* = 8.5 Hz, 3H), 7.17-7.26 (m, 9H), 7.39 (aq, *J* = 8.3 Hz, 6H), 7.50 (d, *J* = 8.9 Hz, 3H), 7.76 (d, *J* = 8.2 Hz, 3H), 7.85 (d, *J* = 8.2 Hz, 3H), 8.00 (d, *J* = 8.9 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 15.7, 20.3, 21.9, 23.2, 25.6, 31.2, 33.8, 40.3, 46.5, 78.8, 119.2, 121.5, 121.8, 121.8, 123.4, 125.6, 126.1, 126.3, 126.8, 127.7, 127.8, 128.0, 130.0, 130.2, 130.9, 131.5, 132.9, 133.0, 145.2, 147.0, 152.9. ^{31}P NMR (162 MHz, $CDCl_3$): δ 108.8.



L_{19}AuCl. ^{1}H NMR (400 MHz, $CDCl_3$): δ 1.95 (s, 18H), 1.98 (s, 18H), 6.04 (s, 3H), 6.65 (d, *J* = 9.0 Hz, 3H), 6.36 (s, 6H), 6.49 (s, 4H), 6.65 (s, 3H), 6.68 (s, 6H), 6.89 (d, *J* = 9.1 Hz, 3H), 6.91-6.94 (m, 3H), 6.99 (d, *J* = 8.4 Hz, 3H), 7.16-7.20 (m, 4H), 7.23-7.26 9m, 6H), 7.37-7.42 (m, 6H), 7.68-7.71 (m, 3H), (7.73 (d, *J* = 8.1 Hz, 3H), 7.89 (d, *J* = 9.1 Hz, 3H). ^{31}P NMR (162 MHz, $CDCl_3$): δ 110.6.

2.4 Preparation and Characterization of Substrates

Scheme 1. *Representative procedure: synthesis of* ***2.***



Prepared by a modification of a procedure reported by Yoshinao.[7] To a solution of 1,4-pentadien-3-ol (4.00 g, 47.6 mmol, 1 equiv) in CH_2Cl_2 (95 mL) at 0 ºC was added dropwise thionyl chloride (6.79 g, 57.1 mmol, 1.2 equiv). The reaction mixture was warmed to room temperature and stirred 2 hours. The reaction was quenched with water, the layers were separated and the aqueous phase was washed with CH_2Cl_2. The combined organic layers were then dried over Na_2SO_4 and concentrated via a rotary evaporator to afford a yellow oil. The crude mixture was purified by Kugelrohr distillation (80 ºC, 1 atm) to give a clear oil (3.07 g, 63%). Spectral data was consistent with that reported in the literature.

To a suspension of NaH (177 mg, 12.3 mmol, 1.2 equiv) in anhydrous DMSO (5 mL) and THF (50 mL) at 0 ºC was added dropwise a solution of dimethyl malonate (2.98 g, 22.56 mmol, 2.2 equiv) in THF (5 mL). After 30 minutes at 0 ºC, a solution of the dienyl chloride (1.00 g, 10.25 mmol, 1.0 equiv) in THF (5 mL) was added dropwise. The mixture was warmed to room temperature and stirred overnight. The reaction was quenched with water (50 mL), diluted with AcOEt (25 mL), the layers were separated and the water layer was washed with AcOEt (3 x 25 mL). The combined organic layers were then dried over Na_2SO_4 and concentrated in a rotary evaporator. The crude oil was purified by flash chromatography (AcOEt:hexanes 1:10) to afford the desired product.

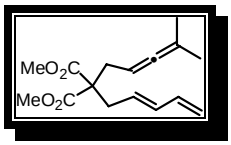
To a solution of 4-methyl-2,3-pentadienol[8] (371 mg, 3.78 mmol, 1.0 equiv), Et_3N (0.78 mL, 5.67 mmol, 1.5 equiv) and DMAP (45 mg, 0.37 mmol, 0.1 equiv) in 20 mL of CH_2Cl_2 at -40 ºC was added dropwise methanesulfonyl chloride (0.45 mL, 5.67 mmol, 1.5 equiv). The reaction was stirred at -40 ºC for one hour. The mixture was quenched with water (20 mL), the layers were separated and the aqueous layer was extracted with CH_2Cl_2 (2x10 mL). The combined

[7] Masanari, K; Ezoe, A; Mori, M; Yoshinao, T. *J. Am. Chem. Soc.* **2005**, *127*, 201.

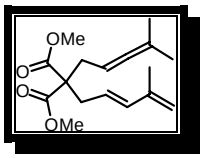
[8] (a) Wender, P. A.; Glorius, F.; Husfeld, C. O.; Langkopf, E.; Love, J. A. *J. Am. Chem. Soc.* **1999**, *121*, 5348. (b) Murakami, M.; Kadowaki, S.; Matsuda, T. *Org. Lett.* **2005**, *7*, 3953.

organic layers were dried over Na_2SO_4 and concentrated in a rotary evaporator. The resulting oil was used without further purification.

To a stirred suspension of NaH (152 mg, 3.78 mmol, 1.5 equiv) in THF (10 mL) at 0 ºC was added a solution of the previously prepared diene-malonate (500 mg, 2.52 mmol, 1.0 equiv) in THF (2 mL). After 30 minutes at 0 ºC, the crude mesylate (1.5 equiv) dissolved in DMSO (1.5 mL) and NaI (566 mg, 3.78 mmol, 1.5 equiv) were sequentially added. The mixture was brought to room temperature and stirred for two hours. The reaction was quenched with saturated $NaHCO_3$ (15 mL), washed with AcOEt (3x10 mL), dried over $MgSO_4$, and concentrated in a rotary evaporator. The resulting oil was purified by flash chromatography (AcOEt: hexanes, 1:15) to afford the desired allene-diene (52%).



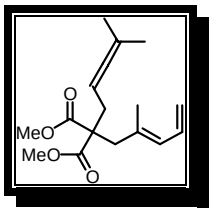
Dimethyl (4-methylpenta-2,3-dien-1-yl)[(2*E*)-penta-2,4-dien-1-yl]propanedioate (2). ^{1}H NMR (400 MHz, $CDCl_3$): δ 1.60 (s, 3H), 1.61 (s, 3H), 2.49 (d, *J* = 7.6 Hz, 2H), 2.68 (d, *J* = 7.6 Hz, 2H), 3.66 (s, 6H), 4.77-4.67 (m, 1H), 4.97 (d, *J* = 10.4 Hz, 1H), 5.08 (d, *J* = 17.2 Hz, 1H), 5.46 (dt, *J* = 17.2 Hz, 10.0 Hz, 1H), 6.05 (dd, *J* = 15.2, 10.4 Hz, 1H), 6.25 (dt, *J* = 17.2 Hz, 10.4 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 20.4, 30.2, 32.6, 32.7, 35.4, 52.3, 58.0, 82.6, 95.1, 116.3, 127.9, 135.0, 136.6, 171.0, 203.7. HRMS (EI) calculated for $C_{16}H_{22}O_4Na$ 301.1410, found 301.1416. All spectroscopic data was in complete agreement with the previously reported literature values.[9]



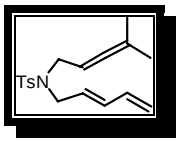
Dimethyl [(2*E*)-4-methylpenta-2,4-dien-1-yl](4-methylpenta-2,3-dien-1-yl)propanedioate.[9] Prepared dimethyl 2-(4-methylpenta-2,3-dienyl)malonate and (*E*)-5-bromo-2-methylpenta-1,3-diene to yield the product (84%) as a colorless oil. ^{1}H NMR ($CDCl_3$, 400 MHz): δ 1.58 (s,

[9] Mauleon, P.; Zeldin, R. M.; Gonzalez, A. Z.; Toste, F. D. *J. Am. Chem. Soc.* **2009**, *131*, 6348-6349.

3H),1.59 (s, 3H), 1.72 (s, 3H), 2.48 (d,, J = 7.6 Hz, 2H), 2.67 (d, J = 7.6 Hz, 2H), 4.68-4.47 (m, 1H), 4.82 (d, J = 6.5 Hz, 1H), 5.38 (dt,, J = 7.6, 15.5 Hz, 1H), 6.10 (d,, J = 15.5 Hz, 1H), . ^{13}C NMR ($CDCl_3$. 100 MHz): δ 18.3, 20.3, 32.3, 35.5, 52.1, 58.0, 82.5, 94.9, 115.6, 123.5, 136.8, 141.4, 171.0, 171.1,203.6.

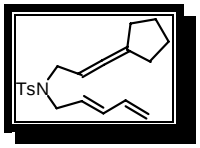


Dimethyl (4-methylpenta-2,3-dien-1-yl)[(2*E*)-2-methylpenta-2,4-dien-1-yl]propanedioate.[9] Prepared using dimethyl 2-(4-methylpenta-2,3-dienyl)malonate and (*E*)-5-bromo-4-methylpenta-1,3-diene to yield the product (96%) as a colorless oil.[10] ^{1}H NMR ($CDCl_3$, 400 MHz): δ 1.65 (s, 3H), 1.66 (s, 3H), 1.67 (s, 3H), 2.55 (d, J = 7.4 Hz, 2H), 2.76 (s, 2H), 3.70 (s, 6H), 4.83-4.74 (m, 1H), 5.02 (d, J = 10.6 Hz, 1H), 5.09 (d, J = 16.8 Hz, 1H), 5.87 (d, J = 10.9 Hz, 1H),6.50 (dt, J = 16.9 Hz, 10.4 Hz, 1H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ 17.3, 20.5, 32.4, 41.9, 52.3, 57.8, 83.0, 95.2, 116.2, 130.6, 132.8, 133.5, 171.4, 203.7. HRMS (EI): calculated for $C_{17}H_{24}O_4$ 292.1675, found 292.1675.

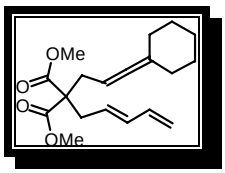


***N,N'*-(4-methylpenta-2,3-dien-1-yl)[(2*E*)-penta-2,4-dien-1-yl]-*N*-toluenesulfonamide (1).**[9] Prepared by the method described by Wender to give the product (78%) as a clear oil. ^{1}H NMR (400 MHz, $CDCl_3$): δ 1.63 (s, 3H) 1.64 (s, 3H), 2.41 (s, 3H), 3.78 (d, J = 7.0 Hz, 2H), 3.89 (d, J = 6.7 Hz, 2H), 4.71 (m, 1H), 5.08 (d, J = 10.4 Hz, 1H), 5.26 (d, J = 15.8 Hz, 1H), 5.47 (dt, J = 6.8, 15.2 Hz, 1H), 6.10 (dd, J = 10.4, 15.2 Hz, 1H), 6.25 (dt, J = 10.0, 17.2 Hz, 1H), 7.29 (d, J = 8.1 Hz, 2H),7.70 (d, J = 8.2 Hz, 2H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 20.3 (2C), 21.5, 46.6, 47.9, 84.2, 96.7, 117.9, 127.2, 127.9, 129.7, 134.6, 135.9, 137.6, 143.6, 203.3. HRMS (FAB+H^+): calculated for $C_{18}H_{24}NO_2S$ 318.1539, found 318.1535.

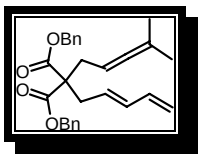
[10] (*E*)-5-Bromo-4-methylpenta-1,3-diene was prepared from acrylaldehyde as previously described in: Piers, E.; Jung, G. L.; Ruediger, E. H. *Can. J. Chem.* **1987**, *65*, 670.



***N,N'*-(3-cyclopentylideneprop-2-en-1-yl)[(2*E*)-penta-2,4-dien-1-yl]-*N*-toluenesulfonamide (15).** ^{1}H NMR (400 MHz, $CDCl_3$): δ 1.53 (bs, 3H), 2.20-2.29 (m, 7H), 3.71 (d, *J* = 6.8 Hz, 2H), 3.75 (d, *J* = 6.6 Hz, 2H), 4.71-4.73 (m, 1H), 4.97 (d, *J* = 10.2 Hz, 1H), 5.04 (d, *J* = 10.2 Hz, 1H), 5.39-5.45 (m, 1H), 5.99-6.20 (m, 2H), 7.18 (d, *J* = 8.1 Hz, 2H), 7.60 (d, *J* = 8.2 Hz, 2H). All spectroscopic data was in complete agreement with reported literature values.[11]



Dimethyl (3-cyclohexylideneprop-2-en-1-yl)[(2*E*)-penta-2,4-dien-1-yl]propanedioate.[9] Prepared using using dimethyl 2-(4-methylpenta-2,3-dienyl)malonate and 3-cyclohexylideneprop-2-en-1-ol to yield the product (59%) as a clear oil.[12] ^{1}H NMR (400 MHz, $CDCl_3$): δ 1.50-1.45 (m, 2H), 1.59-1.51 (m, 4H), 2.08-2.03 (m, 4H), 2.55 (d, *J* = 8.0 Hz, 2H), 2.71 (d, *J* = 7.6 Hz, 2H), 4.76 (m, 1H), 3.70 (s, 6H), 5.00 (d, *J* = 10 Hz, 1H), 5.21 (d, *J* = 17.2 Hz, 1H), 5.50 (dt, *J* = 7.6, 15.2 Hz, 1H), 6.08 (dd, *J* = 10.4, 15.2 Hz, 1H),6.26 (dt, *J* = 10.4, 17.2 Hz, 1H). ^{13}C NMR (100 MHz, $CDCl_3$): δ 25.9, 27.1 (2C), 31.4 (2C), 33.0, 35.3, 52.3 (2C), 58.0, 82.3, 102.3, 116.3, 128.0, 134.9, 136.6, 171.1, 200.4. HRMS (FAB+H^+): calculated for $C_{19}H_{27}O_4$ 319.1909, found 319.1904**.**



Dibenzyl (4-methylpenta-2,3-dien-1-yl)[(2*E*)-penta-2,4-dien-1-yl]propanedioate (16). ^{1}H NMR (500 MHz, $CDCl_3$): δ 1.65 (s, 6H), 2.62 (d, *J* = 7.5 Hz, 2H), 2.77 (d, *J* = 8.0 Hz, 2H), 4.76

[11] Trillo, B.; Lopez, F.; Montserrat, S.; Ujaque, G.; Castedo, L.; Lledós, A.; Mascareñas, J. L. *Chem. Eur. J.* **2009**, *15*, 3336.
[12] Zhang, Z.; Bender, C. F.; Widenhoefer, R. A. *Org. Lett.* **2007**, *9*, 2887.

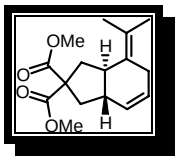
(bs, 1H), 4.99-5.19 (m, 6H), 5.44-5.50 (m, 1H), 6.00-6.05 (m, 1H), 6.18-6.26 (m, 1H), 7.27 (s, 4H), 7.31 (s, 6H). ^{13}C NMR (123 MHz, $CDCl_3$): δ 20.4, 32.6, 35.3, 58.1, 67.0, 82.5, 95.2, 116.4, 127.8, 128.1, 128.2, 128.5, 135.1, 135.4, 136.6, 170.4, 203.9.

2.5. Au(I)-catalyzed [4 + 2]-rearrangements of diene-allenes

Representative procedure for Au(I)-catalyzed [4 + 2] cycloisomerizations:

Unless otherwise noted, most reactions were carried at 25 °C. To a small vial was added $AgSbF_6$[13] (0.005 mmol, 0.05 equiv) and the corresponding **L**AuCl (0.005 mmol, 0.05 equiv) in CH_2Cl_2 (or benzene, 0.2 mL). The mixture was stirred for five minutes at room temperature, and then the suspension was filtered through glass fiber and added to a solution of the corresponding allene-diene (0.1 mmol, 1.0 equiv) in CH_2Cl_2 (0.8 mL). The reaction mixture was stirred for 3 hours at room temperature[14], then filtered through a short pad of silica and washed with CH_2Cl_2. Solvent was removed in a rotary evaporator and the corresponding cycloadduct was isolated by silica gel flash chromatography.

All racemic material where synthesized utilizing 5 mol % tris(2,4-di-*tert*-butyl phenyl)phosphiteAuCl complex and 5 mol % $AgSbF_6$ in dichloromethane at 25 °C, following the above mentioned procedure as previously reported.[9]



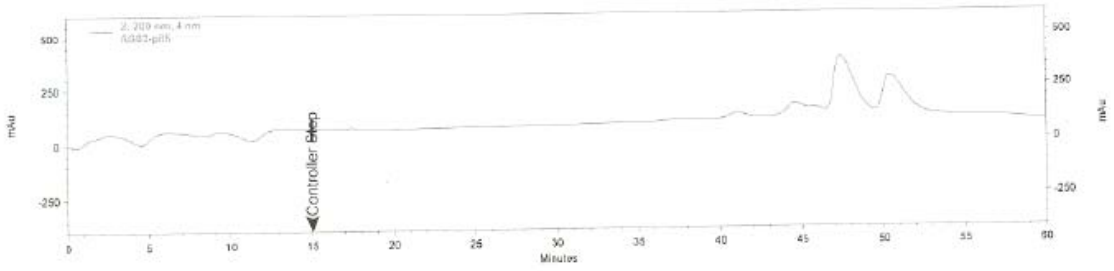
4. Isolated via silica gel column chromatography (hexanes:EtOAc 90:10, Rf = 0.2) as a clear oil. ^{1}H NMR (400 MHz, $CDCl_3$): δ 1.64 (s, 3H), 1.81 (s, 3H), 2.20-2.15 (m, 2H), 2.66 (dd, *J* = 6.8, 13.2 Hz, 1H), 2.73 (broad d, *J* = 20.0 Hz, 1H), 2.86 (d, *J* = 20.0 Hz, 1H), 3.00 (dd, *J* = 11.6, 19.2 Hz, 1H), 3.73 (s, 3H), 3.74 (s, 3H), 5.75-5.71 (m, 1H),5.85 (broad d, *J* = 9.6 Hz, 1H). ^{13}C NMR

[13] When noted $AgBF_4$ was used instead.
[14] Reactions carried utilizing BF_4^- usually require 12 hours to reach completion. See bellow for information on reaction times for each particular substrate.

(100 MHz, $CDCl_3$): δ 21.8, 21.9, 31.8, 37.4, 39.7, 44.2, 48.1, 52.8 (2C), 58.4, 121.7, 123.9, 127.9, 129.1, 173.0, 173.2. HRMS (EI+): calculated for $C_{16}H_{22}O_4$ 278.1518, found 278.1514.[9]

HPLC traces for compound **4**:

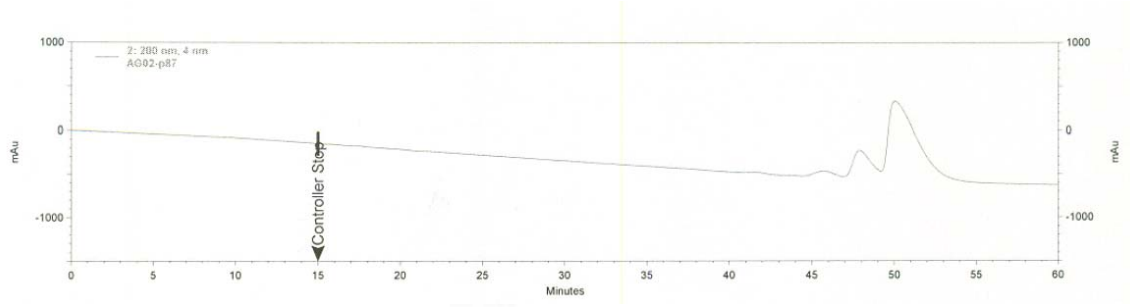
From (*S*)-**L$_{16}$**AuCl, (5 mol %), $AgBF_4$ (5 mol %), 25 °C, 12h, benzene, (92% yield) (Method: Chiracel IA, hexanes:*tert*-butyl methyl ether, 95:5, 0.2 mL/min)**:**



1: 210 nm, 4 nm Results

Retention Time	Area	Area Percent	Lambda Max
47.408	31475969	63.865	208
50.432	17809171	36.135	207

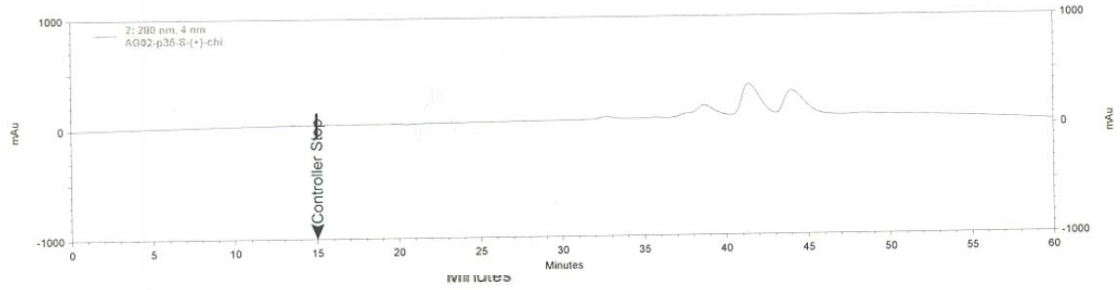
From (*R*)-**L$_5$**AuCl (5 mol %), $AgSbF_6$ (5 mol %), 25 °C, 3h, benzene (90% yield) (Table 1, entry 8) (Method: Chiracel IA, hexanes:*tert*-butyl methyl ether, 95:5, 0.2 mL/min)**:**



1: 210 nm, 4 nm Results

Retention Time	Area	Area Percent	Lambda Max
47.900	12059985	13.372	219
50.052	78125589	86.628	210

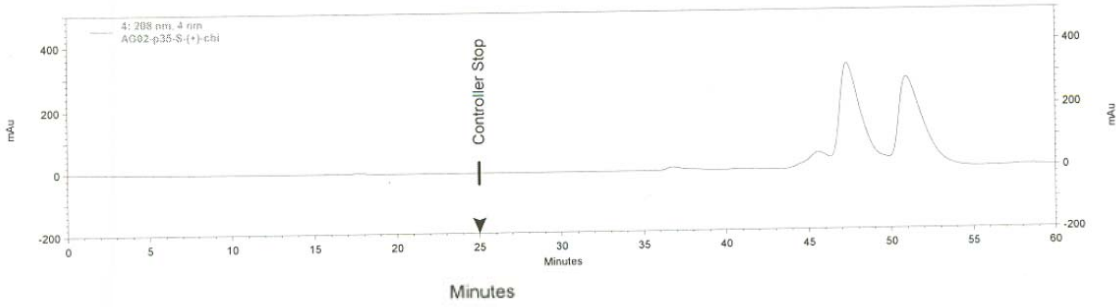
From (*S*)-**L$_{17}$**AuCl (5 mol %), $AgBF_4$ (5 mol %), 25 °C, 12h, benzene (88% yield) (Method: Chiracel IA, hexanes:*tert*-butyl methyl ether, 95:5, 0.2 mL/min)**:**



1: 210 nm, 4 nm Results

Retention Time	Area	Area Percent	Lambda Max
41.408	29284392	53.377	208
44.008	25578786	46.623	207

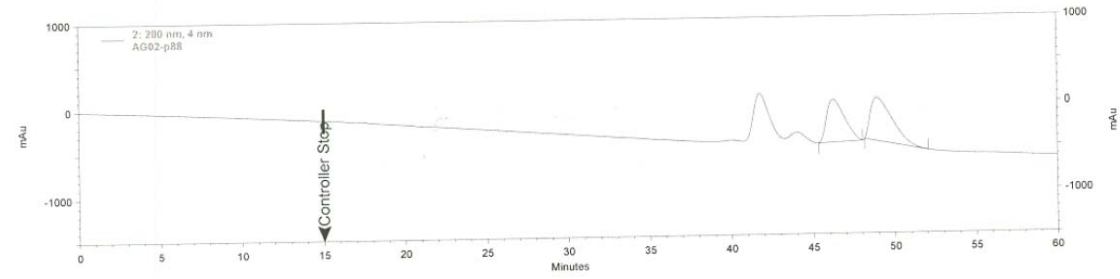
From (*S*)-**L$_{18}$**AuCl (5 mol %), $AgBF_4$ (5 mol %), 25 °C, 12h, benzene, (93% yield) (Method: Chiracel IA, hexanes:*tert*-butyl methyl ether, 95:5, 0.2 mL/min)**:**



1: 200 nm, 4 nm Results

Retention Time	Area	Area Percent	Lambda Max
47.312	35961579	50.126	201
50.932	35780848	49.874	201

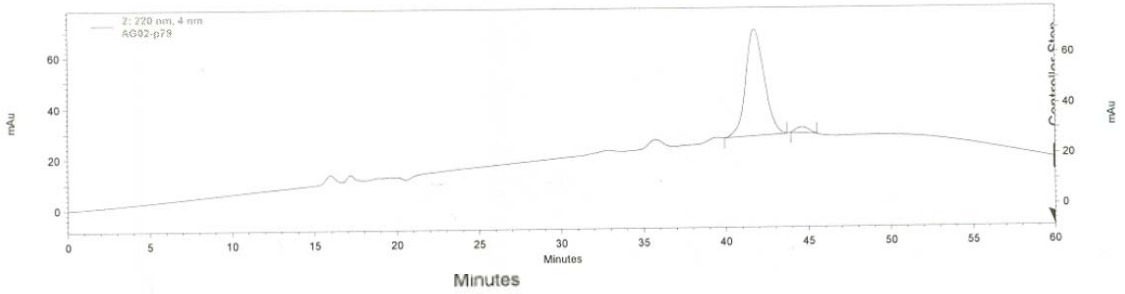
From (*R*)-**L$_{19}$**AuCl (5 mol %), $AgBF_4$ (5 mol %), 25 °C, 12h, benzene (82% yield) (Method: Chiracel IA, hexanes:*tert*-butyl methyl ether, 95:5, 0.2 mL/min)**:**



2: 200 nm, 4 nm Results

Retention Time	Area	Area Percent	Lambda Max
46.248	37195485	44.692	214
48.916	46030804	55.308	213

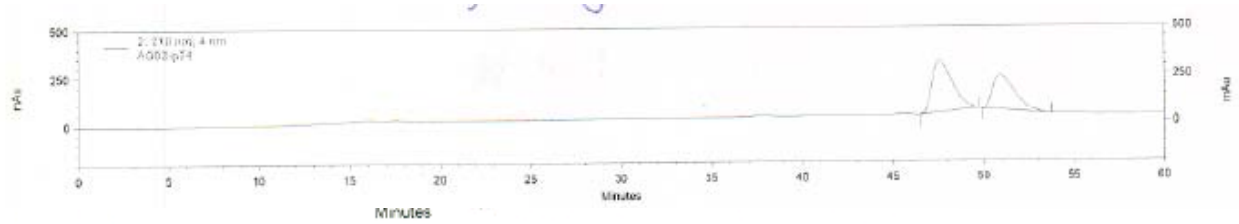
From (*S*)-**L$_6$**AuCl (5 mol %), $AgBF_4$ (5 mol %), 5 °C, 12h, benzene (87% yield) (Table 1, entry 11) (Method: Chiracel IA, hexanes:*tert*-butyl methyl ether, 95:5, 0.2 mL/min)**:**



1: 210 nm, 4 nm Results

Retention Time	Area	Area Percent	Lambda Max
41.744	7870593	96.170	206
44.640	313441	3.830	206

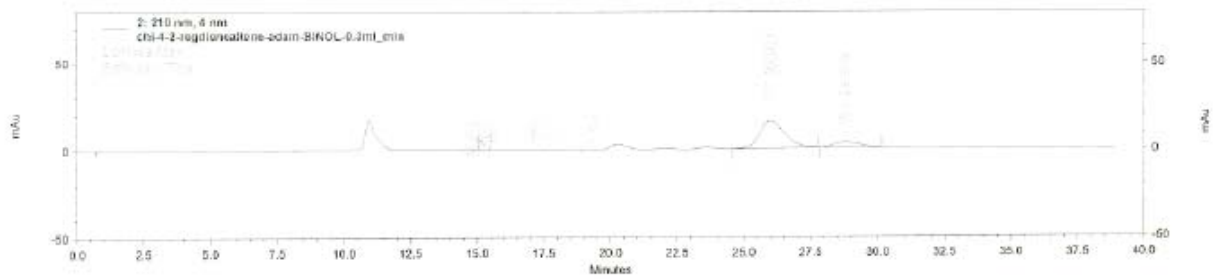
From (*R*)-**L$_4$**AuCl (10 mol %), $AgSbF_6$ (10 mol %), 5 °C, 12h, CH_2Cl_2 (86% yield) (Table 1, entry 5) (Method: Chiracel IA, hexanes:*tert*-butyl methyl ether, 95:5, 0.2 mL/min)**:**



1: 220 nm, 4 nm Results

Retention Time	Area	Area Percent	Lambda Max
47.552	6978365	55.226	201
50.868	5657723	44.774	201

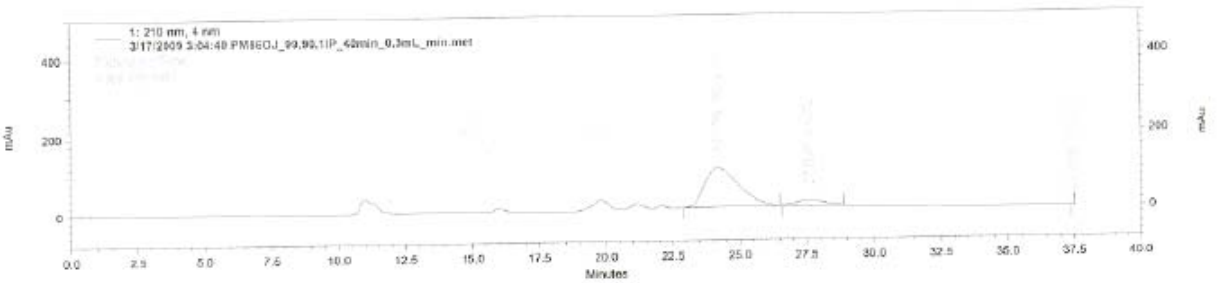
From (*S*)-**L$_6$**AuCl (5 mol %), $AgSbF_6$ (5 mol %), 25 °C, 3h, CH_2Cl_2 (92% yield) (Table 1, entry 9) (Method: Chiracel OJ, hexanes:isopropyl alcohol, 99.1:0.01, 0.3 mL/min)**:**



1: 210 nm, 4 nm Results

Retention Time	Area	Area Percent
24.208	9053181	90.314
27.600	970596	9.683
37.435	340	0.003

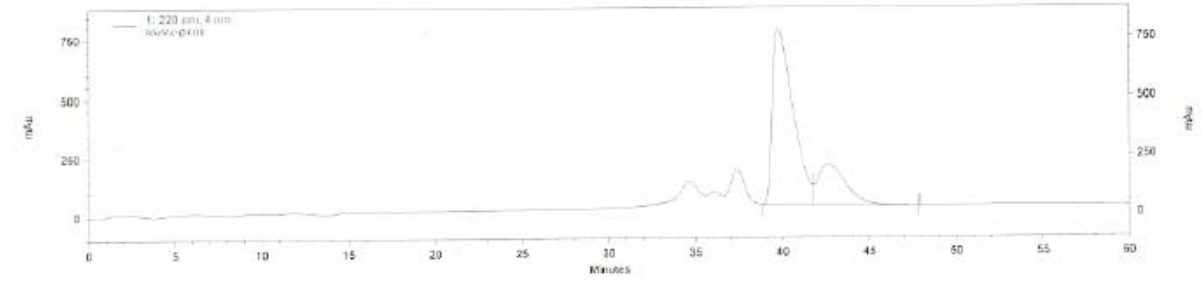
From (*S*)-**L_5AuCl** (5 mol %), $AgSbF_6$ (5 mol %), 25 °C, 3h, CH_2Cl_2 (90% yield) (Table 1, entry 7) (Method: Chiracel OJ, hexanes:isopropyl alcohol, 99.1:0.01, 0.3 mL/min)**:**



1: 210 nm, 4 nm Results

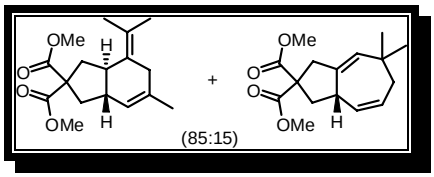
Retention Time	Area	Area Percent
26.021	1023375	82.773
28.816	212989	17.227

From (*R,R,R*)-**L_{10}**AuCl (10 mol %), $AgSbF_6$ (10 mol %), -30 °C, 24h, CH_2Cl_2 (84% yield) (Method: Chiracel IA, hexanes:*tert*-butyl methyl ether, 95:5, 0.2 mL/min)**:**



1: 220 nm, 4 nm Results

Retention Time	Area	Area Percent	Lambda Max
39.784	62716528	76.623	209
42.648	19134566	23.377	207
47.808	177	0.000	206

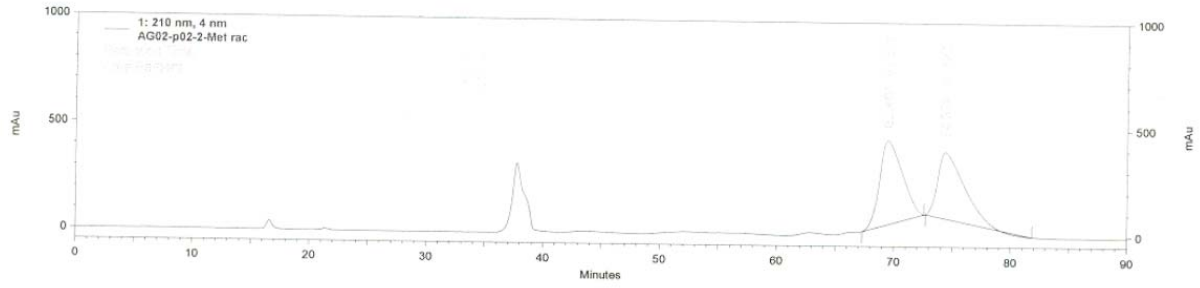


5. Prepared by the method described above to give the above mixture of products, [4+3]:[4+2], 85:15 (93% combined yield,) as a colorless oil. Isolated via silica gel flash column chromatography (hexanes:EtOAc, 90:10, Rf = 0.2). The [4+2] cycloaddition product was subsequently isolated as a sole product in 70% yield. The following assignments correspond to the major resulting isomer. ^{1}H NMR ($CDCl_3$. 400 MHz): δ 1.60 (s, 3H), 1.64 (s, 3H), 1.76 (s, 3H), 2.08 (m, 3H), 2.62-2.55 (m, 3H), 2.65 (s, 1H), 2.98-2.88 (m, 1H), 3.71 (s, 6H),5.51 (s, 1H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ 21.7, 21.8, 22.7, 36.7, 37.7, 39.6, 44.6, 48.2, 52.6, 52.7, 58.5, 123.2, 123.4, 128.0, 135.5,173.2 (2C). HRMS (EI): calculated for $C_{17}H_{24}O_4$ 292.1675, found 292.1673. All spectroscopic data were in complete agreement with reported literature values.[9] For spectroscopic data on the minor isomer see Ref. 9.

HPLC trace for coumpound **5** (Table 2, entry 2):

Method: Whelk-O1, hexanes:isopropanol, 99.9:0.1, 0.2 mL/min.

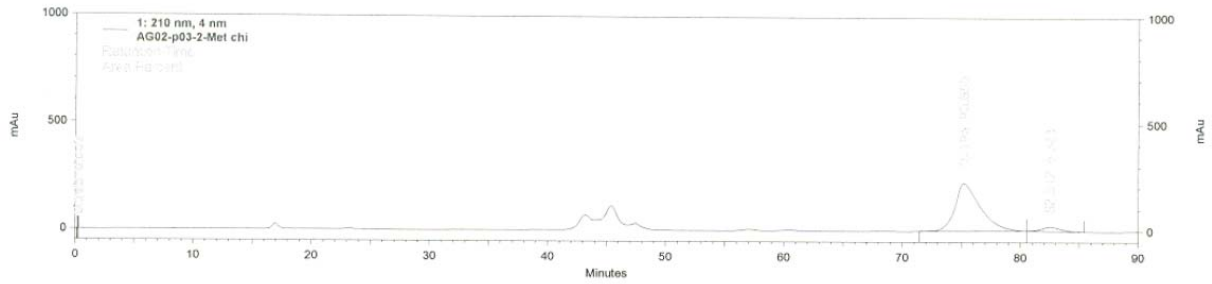
Racemic:



1: 210 nm, 4 nm Results

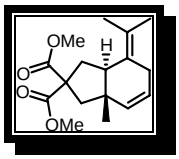
Retention Time	Area	Area Percent
69.461	53088676	51.678
74.379	49641583	48.322

From (*S*)-**L$_6$**AuCl (5 mol %), $AgBF_4$ (5 mol %), 12 h, 25 °C in benzene:



1: 210 nm, 4 nm Results

Retention Time	Area	Area Percent
0.160	323	0.001
0.235	371	0.001
0.272	7	0.000
75.195	33594468	93.655
82.512	2275381	6.343

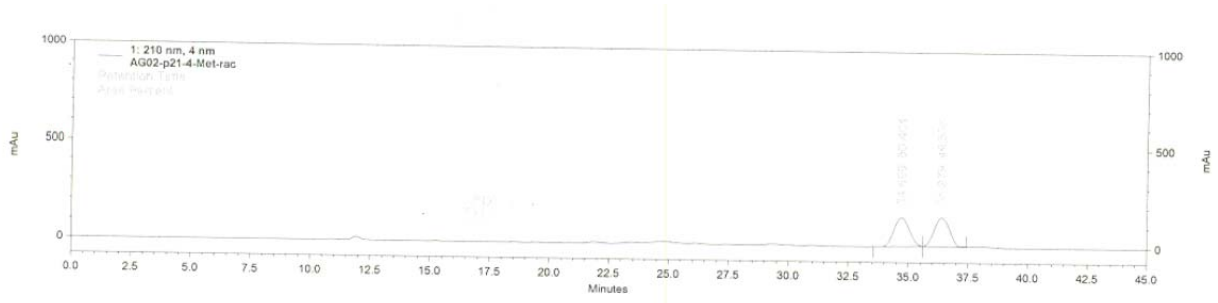


6. Isolated via silica gel flash column chromatography (hexanes:EtOAc 90:10, Rf = 0.3) as a colorless oil (50%). ^{1}H NMR ($CDCl_3$. 400 MHz): δ 0.78 (s, 3H), 1.61 (s, 1H), 1.65 (s, 3H), 1.78 (s, 3H), 2.33 (d, *J* = 16.5 Hz, 1H), 2.48-2.44 (m, 1H), 2.54-2.52 (m, 2H), 2.89 (dd, *J* = 12.3 Hz, 5.2 Hz, 1H), 2.90 (d, *J* = 20.8 Hz, 1H), 3.72-3.67 (m, 1H), 3.71 (s, 3H), 3.74 (s, 3H), 5.49 (dt, *J* = 3.4, 9.5 Hz, 1H), 5.87 (d, *J* = 9.5 Hz, 1H). ^{13}C NMR ($CDCl_3$, 100 MHz): δ 21.2, 21.3, 22.0, 32.2, 37.6, 43.6, 45.0, 51.8, 58.1, 124.5, 124.9, 126.2, 135.9, 173.2, 173.4. HRMS (EI): calculated for $C_{17}H_{24}O_4$ 292.1675, found 292.1669.[9]

HPLC trace for coumpound **6** (Table 2, entry 3):

Method: Chiracel AD, hexanes:isopropanol, 99.9:0.1, 0.3 mL/min.

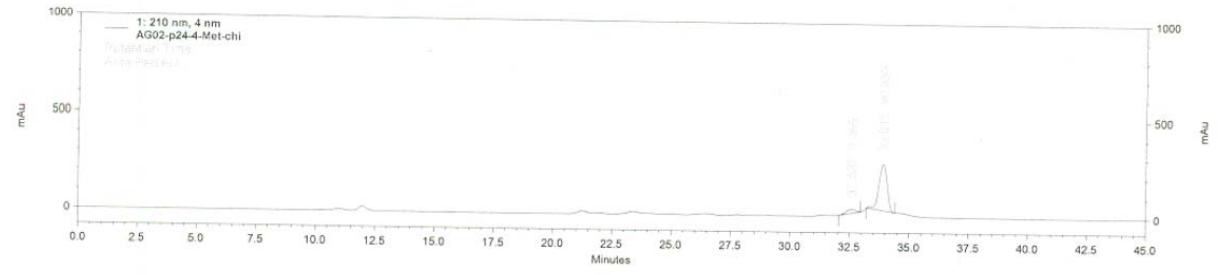
Racemic:



1: 210 nm, 4 nm Results

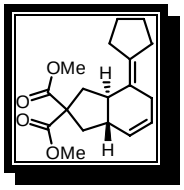
Retention Time	Area	Area Percent
34.699	6559446	50.464
36.379	6438776	49.536

From (*S*)-**L$_6$**AuCl (5 mol %), $AgSbF_6$ (5 mol %), 25 °C, 2 h, CH_2Cl_2:



1: 210 nm, 4 nm Results

Retention Time	Area	Area Percent
32.597	527401	8.477
33.915	5694376	91.523

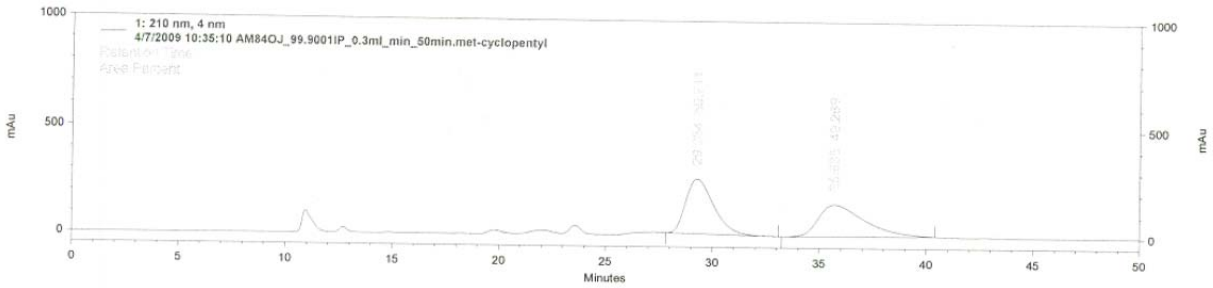


7. Prepared by the method described above to give the product (93%) as a colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$): δ 1.53-1.72 (m, 5H), 1.86 (s, 1H), 2.11-2.18 (m, 4H), 2.40 (s, 2H), 2.63-2.92 (m, 3H), 3.73 (s, 3H), 3.74 (s, 3H), 5.70 (bs, 1H), 5.80-5.83 (m, 1H). All spectroscopic data were in complete agreement with the reported literature values.

HPLC trace for compound **7** (Table 2, entry 4):

Method: Chiracel OJ, hexanes:isopropanol, 99.9:0.1, 0.3 mL/min

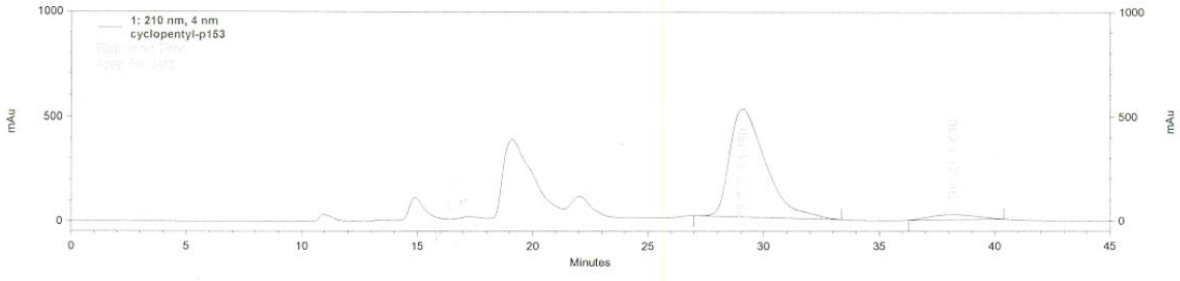
Racemic:



1: 210 nm, 4 nm Results

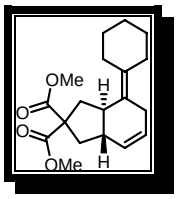
Retention Time	Area	Area Percent
29.264	23541989	50.711
35.685	22881393	49.289

From (*S*)-**L$_6$**AuCl (5 mol %), $AgBF_4$ (5 mol %), 25 °C, 12 h, benzene:



1: 210 nm, 4 nm Results

Retention Time	Area	Area Percent
29.077	56213775	94.390
38.181	3340747	5.610



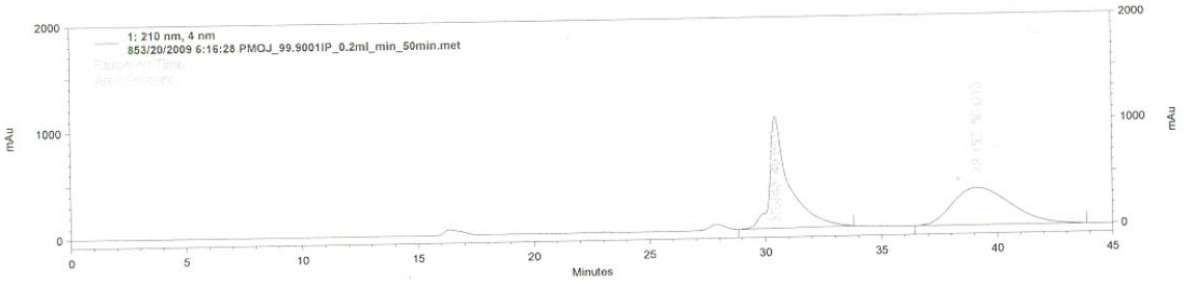
8. Prepared by the method described above to give the product (92%) as a colorless oil. ^{1}H NMR (400 MHz, $CDCl_3$): δ 1.65-1.45 (m, 6H). 1.74 (t, *J* = 12.6 Hz, 2H), 2.30-2.05 (m, 6H), 2.65 (dd,

J = 6.0, 12.8 Hz, 6.0 Hz, 1H), 2.84 (d, J = 9.6 Hz, 2H), 2.98 (d, J = 8.4 Hz, 1H), 3.73 (s, 6H), 5.79-5.71 (m, 1H), 5.86 (d, J = 9.2 Hz, 1H), ^{13}C NMR (100 MHz, $CDCl_3$): δ 26.0, 27.2, 31.4, 33.0, 35.3, 52.4, 58.0, 82.3, 102.3, 116.4, 128.0, 128.2, 129.3, 133.5, 173.2. HRMS (EI): calculated for $C_{19}H_{26}O_4$ 318.1831, found 318.1829. All spectroscopic data were in complete agreement with the reported literature values.[9]

HPLC trace for compound **8** (Table 2, entry 5):

Method: Chiracel OJ, hexanes:isopropanol, 99.9:0.1, 0.2 mL/min

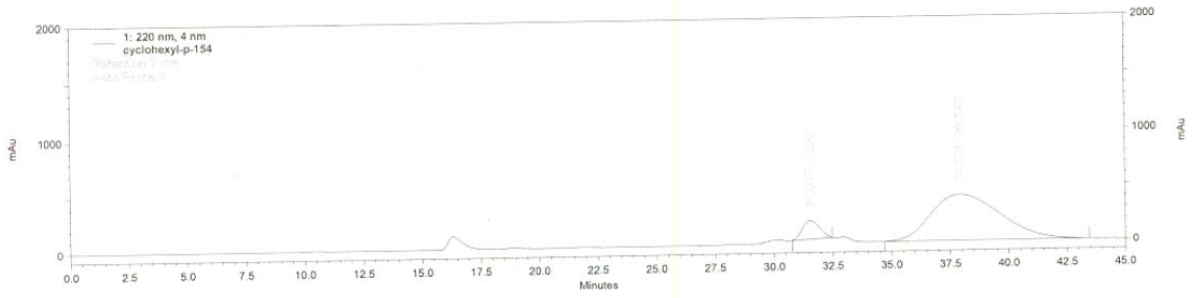
Racemic:



1: 210 nm, 4 nm Results

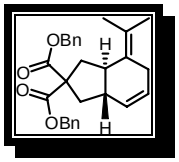
Retention Time	Area	Area Percent
30.443	60546777	49.987
39.152	60577182	50.013

From (*R*)-**L$_6$**AuCl (5 mol %), $AgBF_4$ (5 mol %), 25 °C, 12 h, benzene:



1: 220 nm, 4 nm Results

Retention Time	Area	Area Percent
31.547	8597743	9.253
37.931	84323330	90.747

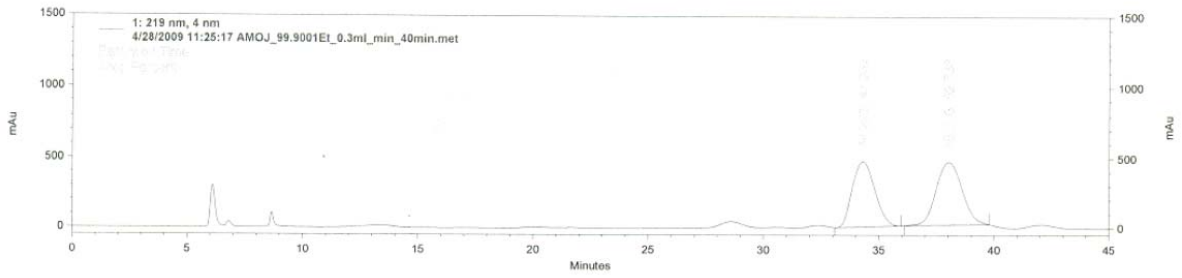


9. Prepared by the method described above to give the product (92%) as a colorless oil. Isolated via silica gel flash column chromatography (hexanes:EtOAc 95:5, Rf = 0.4). ^{1}H NMR (400 MHz, $CDCl_3$): δ 1.26 (s, 1H), 1.44 (s, 3H), 1.67 (s, 3H), 2.20 (bs, 3H), 2.65-2.87 (m, 3H), 3.01 (d, *J* = 7.2 Hz, 1H), 5.09 (bs, 4H), 5.74 (bs, 1H), 5.84 (d, *J* = 9.2 Hz, 1H), 7.25-7.30 (m, 10H). ^{13}C NMR (126 MHz, $CDCl_3$): δ 21.8, 22.0, 31.5, 37.4, 39.6, 44.3, 48.2, 58.6, 67.2, 124.0, 127.9, 128.0, 128.0, 128.3, 128.6, 129.1, 135.6, 135.6, 172.5. HRMS (EI): calculated for [M+1] $C_{28}H_{31}O_4$ 431.2222, found 431.2232.

HPLC trace for compound **9** (Table 2, entry 6):

Method: Chiracel OJ, hexanes:isopropanol, 99.9:0.1, 0.2 mL/min

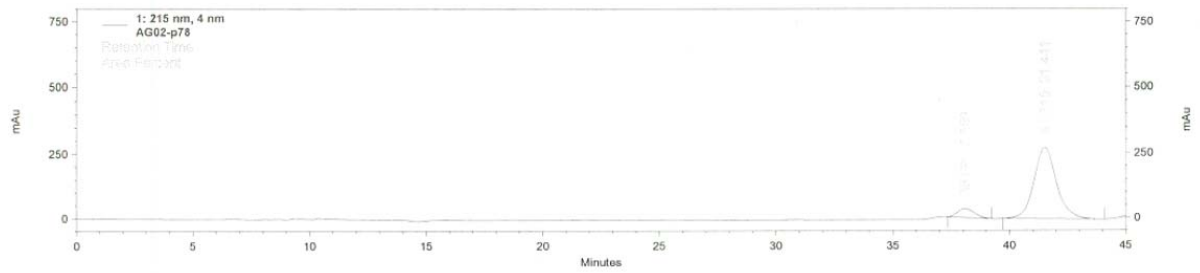
Racemic:



1: 219 nm, 4 nm Results

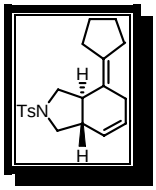
Retention Time	Area	Area Percent
34.293	31782603	47.267
38.016	35458331	52.733

From (*S*)-**L$_6$**AuCl (10 mol %), $AgBF_4$ (10 mol %), -30 °C, CH_2Cl_2, 24 h:



1: 215 nm, 4 nm Results

Retention Time	Area	Area Percent
38.091	1733447	8.559
41.515	18520447	91.441



10. Isolated via silica gel flash column chromatography (hexanes:EtOAc 95:5, Rf = 0.2) as a colorless oil. 1H-NMR (500 MHz, $CDCl_3$): δ 1.50-1.76 (m, 4H), 2.14-2.30 (m, 4H), 2.42 (s, 3H), 2.66 (d, *J* = 21.9 Hz, 1H), 2.70 (d, *J* = 21.2 Hz, 1H), 2.86 (dd, *J* = 10.9, 9.2 Hz, 1H), 3.37 (t, *J* = 10.1 Hz, 3H), 3.63 (dd, *J* = 9.1, 7.1 Hz, 1H), 3.87 (dd, *J* = 9.4, 5.8 Hz, 2H), 5.71 (s, 2H), 7.31 (d, *J* = 8.0 Hz, 2H), 7.73 (d, *J* = 8.3 Hz, 2H). ^{13}C NMR (126 MHz, $CDCl_3$): δ 21.5, 25.8, 27.4, 30.9, 31.6, 32.0, 42.8, 47.1, 50.8, 51.3, 122.2, 125.3, 127.2, 128.8, 129.7, 134.7, 136.1, 143.2 . All spectroscopic data were in complete agreement with the reported literature values.[11]

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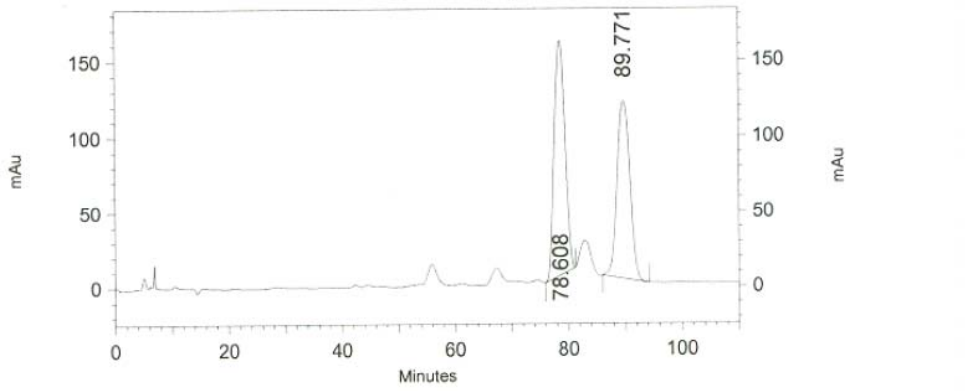
HPLC trace for compound **10**:

Method: Chiracel AD, hexanes:isopropanol, 99:1, 0.5 mL/min

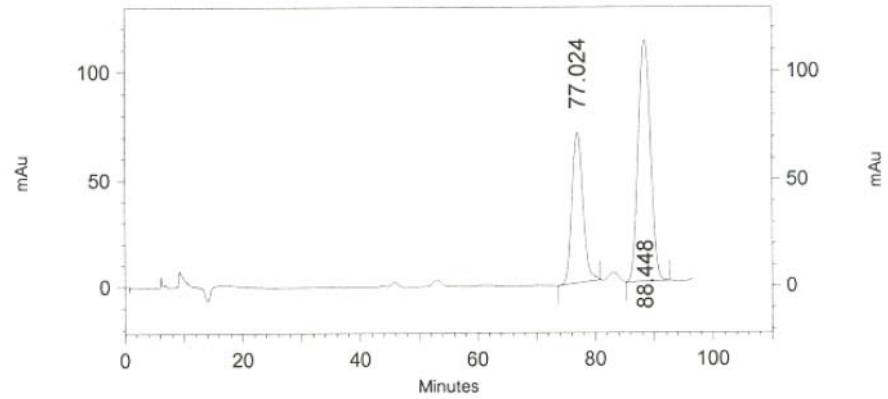
Racemic:



1: 230 nm, 4 nm Results

Retention Time	Area	Area Percent
78.608	20776196	52.790
89.771	18580096	47.210

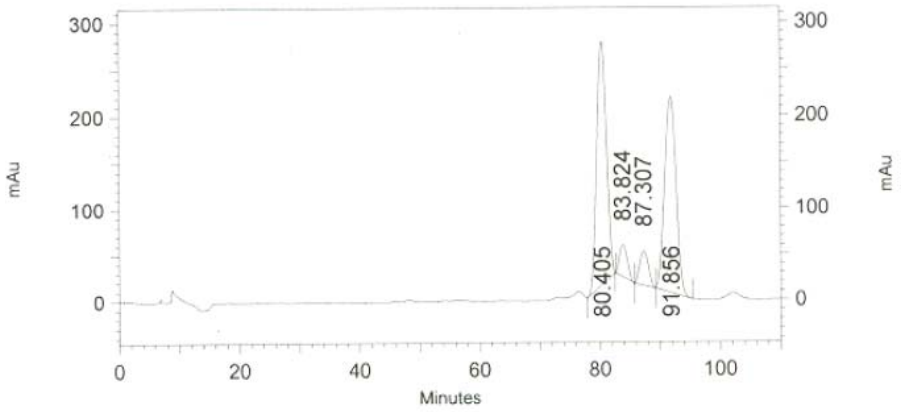
From (*R*)-**L$_6$**AuCl (5 mol %), $AgSbF_6$ (5 mol %), 25 °C, CH_2Cl_2, 12 h (77% yield):



1: 220 nm, 4 nm Results

Retention Time	Area	Area Percent
77.024	9220338	35.825
88.448	16516955	64.175

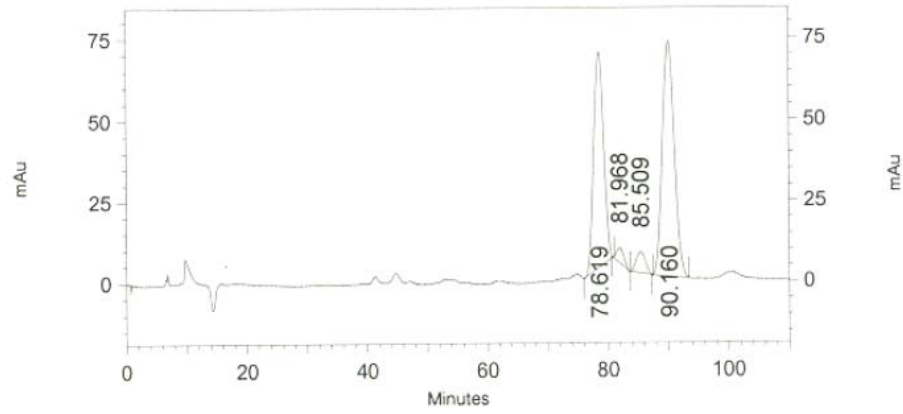
From (*R*)-**L$_4$**AuCl (10 mol %), $AgSbF_6$ (10 mol %), CH_2Cl_2, 25 °C, 12h. Isolated as a 9:1 mixture of [4+2] and [4+3] products, respectively, as shown bellow (92% yield):



1: 235 nm, 4 nm Results

Retention Time	Area	Area Percent
80.405	29892219	46.086
83.824	3102240	4.783
87.307	3746525	5.776
91.856	28120154	43.354

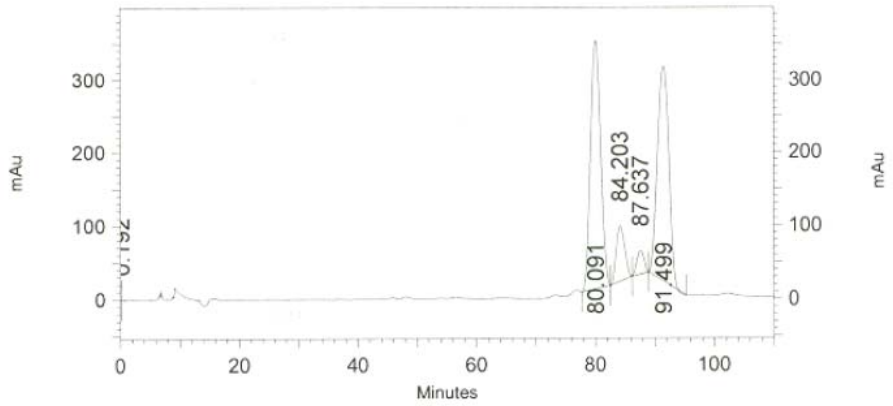
From (*S*,*S*,*S*)-**L**$_7$AuCl (10 mol %), $AgSbF_6$ (10 mol %), CH_2Cl_2, 25 °C, 12 h. Isolated as a 13:1 mixture of [4+2] and [4+3] products, respectively, as shown bellow (87% yield):



1: 210 nm, 4 nm Results

Retention Time	Area	Area Percent
78.619	7667548	40.967
81.968	375457	2.006
85.509	662428	3.539
90.160	10010884	53.487

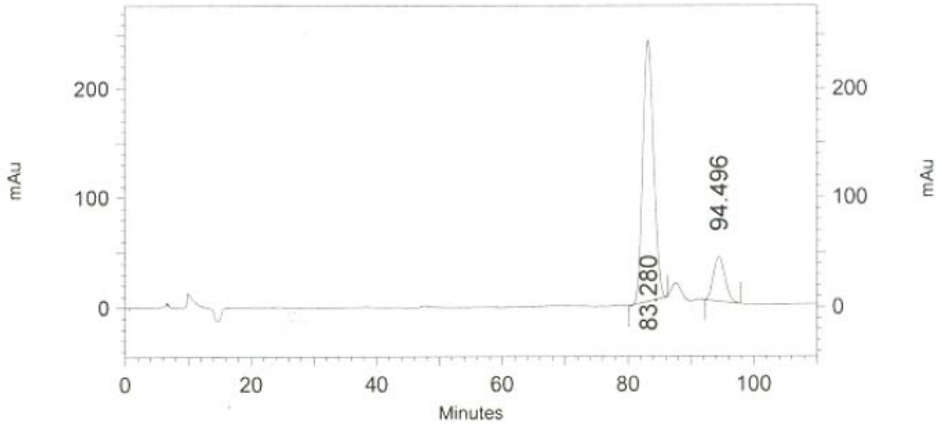
From (*S*,*S*,*S*)-**L**$_{13}$AuCl (10 mol %), $AgSbF_6$ (10 mol %), CH_2Cl_2, 25 °C, 12 h. Isolated as a 7:1 mixture of [4+2] and [4+3] products, respectively, as shown bellow (90% yield):



1: 211 nm, 4 nm Results

Retention Time	Area	Area Percent
0.192	142	0.000
80.091	40256716	44.921
84.203	7473574	8.339
87.637	2710995	3.025
91.499	39176067	43.715

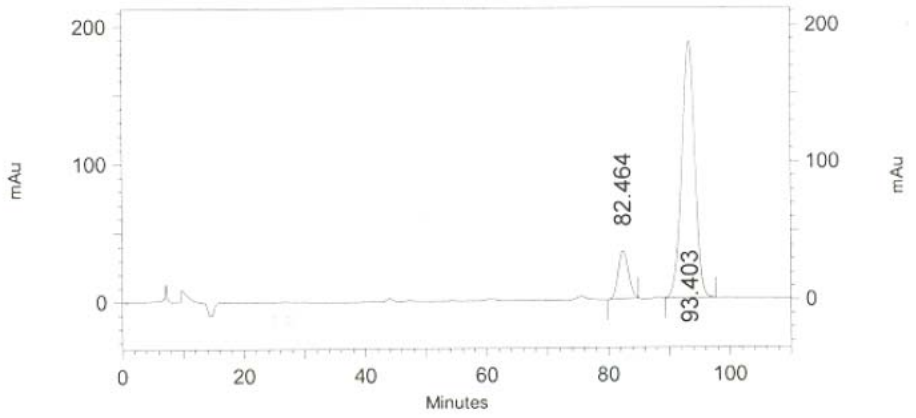
From (*R*,*R*,*R*)-$\mathbf{L_9}$AuCl (10 mol %), $AgSbF_6$ (10 mol %), CH_2Cl_2, -30 °C, 48 h. Isolated as a 13:1 mixture of [4+2] and [4+3] products, respectively (89% yield):



1: 210 nm, 4 nm Results

Retention Time	Area	Area Percent
83.280	28418362	84.535
94.496	5198830	15.465

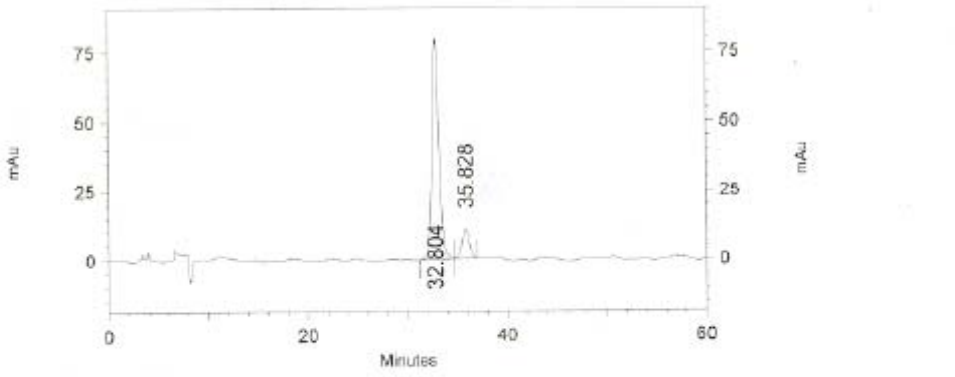
From (*S*,*S*,*S*)-$\mathbf{L_{11}}$AuCl (10 mol %), $AgSbF_6$ (10 mol %), CH_2Cl_2, -30 °C, 48 h. Isolated as a 49:1 mixture of [4+2] and [4+3] products, respectively (85% yield):



1: 230 nm, 4 nm Results

Retention Time	Area	Area Percent
82.464	4108235	12.922
93.403	27683728	87.078

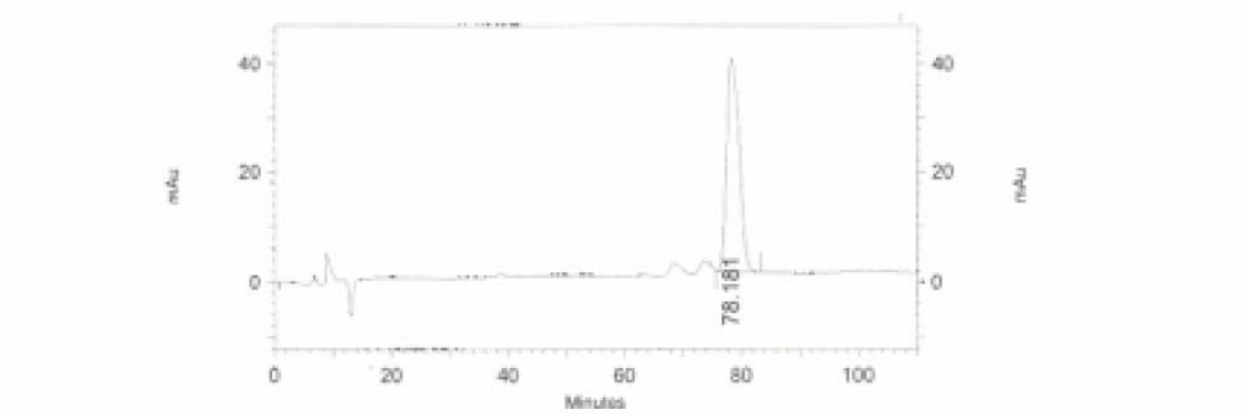
From (*R*,*R*,*R*)-$\mathbf{L_{10}}$AuCl (10 mol %), $AgSbF_6$ (10 mol %), CH_2Cl_2, -30 °C, 48 h. (86% yield) (Method: Chiracel IA, hexanes:isopropyl alcohol, 99:1, 1.0 mL/min):



2: 230 nm, 4 nm Results

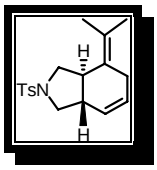
Retention Time	Area	Area Percent	Lambda Max
32.804	3815854	87.743	204
35.828	533031	12.257	204

From (*S*,*S*,*S*)-$\mathbf{L_8}$AuCl (5 mol %), $AgSbF_6$ (5 mol %), CH_2Cl_2, -15 °C, 12h. (91% yield) (Method: Chiracel AD, hexanes:isopropanol (99:1), 0.5 mL/min):



1: 230 nm, 4 nm Results

Retention Time	Area	Area Percent
78.181	5767224	100.000

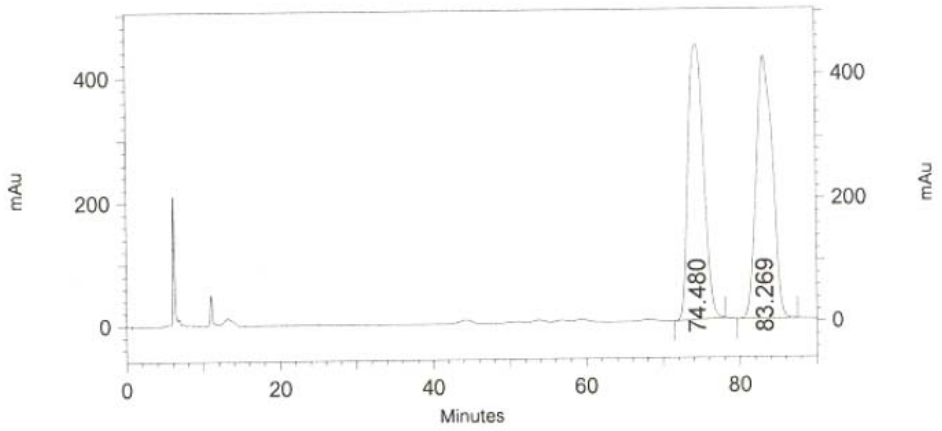


3. Prepared by the method described above to give the product as a colorless oil. Isolated via silica gel flash column chromatography (hexanes:EtOAc 95:5, Rf = 0.2). ^{1}H NMR (400 MHz, C_6D_6): δ 1.38 (s, 3H), 1.46 (s, 3H), 1.93 (s, 3H), 2.01 (m, 2H), 2.38 (d, *J* = 20.4 Hz, 1H), 2.54 (d, *J* = 20.4 Hz, 1H), 2.89 (dd, *J* = 11.2 Hz, 9.2 Hz, 1H), 3.43 (dd, *J* = 9.2, 11.2 Hz, 1H), 3.66 (dd, *J* = 7.6, 9.2 Hz, 1H), 4.12 (dd, *J* = 6.0, 9.2 Hz, 1H), 5.51 (broad s, 2H), 6.85 (d, *J* = 8.4 Hz, 2H), 7.86 (d, *J* = 8.4 Hz, 2H). ^{13}C NMR (400 MHz, C_6D_6): δ 20.7, 21.0, 21.2, 30.9, 42.7, 46.7, 50.4, 52.1, 124.2, 125.2, 125.7, 128.4, 129.3, 129.4, 135.9, 142.4. HRMS (FAB): calculated for $C_{18}H_{24}NO_2S$ 318.1528, found 318.1525.

HPLC traces for compound **3**:

Method: Chiracel AD, hexanes:isopropanol (99:1), 0.5 mL/min

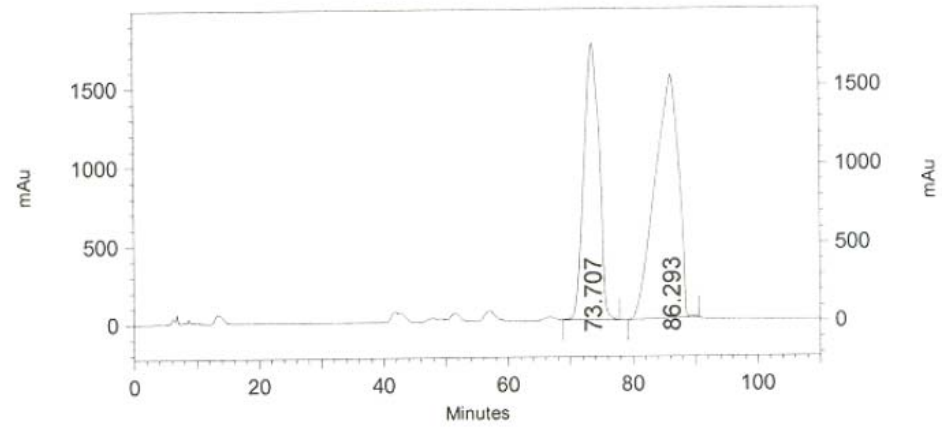
Racemic:



1: 210 nm, 4 nm Results

Retention Time	Area	Area Percent
74.480	62270193	49.919
83.269	62472854	50.081

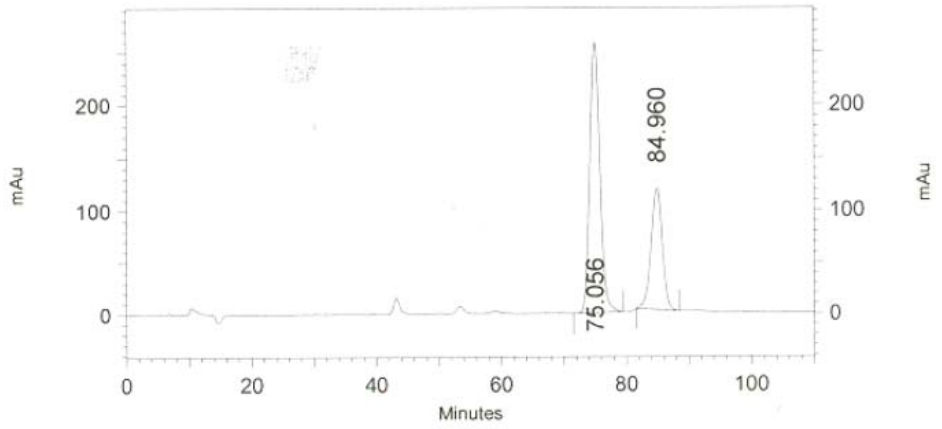
From (*R*)-**L**$_5$AuCl (5 mol %), $AgSbF_6$ (5 mol %), CH_2Cl_2, 25 °C, 12h (92% yield) (Method: Chiracel AD, hexanes:isopropanol (99:1), 0.5 mL/min) (Table 1, entry 6):



1: 210 nm, 4 nm Results

Retention Time	Area	Area Percent
73.707	295873414	42.185
86.293	405502804	57.815

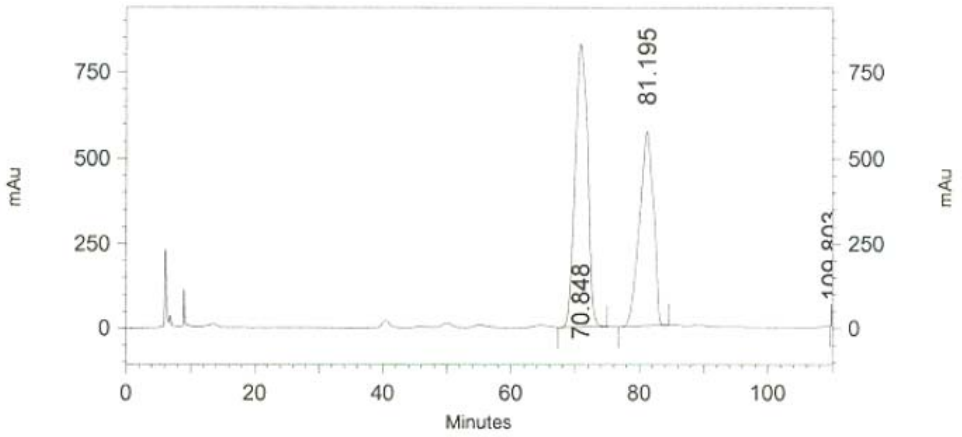
From (*S*)-**L**$_6$AuCl (5 mol %), $AgSbF_6$ (5 mol %), benzene, 5 °C, 24h (86% yield) (Method: Chiracel AD, hexanes:isopropanol (99:1), 0.5 mL/min) (Table 1, entry 12):



1: 230 nm, 4 nm Results

Retention Time	Area	Area Percent
75.056	29301196	66.598
84.960	14696182	33.402

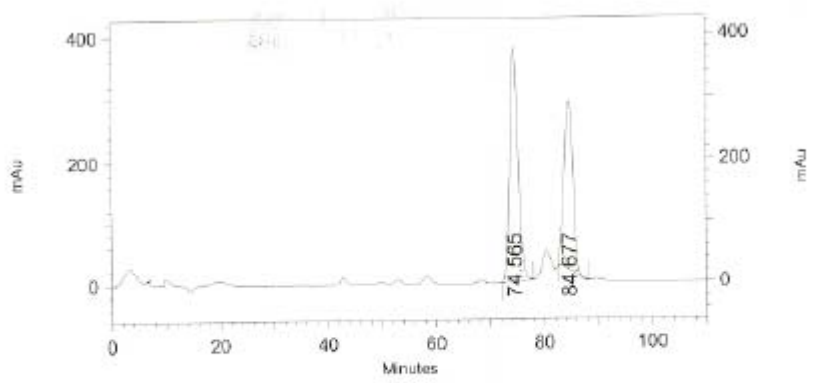
From (*R*)-**L$_{14}$**AuCl (5 mol %), $AgSbF_6$ (5 mol %), CH_2Cl_2, 25 °C, 12h (88% yield) (Method: Chiracel AD, hexanes:isopropanol (99:1), 0.5 mL/min):



1: 210 nm, 4 nm Results

Retention Time	Area	Area Percent
70.848	112121176	56.444
81.195	86520283	43.556
109.803	791	0.000

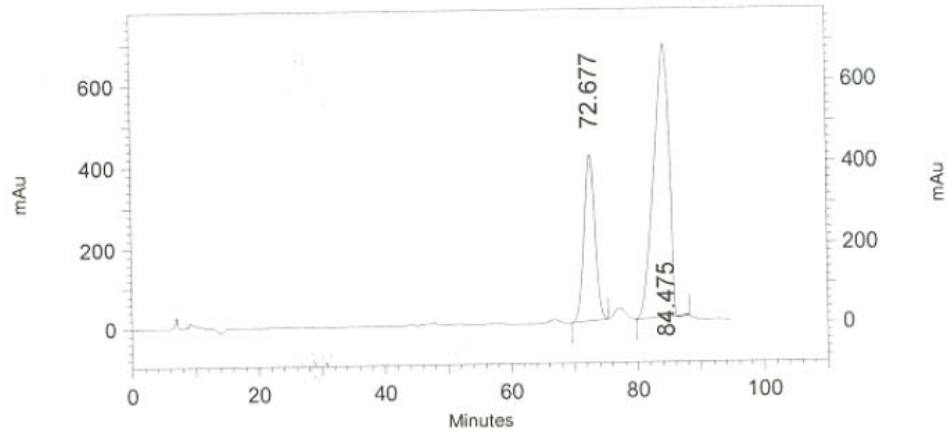
From (*R*)-**L$_4$**AuCl (10 mol %), $AgSbF_6$ (10 mol %), CH_2Cl_2, 25 °C, 12 h. Isolated as a 13:1 mixture of [4+2] and [4+3] products, respectively, as shown bellow (88% yield) (Method: Chiracel AD, hexanes:isopropanol (99:1), 0.5 mL/min) (Table 1, entry 4):



2: 211 nm, 4 nm Results

Retention Time	Area	Area Percent
74.565	41128902	57.130
84.677	30863474	42.870

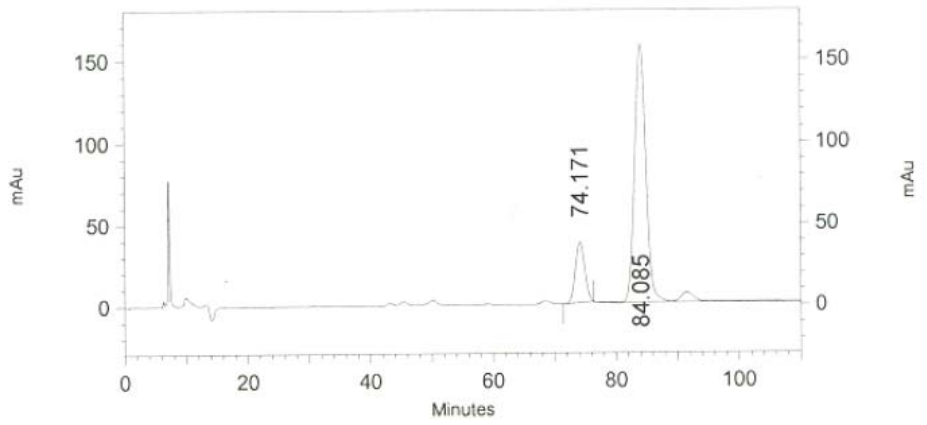
From (*S*,*S*,*S*)-$\mathbf{L_{11}}$AuCl (10 mol %), $AgSbF_6$ (10 mol %), CH_2Cl_2, 25 °C, 12 h. Isolated as a 49:1 mixture of [4+2] and [4+3] products, respectively (83% yield) (Method: Chiracel AD, hexanes:isopropanol (99:1), 0.5 mL/min):



1: 220 nm, 4 nm Results

Retention Time	Area	Area Percent
72.677	49308518	30.284
84.475	113512507	69.716

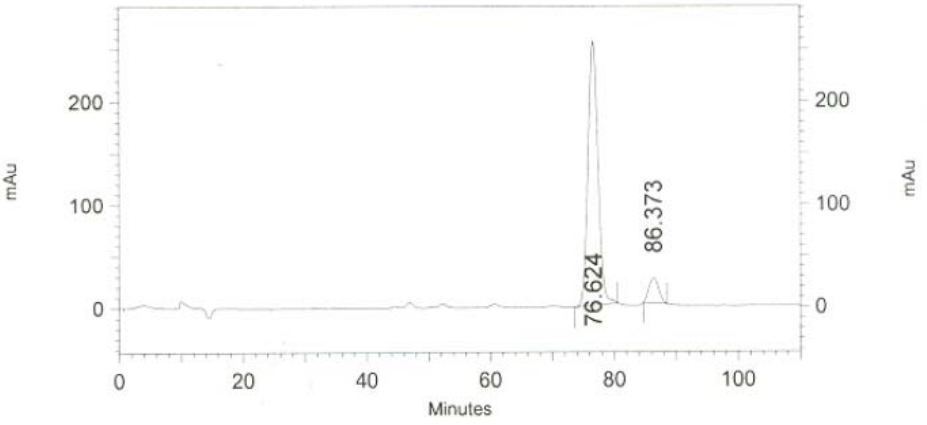
From (*S*,*S*,*S*)-$\mathbf{L_{11}}$AuCl (10 mol %), $AgSbF_6$ (10 mol %), CH_2Cl_2, -30 °C, 24 h (83% yield) (Method: Chiracel AD, hexanes:isopropanol (99:1), 0.5 mL/min):



1: 230 nm, 4 nm Results

Retention Time	Area	Area Percent
74.171	3896786	15.618
84.085	21053418	84.382

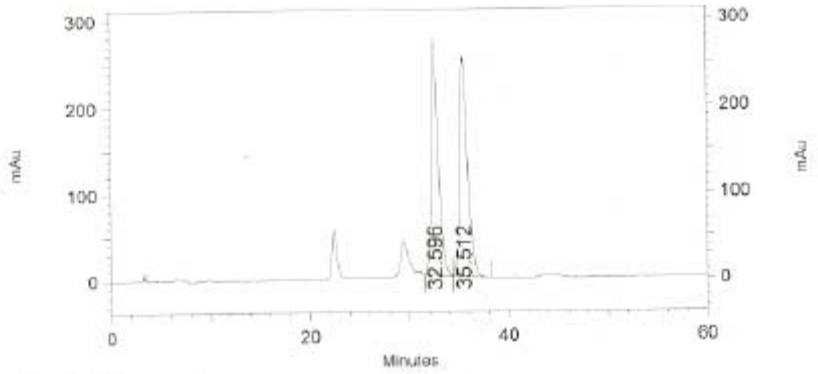
From (*R*,*R*,*R*)-**L**$_{9}$AuCl (10 mol %), $AgSbF_6$ (10 mol %), CH_2Cl_2, -30 °C, 24 h (89% yield) (Method: Chiracel AD, hexanes:isopropanol (99:1), 0.5 mL/min):



1: 230 nm, 4 nm Results

Retention Time	Area	Area Percent
76.624	28965507	91.564
86.373	2668777	8.436

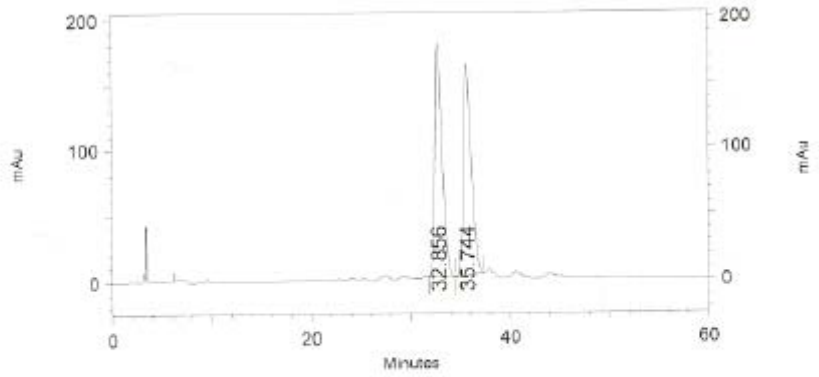
From (*R*,*R*)-**L**$_{15}$AuCl (10 mol %), $AgSbF_6$ (10 mol %), CH_2Cl_2, 25 °C, 12 h. Isolated as a 7:1 mixture of [4+2] and [4+3] products, respectively, as shown bellow (81% yield) (Method: Chiracel IA, hexanes:isopropanol (99:1), 1.0 mL/min):



1: 220 nm, 4 nm Results

Retention Time	Area	Area Percent	Lambda Max
32.596	13551614	49.075	204
35.512	14062484	50.925	204

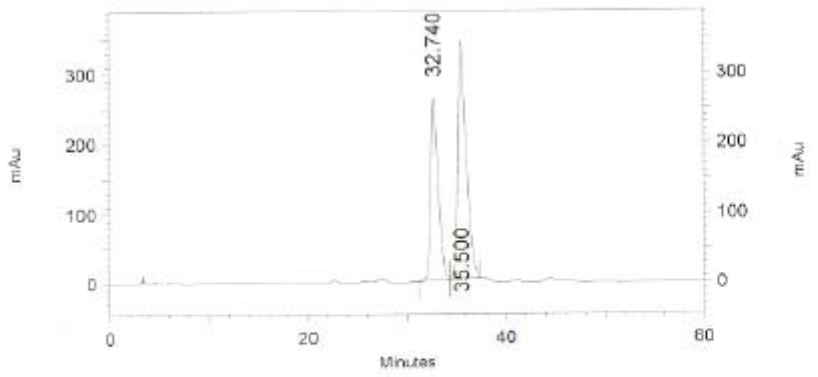
From (*R*,*R*)-$\mathbf{L_3}$AuCl (5 mol %), $AgSbF_6$ (5 mol %), CH_2Cl_2, 25 °C, 12h. (91% yield) (Method: Chiracel IA, hexanes:isopropanol (99:1), 1.0 mL/min) (Table 1, entry 3):



1: 220 nm, 4 nm Results

Retention Time	Area	Area Percent	Lambda Max
32.856	8675059	49.650	204
35.744	8797292	50.350	204

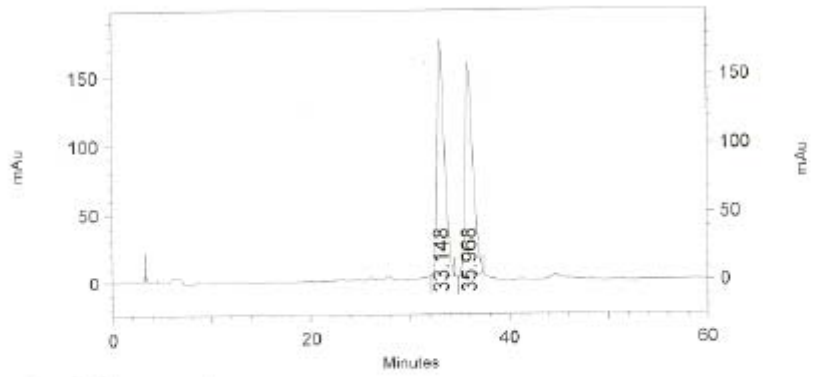
From (*S*,*S*,*S*)-$\mathbf{L_7}$AuCl (10 mol %), $AgSbF_6$ (10 mol %), CH_2Cl_2, 25 °C, 12h. (89% yield) (Method: Chiracel IA, hexanes:isopropanol (99:1), 1.0 mL/min):



1: 220 nm, 4 nm Results

Retention Time	Area	Area Percent	Lambda Max
32.740	13317807	39.551	205
35.500	20355002	60.449	205

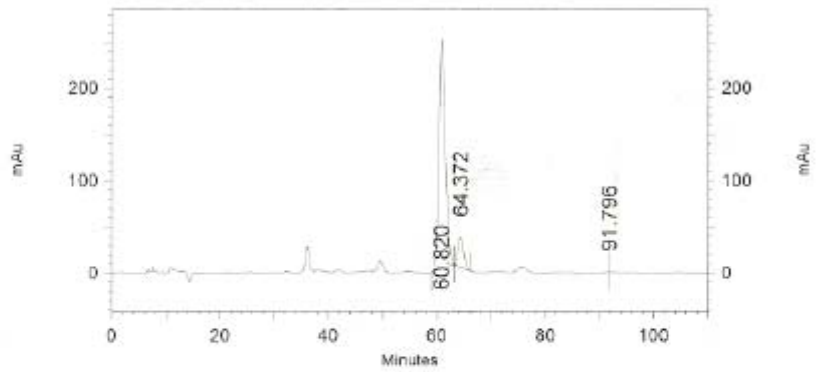
From (*R*,*S*,*S*)-$\mathbf{L_7}$AuCl (10 mol %), $AgSbF_6$ (10 mol %), CH_2Cl_2, 25 °C, 12h. (92% yield) (Method: Chiracel IA, hexanes:isopropanol (99:1), 1.0 mL/min):



1: 220 nm, 4 nm Results

Retention Time	Area	Area Percent	Lambda Max
33.148	8566597	49.860	204
35.968	8614653	50.140	204

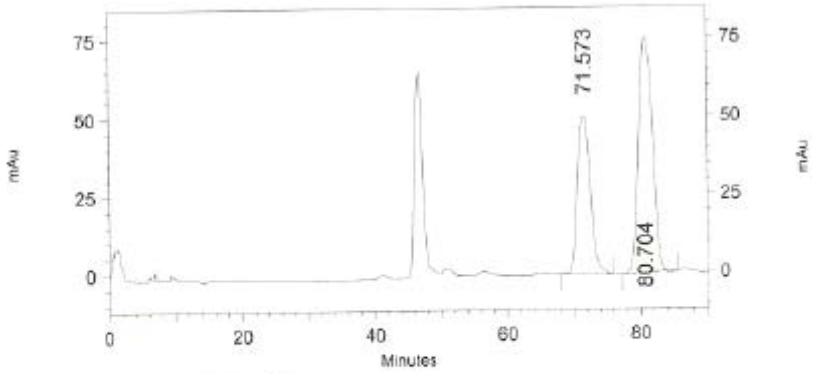
From (*R*,*R*,*R*)-$\mathbf{L_{10}}$AuCl (10 mol %), $AgSbF_6$ (10 mol %), CH_2Cl_2, -30 °C, 12h. (81% yield) (Method: Chiracel IA, hexanes:isopropanol (99:1), 0.5 mL/min):



2: 230 nm, 4 nm Results

Retention Time	Area	Area Percent	Lambda Max
60.820	20919312	89.747	205
64.372	2389840	10.253	205
91.796	40	0.000	204

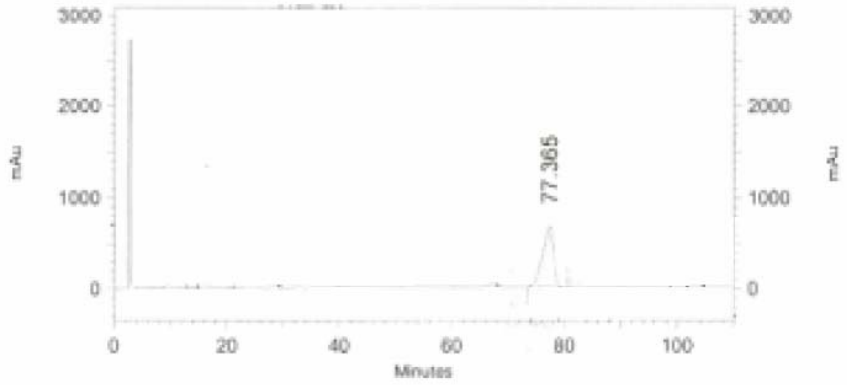
From (*R*)-**L$_6$**AuCl (5 mol %), $AgSbF_6$ (5 mol %), CH_2Cl_2, 25 °C, 12h. (76% yield) (Method: Chiracel AD, hexanes:isopropanol (99:1), 0.5 mL/min) (Table 1, entry 13):



3: 240 nm, 4 nm Results

Retention Time	Area	Area Percent
71.573	6913040	38.541
80.704	11023684	61.459

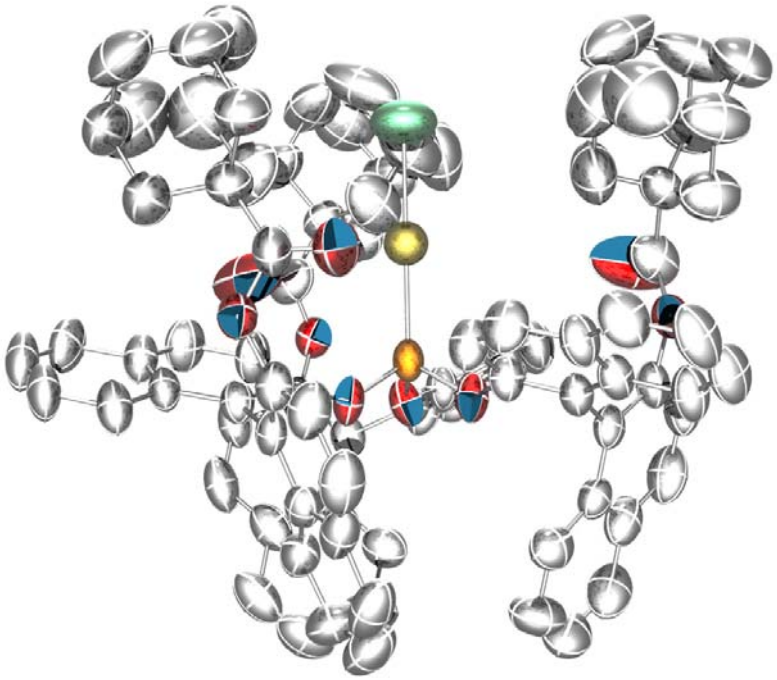
From (*S*,*S*,*S*)-**L$_8$**AuCl (5 mol %), $AgSbF_6$ (5 mol %), CH_2Cl_2, -15 °C, 12h. (83% yield) (Method: Chiracel AD, hexanes:isopropanol (99:1), 0.5 mL/min):



1: 220 nm, 4 nm Results

Retention Time	Area	Area Percent
77.365	86596019	100.000

2.6. X-ray crystal data of L_6AuCl



Experimental

A colorless prism 0.15 x 0.12 x 0.08 mm in size was mounted on a Cryoloop with Paratone oil. Data were collected at 288(2) K using phi and omega scans. Crystal-to-detector distance was 60 mm and exposure time was 30 seconds per frame using a scan width of 0.5°. Data collection was 100.0% complete to 25.00° in θ. A total of 33929 reflections were collected covering the indices, -19<=*h*<=19, -19<=*k*<=19, -22<=*l*<=22. 5044 reflections were found to be symmetry independent, with an R_{int} of 0.0436. Indexing and unit cell refinement indicated a primitive, hexagonal lattice. The space group was found to be P6(3) (No. 173). The data were integrated using the Bruker SAINT software program and scaled using the SADABS software program. Solution by direct methods (SHELXS-97) produced a complete heavy-atom phasing model consistent with the proposed structure. All non-hydrogen atoms were refined anisotropically by full-matrix least-squares (SHELXL-97). All hydrogen atoms were placed using a riding model.

Their positions were constrained relative to their parent atom using the appropriate HFIX command in SHELXL-97.

Table 1. Crystal data and structure refinement.

X-ray ID	shelxl	
Sample/notebook ID	toste06	
Empirical formula	C93 H81 Au Cl O9 P	
Formula weight	1605.96	
Temperature	288(2) K	
Wavelength	0.71073 Å	
Crystal system	Hexagonal	
Space group	P6(3)	
Unit cell dimensions	a = 15.923(2) Å	α= 90°.
	b = 15.923(2) Å	β= 90°.
	c = 18.741(3) Å	γ = 120°.
Volume	4114.9(10) $Å^3$	
Z	2	
Density (calculated)	1.296 Mg/m^3	
Absorption coefficient	1.896 mm^{-1}	
F(000)	1644	
Crystal size	0.15 x 0.12 x 0.08 mm^3	
Crystal color/habit	colorless prism	
Theta range for data collection	1.48 to 25.37°.	
Index ranges	-19<=h<=19, -19<=k<=19, -22<=l<=22	
Reflections collected	33929	
Independent reflections	5044 [R(int) = 0.0436]	
Completeness to theta = 25.00°	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.8631 and 0.7641	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5044 / 1 / 316	
Goodness-of-fit on F^2	1.033	
Final R indices [I>2sigma(I)]	R1 = 0.0498, wR2 = 0.1447	
R indices (all data)	R1 = 0.0703, wR2 = 0.1626	

Absolute structure parameter	-0.015(10)
Largest diff. peak and hole	1.657 and -0.771 e.Å^{-3}

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for toste06. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	5167(4)	8059(4)	6326(4)	54(1)
C(2)	5064(5)	8796(5)	6015(5)	70(2)
C(3)	5886(6)	9653(5)	5879(5)	78(2)
C(4)	6784(5)	9783(5)	6025(5)	70(2)
C(5)	7666(6)	10688(5)	5877(6)	85(2)
C(6)	8534(6)	10797(6)	6048(6)	92(3)
C(7)	8616(5)	10081(6)	6369(6)	86(3)
C(8)	7818(5)	9211(5)	6534(5)	71(2)
C(9)	6883(5)	9041(5)	6357(4)	55(2)
C(10)	6039(4)	8146(4)	6496(4)	51(1)
C(11)	6066(4)	7293(4)	6804(4)	54(2)
C(12)	5720(4)	6930(4)	7494(4)	58(2)
C(13)	5365(5)	7378(6)	7963(4)	77(2)
C(14)	5006(9)	6989(9)	8622(5)	108(3)
C(15)	5000(8)	6156(9)	8847(6)	110(3)
C(16)	5370(7)	5732(8)	8445(6)	100(3)
C(17)	5714(5)	6089(6)	7740(5)	77(2)
C(18)	6101(6)	5638(6)	7282(6)	87(3)
C(19)	6449(5)	5992(5)	6632(5)	73(2)
C(20)	6421(5)	6815(5)	6393(4)	59(2)
C(21)	6460(6)	6772(6)	5135(5)	89(3)
C(22)	6820(7)	7410(7)	4481(5)	75(2)
C(23)	7768(9)	8335(8)	4621(6)	112(3)
C(24)	8094(11)	8965(9)	3935(6)	128(4)
C(25)	7330(20)	9217(17)	3757(14)	192(9)
C(26)	6444(18)	8380(20)	3702(14)	187(9)
C(27)	6473(15)	7772(17)	3063(11)	183(9)
C(28)	7260(15)	7499(11)	3206(8)	150(6)
C(29)	6955(10)	6877(9)	3872(6)	113(4)
C(30)	6119(10)	7713(13)	4342(8)	136(5)
C(31)	8214(11)	8406(13)	3339(8)	145(5)

O(1)	4340(3)	7158(3)	6492(3)	58(1)
O(2)	6824(3)	7241(4)	5734(3)	64(1)
O(3)	5854(9)	5903(6)	5139(4)	181(5)
P(1)	3333	6667	6097(2)	49(1)
Cl(1)	3333	6667	3727(4)	150(3)
Au(1)	3333	6667	4934(1)	79(1)

Table 3. Bond lengths [Å] and angles [°] for toste06.

C(1)-C(10)	1.362(9)	C(19)-C(20)	1.407(10)
C(1)-C(2)	1.392(9)	C(19)-H(19)	0.9300
C(1)-O(1)	1.415(7)	C(20)-O(2)	1.401(9)
C(2)-C(3)	1.362(10)	C(21)-O(3)	1.229(11)
C(2)-H(2)	0.9300	C(21)-O(2)	1.313(10)
C(3)-C(4)	1.367(11)	C(21)-C(22)	1.509(12)
C(3)-H(3)	0.9300	C(22)-C(30)	1.443(16)
C(4)-C(9)	1.412(11)	C(22)-C(29)	1.502(14)
C(4)-C(5)	1.450(11)	C(22)-C(23)	1.514(15)
C(5)-C(6)	1.342(14)	C(23)-C(24)	1.552(15)
C(5)-H(5)	0.9300	C(23)-H(23A)	0.9700
C(6)-C(7)	1.351(14)	C(23)-H(23B)	0.9700
C(6)-H(6)	0.9300	C(24)-C(31)	1.50(2)
C(7)-C(8)	1.368(11)	C(24)-C(25)	1.50(3)
C(7)-H(7)	0.9300	C(24)-H(24)	0.9800
C(8)-C(9)	1.412(10)	C(25)-C(26)	1.38(3)
C(8)-H(8)	0.9300	C(25)-H(25A)	0.9700
C(9)-C(10)	1.410(9)	C(25)-H(25B)	0.9700
C(10)-C(11)	1.496(9)	C(26)-C(30)	1.51(2)
C(11)-C(20)	1.388(9)	C(26)-C(27)	1.55(3)
C(11)-C(12)	1.410(10)	C(26)-H(26)	0.9800
C(12)-C(17)	1.412(10)	C(27)-C(28)	1.54(3)
C(12)-C(13)	1.416(11)	C(27)-H(27A)	0.9700
C(13)-C(14)	1.372(12)	C(27)-H(27B)	0.9700
C(13)-H(13)	0.9300	C(28)-C(31)	1.50(2)
C(14)-C(15)	1.388(17)	C(28)-C(29)	1.51(2)
C(14)-H(14)	0.9300	C(28)-H(28)	0.9800
C(15)-C(16)	1.328(16)	C(29)-H(29A)	0.9700
C(15)-H(15)	0.9300	C(29)-H(29B)	0.9700
C(16)-C(17)	1.435(13)	C(30)-H(30A)	0.9700
C(16)-H(16)	0.9300	C(30)-H(30B)	0.9700
C(17)-C(18)	1.441(13)	C(31)-H(31A)	0.9700
C(18)-C(19)	1.341(13)	C(31)-H(31B)	0.9700
C(18)-H(18)	0.9300	O(1)-P(1)	1.573(4)

P(1)-O(1)#1	1.573(4)	P(1)-Au(1)	2.179(4)
P(1)-O(1)#2	1.573(5)	Cl(1)-Au(1)	2.263(8)

C(10)-C(1)-C(2)	123.8(6)	C(11)-C(12)-C(17)	120.3(7)
C(10)-C(1)-O(1)	115.9(5)	C(11)-C(12)-C(13)	122.3(6)
C(2)-C(1)-O(1)	120.3(5)	C(17)-C(12)-C(13)	117.4(7)
C(3)-C(2)-C(1)	117.6(6)	C(14)-C(13)-C(12)	120.9(9)
C(3)-C(2)-H(2)	121.2	C(14)-C(13)-H(13)	119.5
C(1)-C(2)-H(2)	121.2	C(12)-C(13)-H(13)	119.5
C(2)-C(3)-C(4)	121.6(7)	C(13)-C(14)-C(15)	120.4(11)
C(2)-C(3)-H(3)	119.2	C(13)-C(14)-H(14)	119.8
C(4)-C(3)-H(3)	119.2	C(15)-C(14)-H(14)	119.8
C(3)-C(4)-C(9)	120.5(6)	C(16)-C(15)-C(14)	121.4(10)
C(3)-C(4)-C(5)	122.2(7)	C(16)-C(15)-H(15)	119.3
C(9)-C(4)-C(5)	117.3(7)	C(14)-C(15)-H(15)	119.3
C(6)-C(5)-C(4)	120.4(8)	C(15)-C(16)-C(17)	120.0(9)
C(6)-C(5)-H(5)	119.8	C(15)-C(16)-H(16)	120.0
C(4)-C(5)-H(5)	119.8	C(17)-C(16)-H(16)	120.0
C(5)-C(6)-C(7)	121.6(7)	C(12)-C(17)-C(16)	119.8(9)
C(5)-C(6)-H(6)	119.2	C(12)-C(17)-C(18)	118.5(7)
C(7)-C(6)-H(6)	119.2	C(16)-C(17)-C(18)	121.7(8)
C(6)-C(7)-C(8)	121.5(8)	C(19)-C(18)-C(17)	121.4(7)
C(6)-C(7)-H(7)	119.2	C(19)-C(18)-H(18)	119.3
C(8)-C(7)-H(7)	119.2	C(17)-C(18)-H(18)	119.3
C(7)-C(8)-C(9)	119.8(8)	C(18)-C(19)-C(20)	118.8(8)
C(7)-C(8)-H(8)	120.1	C(18)-C(19)-H(19)	120.6
C(9)-C(8)-H(8)	120.1	C(20)-C(19)-H(19)	120.6
C(10)-C(9)-C(4)	118.5(6)	C(11)-C(20)-O(2)	115.9(6)
C(10)-C(9)-C(8)	122.1(6)	C(11)-C(20)-C(19)	123.1(7)
C(4)-C(9)-C(8)	119.4(6)	O(2)-C(20)-C(19)	120.8(6)
C(1)-C(10)-C(9)	117.9(6)	O(3)-C(21)-O(2)	120.6(8)
C(1)-C(10)-C(11)	119.2(5)	O(3)-C(21)-C(22)	125.7(8)
C(9)-C(10)-C(11)	122.8(5)	O(2)-C(21)-C(22)	113.6(7)
C(20)-C(11)-C(12)	117.8(6)	C(30)-C(22)-C(29)	113.9(11)
C(20)-C(11)-C(10)	119.2(6)	C(30)-C(22)-C(21)	106.0(8)
C(12)-C(11)-C(10)	122.9(6)	C(29)-C(22)-C(21)	110.5(8)

C(30)-C(22)-C(23)	105.5(10)	C(31)-C(28)-H(28)	110.5
C(29)-C(22)-C(23)	109.0(9)	C(29)-C(28)-H(28)	110.5
C(21)-C(22)-C(23)	111.9(8)	C(27)-C(28)-H(28)	110.5
C(22)-C(23)-C(24)	109.5(9)	C(22)-C(29)-C(28)	110.3(10)
C(22)-C(23)-H(23A)	109.8	C(22)-C(29)-H(29A)	109.6
C(24)-C(23)-H(23A)	109.8	C(28)-C(29)-H(29A)	109.6
C(22)-C(23)-H(23B)	109.8	C(22)-C(29)-H(29B)	109.6
C(24)-C(23)-H(23B)	109.8	C(28)-C(29)-H(29B)	109.6
H(23A)-C(23)-H(23B)	108.2	H(29A)-C(29)-H(29B)	108.1
C(31)-C(24)-C(25)	110.8(15)	C(22)-C(30)-C(26)	109.1(12)
C(31)-C(24)-C(23)	109.5(12)	C(22)-C(30)-H(30A)	109.9
C(25)-C(24)-C(23)	107.7(14)	C(26)-C(30)-H(30A)	109.9
C(31)-C(24)-H(24)	109.6	C(22)-C(30)-H(30B)	109.9
C(25)-C(24)-H(24)	109.6	C(26)-C(30)-H(30B)	109.9
C(23)-C(24)-H(24)	109.6	H(30A)-C(30)-H(30B)	108.3
C(26)-C(25)-C(24)	109.2(15)	C(24)-C(31)-C(28)	109.1(11)
C(26)-C(25)-H(25A)	109.8	C(24)-C(31)-H(31A)	109.9
C(24)-C(25)-H(25A)	109.8	C(28)-C(31)-H(31A)	109.9
C(26)-C(25)-H(25B)	109.8	C(24)-C(31)-H(31B)	109.9
C(24)-C(25)-H(25B)	109.8	C(28)-C(31)-H(31B)	109.9
H(25A)-C(25)-H(25B)	108.3	H(31A)-C(31)-H(31B)	108.3
C(25)-C(26)-C(30)	117(2)	C(1)-O(1)-P(1)	126.9(4)
C(25)-C(26)-C(27)	109(2)	C(21)-O(2)-C(20)	120.9(6)
C(30)-C(26)-C(27)	106(2)	O(1)#1-P(1)-O(1)	99.6(3)
C(25)-C(26)-H(26)	108.1	O(1)#1-P(1)-O(1)#2	99.6(3)
C(30)-C(26)-H(26)	108.1	O(1)-P(1)-O(1)#2	99.6(3)
C(27)-C(26)-H(26)	108.1	O(1)#1-P(1)-Au(1)	118.1(2)
C(28)-C(27)-C(26)	108.8(12)	O(1)-P(1)-Au(1)	118.1(2)
C(28)-C(27)-H(27A)	109.9	O(1)#2-P(1)-Au(1)	118.1(2)
C(26)-C(27)-H(27A)	109.9	P(1)-Au(1)-Cl(1)	180.000(2)
C(28)-C(27)-H(27B)	109.9		
C(26)-C(27)-H(27B)	109.9		
H(27A)-C(27)-H(27B)	108.3		
C(31)-C(28)-C(29)	109.3(14)		
C(31)-C(28)-C(27)	109.3(14)		
C(29)-C(28)-C(27)	106.7(13)		

Symmetry transformations used to generate equivalent atoms:

#1 -y+1,x-y+1,z #2 -x+y,-x+1,z

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for toste06. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

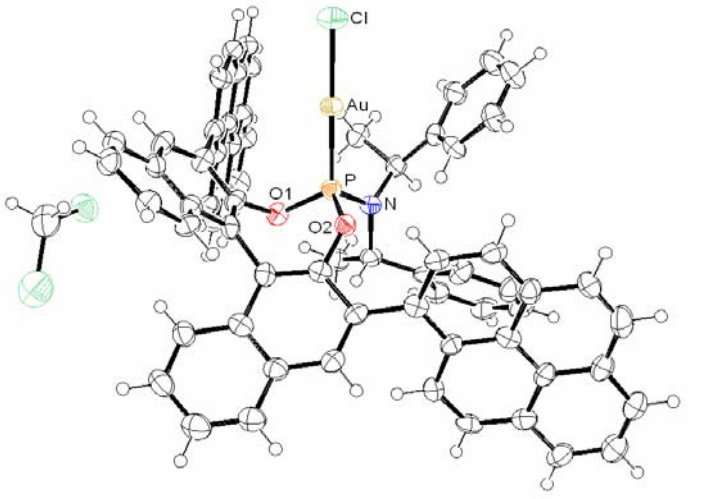
	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	44(3)	40(3)	73(4)	1(3)	1(3)	17(2)
C(2)	57(4)	51(4)	100(5)	14(4)	-2(4)	24(3)
C(3)	79(5)	53(4)	103(6)	17(4)	-1(4)	33(4)
C(4)	51(4)	54(4)	93(6)	0(4)	9(4)	18(3)
C(5)	79(5)	45(4)	111(7)	11(4)	19(5)	16(4)
C(6)	56(5)	59(5)	130(8)	-11(5)	20(5)	5(4)
C(7)	47(4)	66(5)	118(7)	-11(5)	4(4)	8(3)
C(8)	49(4)	55(4)	101(6)	-13(4)	1(4)	20(3)
C(9)	43(3)	44(3)	68(4)	-9(3)	2(3)	14(3)
C(10)	44(3)	48(3)	63(4)	-3(3)	1(3)	23(3)
C(11)	35(3)	48(3)	69(4)	4(3)	-1(3)	15(3)
C(12)	46(3)	57(3)	66(4)	4(3)	-7(3)	22(3)
C(13)	67(4)	74(5)	73(5)	9(4)	1(4)	23(4)
C(14)	120(8)	122(8)	67(5)	14(5)	20(5)	49(7)
C(15)	96(7)	130(9)	89(7)	40(6)	23(6)	47(7)
C(16)	79(6)	96(7)	114(8)	45(6)	8(5)	35(5)
C(17)	55(4)	71(4)	92(5)	23(4)	-2(3)	22(4)
C(18)	77(5)	64(4)	127(8)	17(5)	-6(5)	40(4)
C(19)	63(4)	62(4)	102(6)	14(4)	5(4)	37(4)
C(20)	50(3)	53(3)	78(5)	0(3)	2(3)	28(3)
C(21)	75(5)	68(5)	92(7)	-8(4)	9(4)	11(4)
C(22)	78(5)	78(5)	66(5)	-4(4)	10(4)	36(4)
C(23)	116(8)	92(7)	93(6)	7(5)	2(6)	25(6)
C(24)	132(10)	95(7)	96(8)	11(6)	16(7)	10(7)
C(25)	240(20)	156(17)	220(20)	49(17)	50(20)	122(19)
C(26)	178(19)	240(30)	190(20)	40(20)	-17(17)	140(20)
C(27)	154(14)	188(18)	124(13)	49(13)	-47(12)	25(13)
C(28)	198(16)	127(10)	95(9)	-3(7)	61(10)	58(11)
C(29)	133(9)	106(8)	85(7)	-12(6)	22(7)	49(7)
C(30)	112(10)	180(14)	146(11)	36(10)	28(8)	96(11)
C(31)	134(11)	182(14)	113(9)	44(9)	48(8)	73(11)

O(1)	38(2)	44(2)	86(3)	13(2)	2(2)	16(2)
O(2)	57(3)	60(3)	70(3)	-2(2)	2(2)	27(2)
O(3)	212(10)	88(5)	107(7)	-14(4)	20(6)	-28(6)
P(1)	40(1)	40(1)	68(2)	0	0	20(1)
Cl(1)	190(5)	190(5)	71(4)	0	0	95(3)
Au(1)	83(1)	83(1)	72(1)	0	0	41(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for toste06.

	x	y	z	U(eq)
H(2)	4455	8707	5905	85
H(3)	5835	10161	5682	94
H(5)	7631	11195	5662	102
H(6)	9093	11380	5944	111
H(7)	9229	10183	6480	103
H(8)	7891	8732	6761	85
H(13)	5376	7943	7822	92
H(14)	4764	7286	8920	130
H(15)	4732	5888	9288	132
H(16)	5406	5205	8621	121
H(18)	6110	5089	7441	105
H(19)	6704	5698	6344	88
H(23A)	8260	8178	4761	135
H(23B)	7686	8693	5007	135
H(24)	8711	9560	4022	154
H(25A)	7299	9628	4127	230
H(25B)	7483	9570	3309	230
H(26)	5950	8557	3602	224
H(27A)	5847	7189	3008	219
H(27B)	6620	8147	2626	219
H(28)	7313	7139	2800	180
H(29A)	6352	6279	3782	136
H(29B)	7446	6711	3995	136
H(30A)	6064	8050	4755	163
H(30B)	5488	7150	4250	163
H(31A)	8702	8239	3466	175
H(31B)	8425	8800	2910	175

2.7. X-ray crystal data of L_8AuCl



Experimental

A colorless needle 0.08 x 0.04 x 0.04 mm in size was mounted on a Cryoloop with Paratone oil. Data were collected in a nitrogen gas stream at 100(2) K using phi and omega scans. Crystal-to-detector distance was 60 mm and exposure time was 10 seconds per frame using a scan width of 1.0°. Data collection was 99.0% complete to 67.00° in θ. A total of 64681 reflections were collected covering the indices, -15<=*h*<=10, -20<=*k*<=20, -30<=*l*<=30. 10493 reflections were found to be symmetry independent, with an R_{int} of 0.0869. Indexing and unit cell refinement indicated a primitive, orthorhombic lattice. The space group was found to be P2(1)2(1)2(1) (No. 19). The data were integrated using the Bruker SAINT software program and scaled using the SADABS software program. Solution by direct methods (SIR-97) produced a complete heavy-atom phasing model consistent with the proposed structure. All non-hydrogen atoms were refined anisotropically by full-matrix least-squares (SHELXL-97). All hydrogen atoms were placed using a riding model. Their positions were constrained relative to their parent atom using the appropriate HFIX command in SHELXL-97. Disordered solvent contributions were treated using the SQUEEZE routine and its use is detailed in the CIF file.

Table 1. Crystal data and structure refinement.

Table 1. Crystal data and structure refinement for toste16.

X-ray ID	toste16	
Sample/notebook ID	AG03-p34	
Empirical formula	C69 H48 Au Cl3 N O2 P	
Formula weight	1257.37	
Temperature	100(2) K	
Wavelength	1.54178 Å	
Crystal system	Orthorhombic	
Space group	P2(1)2(1)2(1)	
Unit cell dimensions	a = 13.0180(4) Å	α= 90°.
	b = 17.4743(7) Å	β= 90°.
	c = 25.6126(10) Å	γ = 90°.
Volume	5826.4(4) $Å^3$	
Z	4	
Density (calculated)	1.433 Mg/m^3	
Absorption coefficient	6.626 mm^{-1}	
F(000)	2520	
Crystal size	0.08 x 0.04 x 0.04 mm^3	
Crystal color/habit	colorless needle	
Theta range for data collection	3.06 to 68.29°.	
Index ranges	-15<=h<=10, -20<=k<=20, -30<=l<=30	
Reflections collected	64681	
Independent reflections	10493 [R(int) = 0.0869]	
Completeness to theta = 67.00°	99.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7775 and 0.6192	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	10493 / 0 / 696	
Goodness-of-fit on F^2	1.017	
Final R indices [I>2sigma(I)]	R1 = 0.0404, wR2 = 0.0829	
R indices (all data)	R1 = 0.0525, wR2 = 0.0871	
Absolute structure parameter	-0.028(8)	
Largest diff. peak and hole	1.400 and -0.687 e.$Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for toste16. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	3821(5)	-1112(3)	6638(2)	33(1)
C(2)	2786(5)	-1380(3)	6850(2)	31(1)
C(3)	2553(6)	-1240(4)	7367(3)	42(2)
C(4)	1634(6)	-1499(5)	7592(3)	51(2)
C(5)	953(6)	-1904(5)	7289(3)	50(2)
C(6)	1174(5)	-2051(4)	6776(3)	43(2)
C(7)	2086(5)	-1795(4)	6560(2)	36(1)
C(8)	4142(5)	-308(4)	6822(3)	38(1)
C(9)	4827(5)	-1597(4)	5854(3)	34(2)
C(10)	4883(5)	-2405(3)	6090(3)	37(1)
C(11)	4045(5)	-2882(3)	6058(3)	41(1)
C(12)	4086(6)	-3625(4)	6256(3)	47(2)
C(13)	4986(6)	-3883(4)	6486(3)	48(2)
C(14)	5833(6)	-3417(4)	6514(3)	47(2)
C(15)	5786(6)	-2673(4)	6320(3)	44(2)
C(16)	5795(5)	-1123(4)	5933(3)	40(2)
C(17)	3526(5)	356(3)	5008(3)	33(1)
C(18)	3482(5)	1125(4)	5175(3)	35(1)
C(19)	2936(5)	1623(4)	4869(3)	38(2)
C(20)	2398(5)	1375(4)	4417(2)	34(1)
C(21)	1770(5)	1887(4)	4134(2)	38(2)
C(22)	1172(6)	1635(4)	3732(3)	39(2)
C(23)	1171(5)	844(4)	3605(2)	35(1)
C(24)	1794(5)	351(3)	3858(2)	33(1)
C(25)	2435(5)	594(4)	4269(2)	33(1)
C(26)	3092(5)	86(4)	4562(2)	31(1)
C(27)	3241(4)	-725(3)	4386(2)	31(1)
C(28)	3567(4)	-883(3)	3860(2)	32(1)
C(29)	3877(5)	-306(4)	3507(3)	38(1)
C(30)	4129(5)	-487(4)	2998(3)	45(2)
C(31)	4085(6)	-1255(4)	2822(3)	48(2)

C(32)	3824(5)	-1817(4)	3155(3)	41(2)
C(33)	3581(5)	-1662(4)	3686(2)	35(1)
C(34)	3307(4)	-2241(3)	4038(2)	31(1)
C(35)	3033(5)	-2113(3)	4544(2)	30(1)
C(36)	3032(5)	-1326(3)	4713(2)	31(1)
C(37)	3867(5)	1376(3)	5709(3)	36(1)
C(38)	3147(5)	1719(3)	6035(3)	39(1)
C(39)	3413(5)	1941(3)	6535(3)	37(1)
C(40)	4408(5)	1850(3)	6719(2)	34(1)
C(41)	4713(6)	2088(4)	7225(3)	41(2)
C(42)	5680(6)	2013(4)	7395(3)	40(2)
C(43)	6460(6)	1686(4)	7069(3)	40(2)
C(44)	7492(6)	1603(4)	7234(3)	44(2)
C(45)	8206(6)	1298(4)	6904(3)	50(2)
C(46)	7947(6)	1056(4)	6406(3)	44(2)
C(47)	6944(6)	1115(3)	6224(2)	38(1)
C(48)	6651(5)	892(3)	5706(3)	34(1)
C(49)	5676(5)	974(3)	5538(2)	33(1)
C(50)	4889(5)	1282(3)	5865(3)	32(2)
C(51)	5152(5)	1521(3)	6376(2)	31(1)
C(52)	6189(5)	1435(3)	6562(2)	33(1)
C(53)	2632(5)	-2739(4)	4877(2)	32(1)
C(54)	1676(4)	-2647(3)	5114(2)	33(1)
C(55)	1217(5)	-3237(4)	5388(3)	36(1)
C(56)	1694(5)	-3945(3)	5440(2)	37(2)
C(57)	1256(6)	-4571(4)	5731(3)	44(2)
C(58)	1722(7)	-5235(4)	5772(3)	54(2)
C(59)	2693(5)	-5381(4)	5552(3)	39(2)
C(60)	3212(6)	-6082(4)	5590(3)	44(2)
C(61)	4146(6)	-6201(4)	5365(3)	48(2)
C(62)	4632(6)	-5620(4)	5092(3)	46(2)
C(63)	4163(5)	-4894(4)	5041(2)	37(1)
C(64)	4635(5)	-4274(4)	4783(3)	35(1)
C(65)	4184(5)	-3577(3)	4727(2)	33(1)
C(66)	3165(5)	-3445(3)	4930(2)	31(1)
C(67)	2675(5)	-4051(4)	5208(2)	32(1)

C(68)	3174(5)	-4774(3)	5267(2)	33(1)
C(69)	4964(6)	2515(5)	3993(4)	64(2)
N(1)	3892(4)	-1187(3)	6057(2)	31(1)
O(1)	4022(3)	-176(2)	5344(2)	31(1)
O(2)	2717(3)	-1216(2)	5227(2)	30(1)
P(1)	3196(1)	-666(1)	5674(1)	29(1)
Cl(1)	640(1)	612(1)	6444(1)	47(1)
Cl(2)	5612(2)	2367(1)	4586(1)	57(1)
Cl(3)	5616(2)	2049(2)	3472(1)	82(1)
Au(1)	1948(1)	-30(1)	6055(1)	31(1)

Table 3. Bond lengths [Å] and angles [°] for toste16.

C(1)-N(1)	1.497(8)	C(16)-H(16B)	0.9800
C(1)-C(2)	1.526(8)	C(16)-H(16C)	0.9800
C(1)-C(8)	1.540(9)	C(17)-C(26)	1.360(8)
C(1)-H(1)	1.0000	C(17)-C(18)	1.410(9)
C(2)-C(7)	1.381(9)	C(17)-O(1)	1.422(7)
C(2)-C(3)	1.381(9)	C(18)-C(19)	1.370(9)
C(3)-C(4)	1.403(10)	C(18)-C(37)	1.522(9)
C(3)-H(3)	0.9500	C(19)-C(20)	1.421(9)
C(4)-C(5)	1.375(10)	C(19)-H(19)	0.9500
C(4)-H(4)	0.9500	C(20)-C(21)	1.413(9)
C(5)-C(6)	1.370(10)	C(20)-C(25)	1.416(9)
C(5)-H(5)	0.9500	C(21)-C(22)	1.363(9)
C(6)-C(7)	1.384(9)	C(21)-H(21)	0.9500
C(6)-H(6)	0.9500	C(22)-C(23)	1.420(9)
C(7)-H(7)	0.9500	C(22)-H(22)	0.9500
C(8)-H(8A)	0.9800	C(23)-C(24)	1.349(8)
C(8)-H(8B)	0.9800	C(23)-H(23)	0.9500
C(8)-H(8C)	0.9800	C(24)-C(25)	1.409(8)
C(9)-N(1)	1.505(7)	C(24)-H(24)	0.9500
C(9)-C(16)	1.521(9)	C(25)-C(26)	1.443(8)
C(9)-C(10)	1.537(9)	C(26)-C(27)	1.500(8)
C(9)-H(9)	1.0000	C(27)-C(36)	1.372(8)
C(10)-C(11)	1.376(9)	C(27)-C(28)	1.440(8)
C(10)-C(15)	1.395(10)	C(28)-C(29)	1.413(9)
C(11)-C(12)	1.395(9)	C(28)-C(33)	1.432(9)
C(11)-H(11)	0.9500	C(29)-C(30)	1.380(9)
C(12)-C(13)	1.387(11)	C(29)-H(29)	0.9500
C(12)-H(12)	0.9500	C(30)-C(31)	1.417(11)
C(13)-C(14)	1.374(11)	C(30)-H(30)	0.9500
C(13)-H(13)	0.9500	C(31)-C(32)	1.344(10)
C(14)-C(15)	1.393(10)	C(31)-H(31)	0.9500
C(14)-H(14)	0.9500	C(32)-C(33)	1.423(9)
C(15)-H(15)	0.9500	C(32)-H(32)	0.9500
C(16)-H(16A)	0.9800	C(33)-C(34)	1.401(9)

C(34)-C(35)	1.362(8)	C(54)-C(55)	1.383(9)
C(34)-H(34)	0.9500	C(54)-H(54)	0.9500
C(35)-C(36)	1.441(8)	C(55)-C(56)	1.390(9)
C(35)-C(53)	1.484(8)	C(55)-H(55)	0.9500
C(36)-O(2)	1.393(7)	C(56)-C(67)	1.421(9)
C(37)-C(38)	1.391(9)	C(56)-C(57)	1.441(9)
C(37)-C(50)	1.398(10)	C(57)-C(58)	1.314(10)
C(38)-C(39)	1.382(9)	C(57)-H(57)	0.9500
C(38)-H(38)	0.9500	C(58)-C(59)	1.408(11)
C(39)-C(40)	1.387(9)	C(58)-H(58)	0.9500
C(39)-H(39)	0.9500	C(59)-C(60)	1.403(9)
C(40)-C(41)	1.420(9)	C(59)-C(68)	1.431(8)
C(40)-C(51)	1.427(8)	C(60)-C(61)	1.361(11)
C(41)-C(42)	1.339(11)	C(60)-H(60)	0.9500
C(41)-H(41)	0.9500	C(61)-C(62)	1.385(11)
C(42)-C(43)	1.433(10)	C(61)-H(61)	0.9500
C(42)-H(42)	0.9500	C(62)-C(63)	1.414(9)
C(43)-C(52)	1.415(9)	C(62)-H(62)	0.9500
C(43)-C(44)	1.416(10)	C(63)-C(64)	1.410(9)
C(44)-C(45)	1.365(10)	C(63)-C(68)	1.428(9)
C(44)-H(44)	0.9500	C(64)-C(65)	1.359(9)
C(45)-C(46)	1.384(10)	C(64)-H(64)	0.9500
C(45)-H(45)	0.9500	C(65)-C(66)	1.444(9)
C(46)-C(47)	1.391(11)	C(65)-H(65)	0.9500
C(46)-H(46)	0.9500	C(66)-C(67)	1.425(8)
C(47)-C(52)	1.425(9)	C(67)-C(68)	1.428(8)
C(47)-C(48)	1.435(9)	C(69)-Cl(2)	1.757(9)
C(48)-C(49)	1.348(9)	C(69)-Cl(3)	1.779(10)
C(48)-H(48)	0.9500	C(69)-H(69A)	0.9900
C(49)-C(50)	1.428(9)	C(69)-H(69B)	0.9900
C(49)-H(49)	0.9500	N(1)-P(1)	1.616(5)
C(50)-C(51)	1.418(9)	O(1)-P(1)	1.614(4)
C(51)-C(52)	1.438(9)	O(2)-P(1)	1.619(4)
C(53)-C(54)	1.394(8)	P(1)-Au(1)	2.1970(16)
C(53)-C(66)	1.421(8)	Cl(1)-Au(1)	2.2692(17)

N(1)-C(1)-C(2)	112.4(5)	C(11)-C(10)-C(15)	119.3(6)
N(1)-C(1)-C(8)	111.7(5)	C(11)-C(10)-C(9)	119.7(6)
C(2)-C(1)-C(8)	114.2(5)	C(15)-C(10)-C(9)	120.9(6)
N(1)-C(1)-H(1)	105.9	C(10)-C(11)-C(12)	120.8(6)
C(2)-C(1)-H(1)	105.9	C(10)-C(11)-H(11)	119.6
C(8)-C(1)-H(1)	105.9	C(12)-C(11)-H(11)	119.6
C(7)-C(2)-C(3)	117.6(6)	C(13)-C(12)-C(11)	119.3(7)
C(7)-C(2)-C(1)	123.5(6)	C(13)-C(12)-H(12)	120.3
C(3)-C(2)-C(1)	118.7(6)	C(11)-C(12)-H(12)	120.3
C(2)-C(3)-C(4)	121.6(7)	C(14)-C(13)-C(12)	120.5(7)
C(2)-C(3)-H(3)	119.2	C(14)-C(13)-H(13)	119.8
C(4)-C(3)-H(3)	119.2	C(12)-C(13)-H(13)	119.8
C(5)-C(4)-C(3)	119.0(7)	C(13)-C(14)-C(15)	120.0(7)
C(5)-C(4)-H(4)	120.5	C(13)-C(14)-H(14)	120.0
C(3)-C(4)-H(4)	120.5	C(15)-C(14)-H(14)	120.0
C(6)-C(5)-C(4)	120.1(7)	C(14)-C(15)-C(10)	120.1(7)
C(6)-C(5)-H(5)	119.9	C(14)-C(15)-H(15)	120.0
C(4)-C(5)-H(5)	119.9	C(10)-C(15)-H(15)	120.0
C(5)-C(6)-C(7)	120.2(7)	C(9)-C(16)-H(16A)	109.5
C(5)-C(6)-H(6)	119.9	C(9)-C(16)-H(16B)	109.5
C(7)-C(6)-H(6)	119.9	H(16A)-C(16)-H(16B)	109.5
C(2)-C(7)-C(6)	121.4(6)	C(9)-C(16)-H(16C)	109.5
C(2)-C(7)-H(7)	119.3	H(16A)-C(16)-H(16C)	109.5
C(6)-C(7)-H(7)	119.3	H(16B)-C(16)-H(16C)	109.5
C(1)-C(8)-H(8A)	109.5	C(26)-C(17)-C(18)	124.6(6)
C(1)-C(8)-H(8B)	109.5	C(26)-C(17)-O(1)	118.1(5)
H(8A)-C(8)-H(8B)	109.5	C(18)-C(17)-O(1)	117.2(5)
C(1)-C(8)-H(8C)	109.5	C(19)-C(18)-C(17)	117.0(6)
H(8A)-C(8)-H(8C)	109.5	C(19)-C(18)-C(37)	120.0(6)
H(8B)-C(8)-H(8C)	109.5	C(17)-C(18)-C(37)	122.3(6)
N(1)-C(9)-C(16)	111.5(5)	C(18)-C(19)-C(20)	121.8(6)
N(1)-C(9)-C(10)	109.9(5)	C(18)-C(19)-H(19)	119.1
C(16)-C(9)-C(10)	114.1(6)	C(20)-C(19)-H(19)	119.1
N(1)-C(9)-H(9)	107.0	C(21)-C(20)-C(25)	119.5(6)
C(16)-C(9)-H(9)	107.0	C(21)-C(20)-C(19)	120.7(6)
C(10)-C(9)-H(9)	107.0	C(25)-C(20)-C(19)	119.7(6)

C(22)-C(21)-C(20)	120.9(6)	C(34)-C(33)-C(32)	122.3(6)
C(22)-C(21)-H(21)	119.5	C(34)-C(33)-C(28)	119.0(6)
C(20)-C(21)-H(21)	119.5	C(32)-C(33)-C(28)	118.7(6)
C(21)-C(22)-C(23)	119.2(6)	C(35)-C(34)-C(33)	124.0(6)
C(21)-C(22)-H(22)	120.4	C(35)-C(34)-H(34)	118.0
C(23)-C(22)-H(22)	120.4	C(33)-C(34)-H(34)	118.0
C(24)-C(23)-C(22)	120.7(6)	C(34)-C(35)-C(36)	116.4(5)
C(24)-C(23)-H(23)	119.6	C(34)-C(35)-C(53)	121.2(5)
C(22)-C(23)-H(23)	119.6	C(36)-C(35)-C(53)	122.0(5)
C(23)-C(24)-C(25)	121.5(6)	C(27)-C(36)-O(2)	122.0(5)
C(23)-C(24)-H(24)	119.2	C(27)-C(36)-C(35)	123.1(5)
C(25)-C(24)-H(24)	119.2	O(2)-C(36)-C(35)	114.7(5)
C(24)-C(25)-C(20)	118.0(6)	C(38)-C(37)-C(50)	121.3(6)
C(24)-C(25)-C(26)	123.6(5)	C(38)-C(37)-C(18)	116.3(6)
C(20)-C(25)-C(26)	118.3(6)	C(50)-C(37)-C(18)	122.4(6)
C(17)-C(26)-C(25)	118.0(6)	C(39)-C(38)-C(37)	120.6(6)
C(17)-C(26)-C(27)	121.8(5)	C(39)-C(38)-H(38)	119.7
C(25)-C(26)-C(27)	120.2(5)	C(37)-C(38)-H(38)	119.7
C(36)-C(27)-C(28)	118.9(5)	C(38)-C(39)-C(40)	121.0(6)
C(36)-C(27)-C(26)	121.0(5)	C(38)-C(39)-H(39)	119.5
C(28)-C(27)-C(26)	120.1(5)	C(40)-C(39)-H(39)	119.5
C(29)-C(28)-C(33)	118.4(6)	C(39)-C(40)-C(41)	122.4(6)
C(29)-C(28)-C(27)	123.1(6)	C(39)-C(40)-C(51)	118.2(6)
C(33)-C(28)-C(27)	118.4(5)	C(41)-C(40)-C(51)	119.3(6)
C(30)-C(29)-C(28)	120.6(6)	C(42)-C(41)-C(40)	122.0(6)
C(30)-C(29)-H(29)	119.7	C(42)-C(41)-H(41)	119.0
C(28)-C(29)-H(29)	119.7	C(40)-C(41)-H(41)	119.0
C(29)-C(30)-C(31)	120.5(6)	C(41)-C(42)-C(43)	121.1(6)
C(29)-C(30)-H(30)	119.8	C(41)-C(42)-H(42)	119.5
C(31)-C(30)-H(30)	119.8	C(43)-C(42)-H(42)	119.5
C(32)-C(31)-C(30)	120.1(7)	C(52)-C(43)-C(44)	118.7(7)
C(32)-C(31)-H(31)	120.0	C(52)-C(43)-C(42)	118.8(6)
C(30)-C(31)-H(31)	120.0	C(44)-C(43)-C(42)	122.6(7)
C(31)-C(32)-C(33)	121.6(7)	C(45)-C(44)-C(43)	120.1(7)
C(31)-C(32)-H(32)	119.2	C(45)-C(44)-H(44)	120.0
C(33)-C(32)-H(32)	119.2	C(43)-C(44)-H(44)	120.0

C(44)-C(45)-C(46)	121.6(7)	C(58)-C(57)-C(56)	122.0(7)
C(44)-C(45)-H(45)	119.2	C(58)-C(57)-H(57)	119.0
C(46)-C(45)-H(45)	119.2	C(56)-C(57)-H(57)	119.0
C(45)-C(46)-C(47)	121.0(7)	C(57)-C(58)-C(59)	122.8(7)
C(45)-C(46)-H(46)	119.5	C(57)-C(58)-H(58)	118.6
C(47)-C(46)-H(46)	119.5	C(59)-C(58)-H(58)	118.6
C(46)-C(47)-C(52)	118.2(6)	C(60)-C(59)-C(58)	124.2(7)
C(46)-C(47)-C(48)	122.7(6)	C(60)-C(59)-C(68)	118.2(6)
C(52)-C(47)-C(48)	119.1(6)	C(58)-C(59)-C(68)	117.6(6)
C(49)-C(48)-C(47)	121.0(6)	C(61)-C(60)-C(59)	122.3(7)
C(49)-C(48)-H(48)	119.5	C(61)-C(60)-H(60)	118.9
C(47)-C(48)-H(48)	119.5	C(59)-C(60)-H(60)	118.9
C(48)-C(49)-C(50)	122.0(6)	C(60)-C(61)-C(62)	120.6(7)
C(48)-C(49)-H(49)	119.0	C(60)-C(61)-H(61)	119.7
C(50)-C(49)-H(49)	119.0	C(62)-C(61)-H(61)	119.7
C(37)-C(50)-C(51)	117.3(6)	C(61)-C(62)-C(63)	120.4(7)
C(37)-C(50)-C(49)	124.1(6)	C(61)-C(62)-H(62)	119.8
C(51)-C(50)-C(49)	118.6(6)	C(63)-C(62)-H(62)	119.8
C(50)-C(51)-C(40)	121.4(6)	C(64)-C(63)-C(62)	123.0(6)
C(50)-C(51)-C(52)	120.1(6)	C(64)-C(63)-C(68)	118.0(6)
C(40)-C(51)-C(52)	118.4(6)	C(62)-C(63)-C(68)	119.0(6)
C(43)-C(52)-C(47)	120.4(6)	C(65)-C(64)-C(63)	123.4(6)
C(43)-C(52)-C(51)	120.4(6)	C(65)-C(64)-H(64)	118.3
C(47)-C(52)-C(51)	119.2(6)	C(63)-C(64)-H(64)	118.3
C(54)-C(53)-C(66)	119.6(6)	C(64)-C(65)-C(66)	120.1(6)
C(54)-C(53)-C(35)	118.6(6)	C(64)-C(65)-H(65)	120.0
C(66)-C(53)-C(35)	121.6(5)	C(66)-C(65)-H(65)	120.0
C(55)-C(54)-C(53)	121.4(6)	C(53)-C(66)-C(67)	118.3(6)
C(55)-C(54)-H(54)	119.3	C(53)-C(66)-C(65)	123.5(5)
C(53)-C(54)-H(54)	119.3	C(67)-C(66)-C(65)	118.2(5)
C(54)-C(55)-C(56)	121.3(6)	C(56)-C(67)-C(66)	121.0(6)
C(54)-C(55)-H(55)	119.3	C(56)-C(67)-C(68)	118.6(6)
C(56)-C(55)-H(55)	119.3	C(66)-C(67)-C(68)	120.4(6)
C(55)-C(56)-C(67)	118.4(6)	C(63)-C(68)-C(67)	119.8(6)
C(55)-C(56)-C(57)	123.3(6)	C(63)-C(68)-C(59)	119.4(6)
C(67)-C(56)-C(57)	118.2(6)	C(67)-C(68)-C(59)	120.7(6)

Cl(2)-C(69)-Cl(3)	110.6(4)
Cl(2)-C(69)-H(69A)	109.5
Cl(3)-C(69)-H(69A)	109.5
Cl(2)-C(69)-H(69B)	109.5
Cl(3)-C(69)-H(69B)	109.5
H(69A)-C(69)-H(69B)	108.1
C(1)-N(1)-C(9)	115.8(5)
C(1)-N(1)-P(1)	121.2(4)
C(9)-N(1)-P(1)	120.9(4)
C(17)-O(1)-P(1)	111.2(4)
C(36)-O(2)-P(1)	129.6(4)
O(1)-P(1)-N(1)	104.1(2)
O(1)-P(1)-O(2)	101.6(2)
N(1)-P(1)-O(2)	108.0(2)
O(1)-P(1)-Au(1)	117.17(15)
N(1)-P(1)-Au(1)	115.5(2)
O(2)-P(1)-Au(1)	109.24(17)
P(1)-Au(1)-Cl(1)	179.03(6)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2$x 10^3)for toste16. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	33(3)	32(3)	35(3)	6(3)	-3(2)	6(2)
C(2)	33(3)	28(3)	31(3)	5(2)	-3(2)	0(2)
C(3)	42(4)	39(4)	43(4)	-5(3)	5(3)	-7(3)
C(4)	56(5)	58(5)	39(4)	-10(3)	12(3)	-14(3)
C(5)	41(4)	59(5)	49(4)	6(3)	12(3)	-10(3)
C(6)	37(4)	48(4)	43(4)	6(3)	-1(3)	-11(3)
C(7)	29(3)	47(4)	32(3)	3(3)	7(3)	-1(3)
C(8)	34(3)	36(3)	45(4)	0(3)	-6(3)	-3(2)
C(9)	33(4)	34(4)	35(3)	0(3)	3(3)	9(3)
C(10)	45(4)	34(3)	31(3)	-11(3)	6(3)	6(2)
C(11)	56(4)	33(3)	33(3)	-1(3)	-11(3)	8(3)
C(12)	65(5)	33(4)	42(4)	-7(3)	-3(3)	-11(3)
C(13)	48(4)	41(4)	55(4)	4(3)	4(3)	18(3)
C(14)	38(4)	47(4)	55(5)	-2(3)	-1(3)	18(3)
C(15)	38(4)	42(4)	52(4)	0(3)	6(3)	7(3)
C(16)	32(4)	42(4)	47(4)	4(3)	6(3)	3(3)
C(17)	30(3)	27(3)	41(3)	2(3)	-2(3)	5(2)
C(18)	30(3)	33(3)	41(4)	1(3)	-8(3)	-1(2)
C(19)	30(4)	27(3)	57(4)	0(3)	-3(3)	-3(3)
C(20)	35(3)	34(3)	32(3)	8(3)	2(3)	2(2)
C(21)	41(4)	32(3)	41(3)	2(2)	2(3)	-6(3)
C(22)	47(4)	36(4)	34(3)	5(3)	-6(3)	5(3)
C(23)	36(3)	37(3)	31(3)	-1(3)	-8(2)	0(3)
C(24)	32(3)	31(3)	36(3)	-6(2)	-4(3)	1(2)
C(25)	30(3)	32(3)	38(4)	1(3)	1(3)	-5(2)
C(26)	28(2)	30(3)	35(2)	6(3)	1(2)	-6(3)
C(27)	23(3)	32(3)	37(3)	3(2)	-2(2)	-4(2)
C(28)	22(3)	44(3)	30(3)	0(3)	-3(2)	2(2)
C(29)	35(4)	38(3)	41(4)	6(3)	3(3)	-2(3)
C(30)	37(4)	58(5)	41(4)	14(3)	9(3)	7(3)
C(31)	50(5)	61(5)	33(4)	3(3)	-3(3)	16(4)
C(32)	40(4)	48(4)	33(3)	-2(3)	-4(3)	6(3)
C(33)	31(3)	39(4)	35(3)	0(3)	0(3)	6(3)

C(34)	21(3)	30(3)	41(4)	-1(2)	-4(2)	3(2)
C(35)	24(3)	30(3)	37(3)	0(2)	-6(3)	8(3)
C(36)	29(3)	36(3)	29(3)	-3(2)	-2(3)	-1(3)
C(37)	44(4)	24(3)	39(4)	-1(3)	0(3)	-4(2)
C(38)	38(3)	41(3)	37(3)	5(3)	7(3)	7(3)
C(39)	37(4)	29(3)	45(4)	2(3)	7(3)	3(2)
C(40)	33(3)	29(3)	40(3)	3(3)	1(3)	0(2)
C(41)	52(4)	33(3)	38(4)	-3(3)	10(3)	0(3)
C(42)	48(4)	44(4)	29(3)	0(3)	-2(3)	0(3)
C(43)	40(4)	36(3)	43(4)	2(3)	1(3)	-8(3)
C(44)	38(4)	54(4)	41(4)	0(3)	-5(3)	-4(3)
C(45)	33(4)	63(4)	53(4)	-2(3)	-8(3)	-3(3)
C(46)	30(4)	46(4)	56(4)	-4(3)	11(3)	-2(3)
C(47)	34(3)	38(3)	43(3)	4(2)	3(3)	2(3)
C(48)	29(3)	30(3)	41(3)	-3(3)	8(2)	-1(2)
C(49)	36(4)	24(3)	37(3)	-4(2)	3(3)	-3(2)
C(50)	35(4)	21(3)	38(3)	3(2)	-1(3)	-2(2)
C(51)	31(3)	26(3)	36(3)	5(2)	3(2)	-6(2)
C(52)	34(3)	27(3)	37(3)	5(2)	-2(3)	-6(2)
C(53)	26(3)	39(3)	31(3)	-5(3)	-4(2)	-3(2)
C(54)	28(3)	32(3)	37(3)	-8(2)	-1(2)	3(2)
C(55)	24(3)	34(3)	50(4)	-12(3)	3(3)	-2(2)
C(56)	47(4)	31(3)	33(3)	-2(2)	-3(3)	-9(3)
C(57)	35(4)	44(4)	53(5)	2(3)	13(3)	-8(3)
C(58)	55(5)	46(4)	60(5)	6(3)	2(4)	-20(3)
C(59)	41(4)	31(3)	45(4)	-1(3)	-8(3)	-6(3)
C(60)	50(5)	33(3)	49(4)	5(3)	-9(3)	1(3)
C(61)	50(4)	40(4)	54(4)	5(3)	-9(3)	9(3)
C(62)	57(5)	34(4)	46(4)	-3(3)	-3(3)	11(3)
C(63)	39(3)	39(4)	32(3)	-4(3)	-2(2)	7(3)
C(64)	20(3)	46(4)	37(3)	-8(3)	5(2)	3(2)
C(65)	33(3)	34(3)	32(3)	4(2)	-3(3)	-4(2)
C(66)	33(3)	27(3)	33(3)	-4(2)	-1(3)	-1(2)
C(67)	26(3)	43(3)	28(3)	-6(3)	-3(2)	-3(2)
C(68)	38(3)	25(3)	36(3)	-3(2)	-5(3)	-4(2)
C(69)	44(4)	66(5)	81(6)	19(5)	-3(4)	6(4)
N(1)	31(3)	32(2)	29(3)	-4(2)	2(2)	3(2)
O(1)	26(2)	32(3)	35(2)	-1(2)	-5(2)	-2(2)

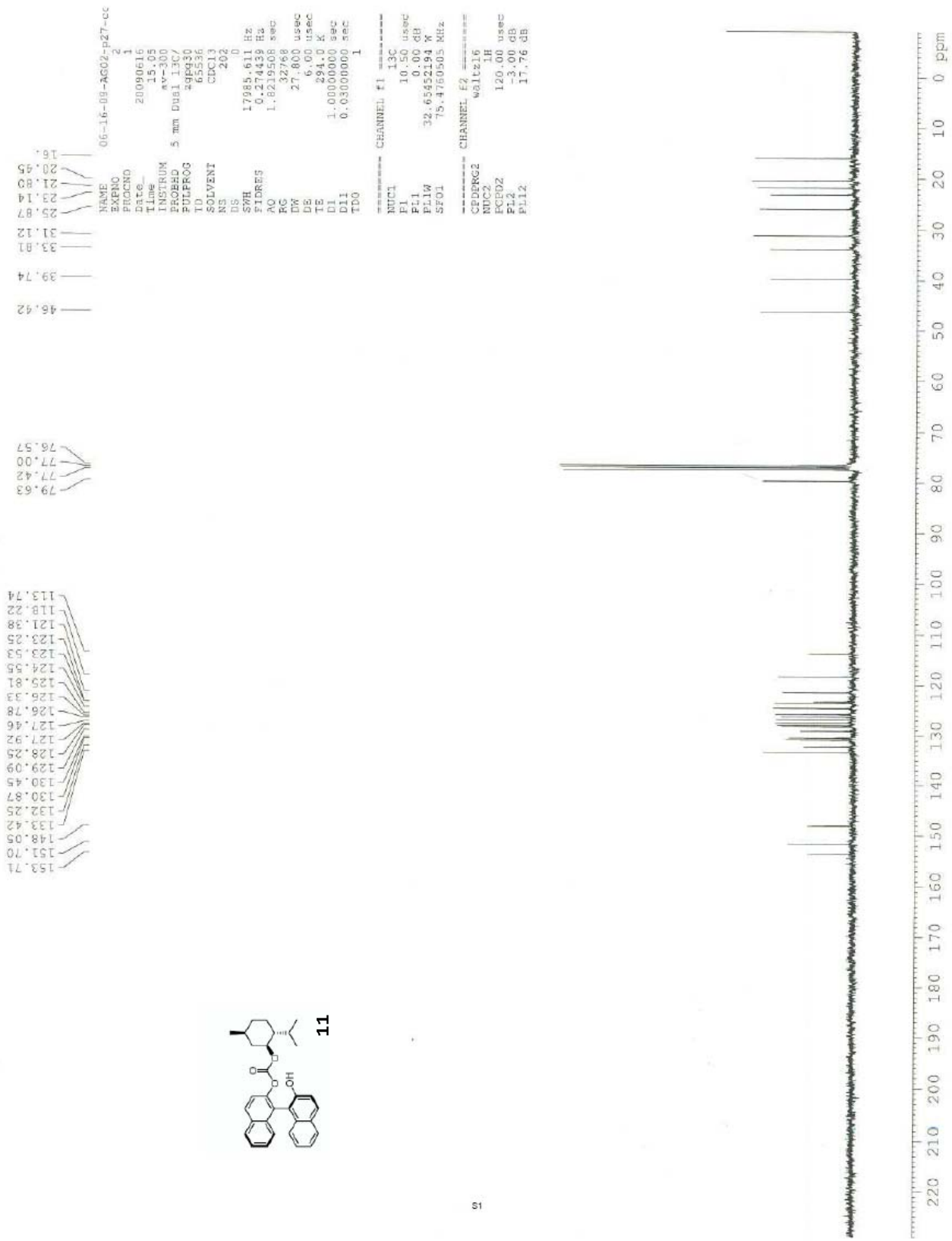
O(2)	32(2)	28(2)	31(2)	-1(2)	0(2)	-5(2)
P(1)	28(1)	29(1)	30(1)	0(1)	0(1)	0(1)
Cl(1)	37(1)	57(1)	46(1)	-10(1)	1(1)	10(1)
Cl(2)	51(1)	65(1)	56(1)	6(1)	2(1)	1(1)
Cl(3)	104(2)	79(2)	62(1)	-3(1)	-29(1)	6(1)
Au(1)	28(1)	33(1)	32(1)	-3(1)	-1(1)	2(1)

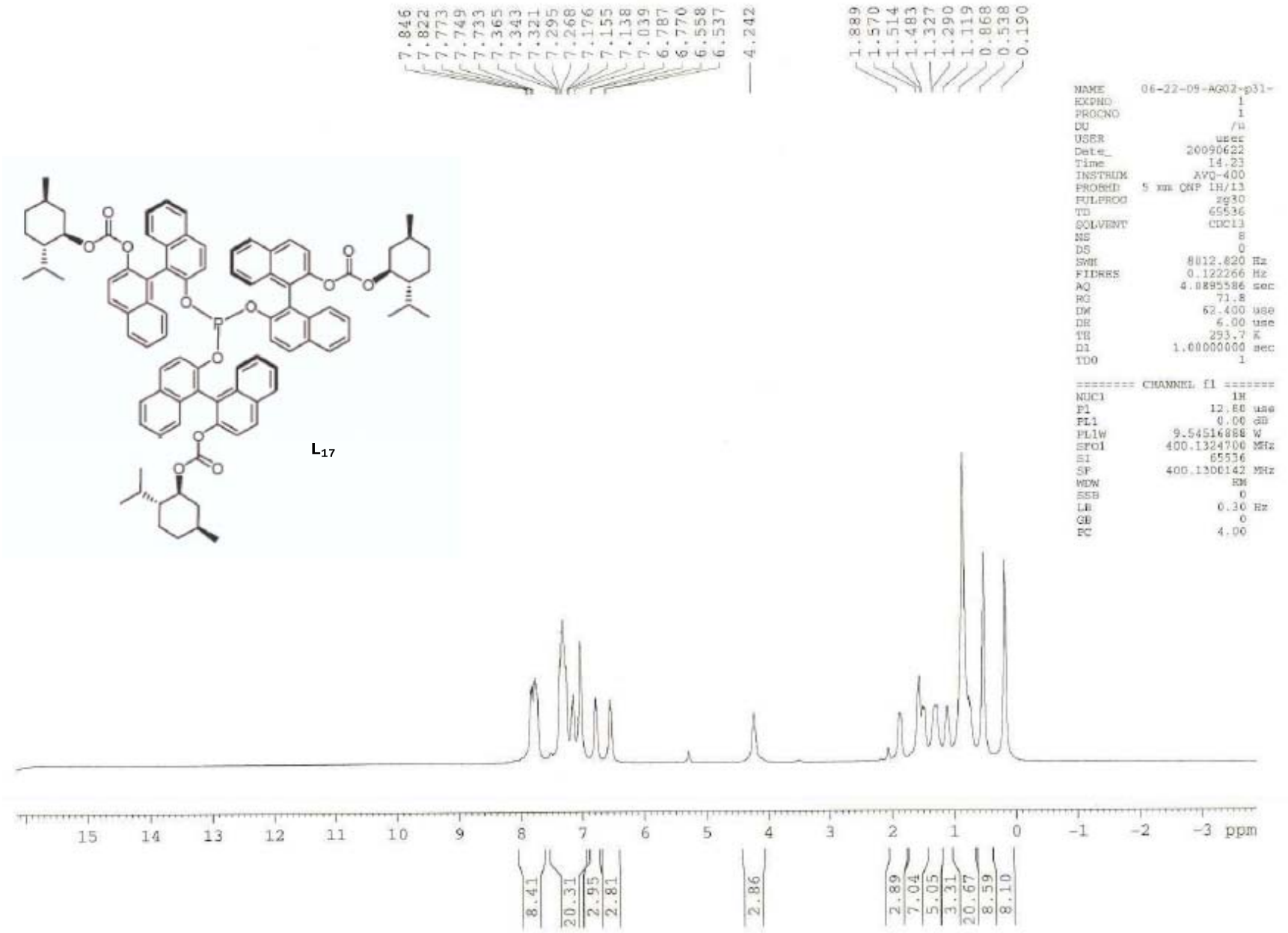
Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for toste16.

	x	y	z	U(eq)
H(1)	4344	-1472	6784	40
H(3)	3026	-961	7575	50
H(4)	1486	-1397	7948	61
H(5)	327	-2083	7436	59
H(6)	701	-2331	6568	51
H(7)	2234	-1906	6205	43
H(8A)	4797	-167	6659	58
H(8B)	4222	-308	7203	58
H(8C)	3614	64	6723	58
H(9)	4733	-1660	5469	41
H(11)	3431	-2704	5899	49
H(12)	3504	-3951	6233	56
H(13)	5017	-4386	6626	58
H(14)	6452	-3601	6665	56
H(15)	6369	-2348	6344	53
H(16A)	5690	-609	5789	60
H(16B)	6372	-1370	5754	60
H(16C)	5946	-1085	6307	60
H(19)	2916	2149	4962	45
H(21)	1764	2414	4224	46
H(22)	762	1985	3539	47
H(23)	726	660	3339	42
H(24)	1801	-172	3757	39
H(29)	3913	211	3620	46
H(30)	4334	-93	2764	54
H(31)	4241	-1373	2469	58
H(32)	3801	-2330	3032	49
H(34)	3312	-2755	3916	37
H(38)	2467	1801	5914	47
H(39)	2907	2160	6757	44
H(41)	4215	2308	7451	49
H(42)	5853	2178	7737	48

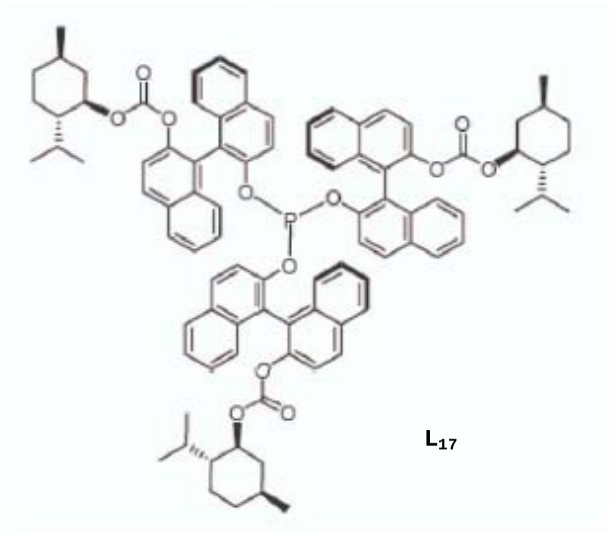
H(44)	7687	1759	7575	53
H(45)	8897	1250	7018	60
H(46)	8462	847	6186	53
H(48)	7153	683	5477	40
H(49)	5508	823	5192	39
H(54)	1333	-2169	5087	39
H(55)	563	-3158	5543	43
H(57)	611	-4501	5898	53
H(58)	1388	-5635	5958	64
H(60)	2902	-6488	5780	53
H(61)	4467	-6687	5395	58
H(62)	5285	-5710	4938	55
H(64)	5302	-4346	4642	42
H(65)	4540	-3176	4553	40
H(69A)	4922	3071	3921	76
H(69B)	4255	2314	4021	76

3. Selected Spectal Data



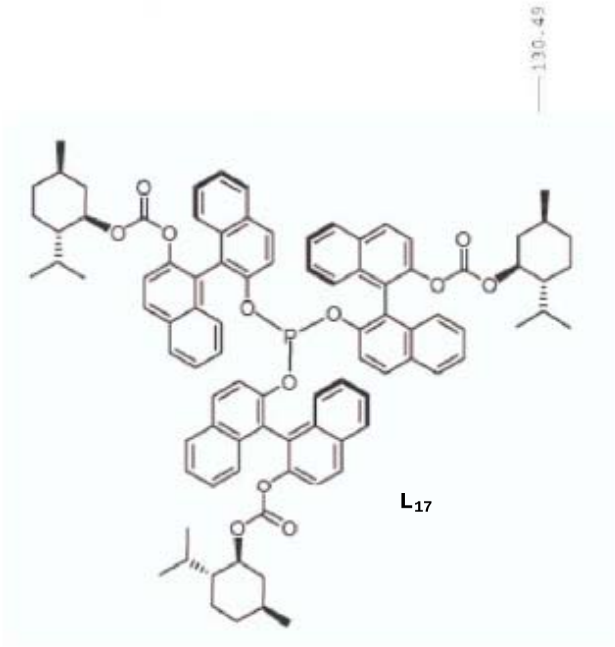

7.846
7.822
7.773
7.749
7.733
7.365
7.343
7.321
7.295
7.268
7.176
7.155
7.138
7.039
6.787
6.770
6.558
6.537
4.242
1.889
1.570
1.514
1.483
1.327
1.290
1.119
0.868
0.538
0.190
NAME 06-22-09-AG02-p31-
EXPNO 1
PROCNO 1
DU /u
USER user
Date_ 20090622
Time 14.23
INSTRUM AVQ-400
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0895586 sec
RG 71.8
DW 62.400 use
DE 6.00 use
TE 293.7 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 =======
NUC1 1H
P1 12.80 use
PL1 0.00 dB
PL1W 9.54516888 W
SFO1 400.1324700 MHz
SI 65536
SF 400.1300142 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 4.00
15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3 ppm
8.41
20.31
2.95
2.81
2.86
2.89
7.04
5.05
3.31
20.67
8.59
8.10

L_{17}



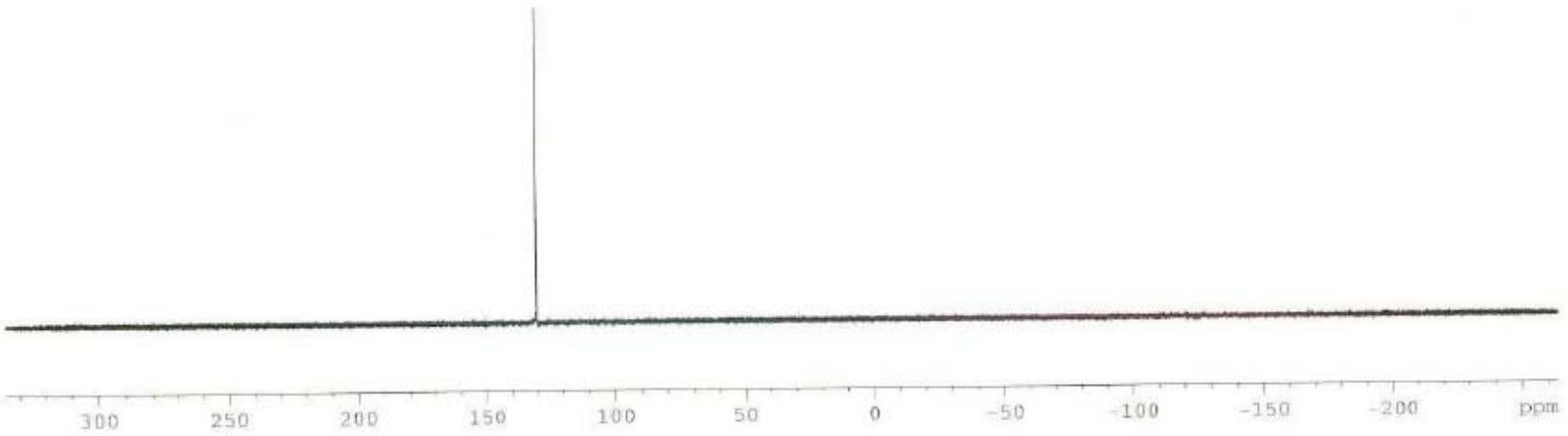
L_{17}

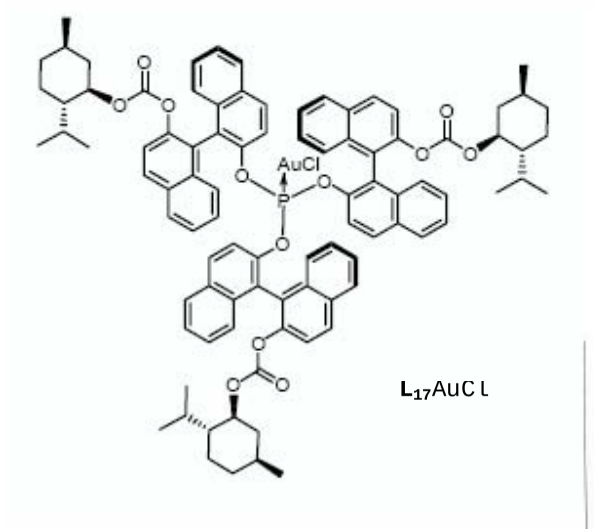
153.02
147.36
146.87
133.25
133.08
131.55
130.10
129.26
127.69
127.55
126.33
126.18
125.68
125.27
124.40
121.55
120.74
120.58
78.51
77.33
77.01
76.69
46.64
40.41
33.90
31.22
25.63
23.25
21.93
20.31
15.86
NAME 06-22-09-AG03-p31-col
EXPNO 3
PROCNO 1
DU /u
USER user
Date_ 20090622
Time 14.30
INSTRUM AVQ-400
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 196
DS 0
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3632196 sec
RG 16384
DW 20.800 usec
DE 6.00 usec
TE 294.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 8.50 usec
PL1 -2.00 dB
PL1W 47.77286148 W
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 70.00 usec
PL2 0.00 dB
PL12 15.00 dB
PL13 17.00 dB
PL2W 9.54516888 W
PL12W 0.30184472 W
PL13W 0.19045115 W
SFO2 400.1316000 MHz
SI 32768
SF 100.6127762 MHz
WDW EM
SSB 0
LB 1.50 Hz
GB 0
PC 1.40
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm



L_{17}

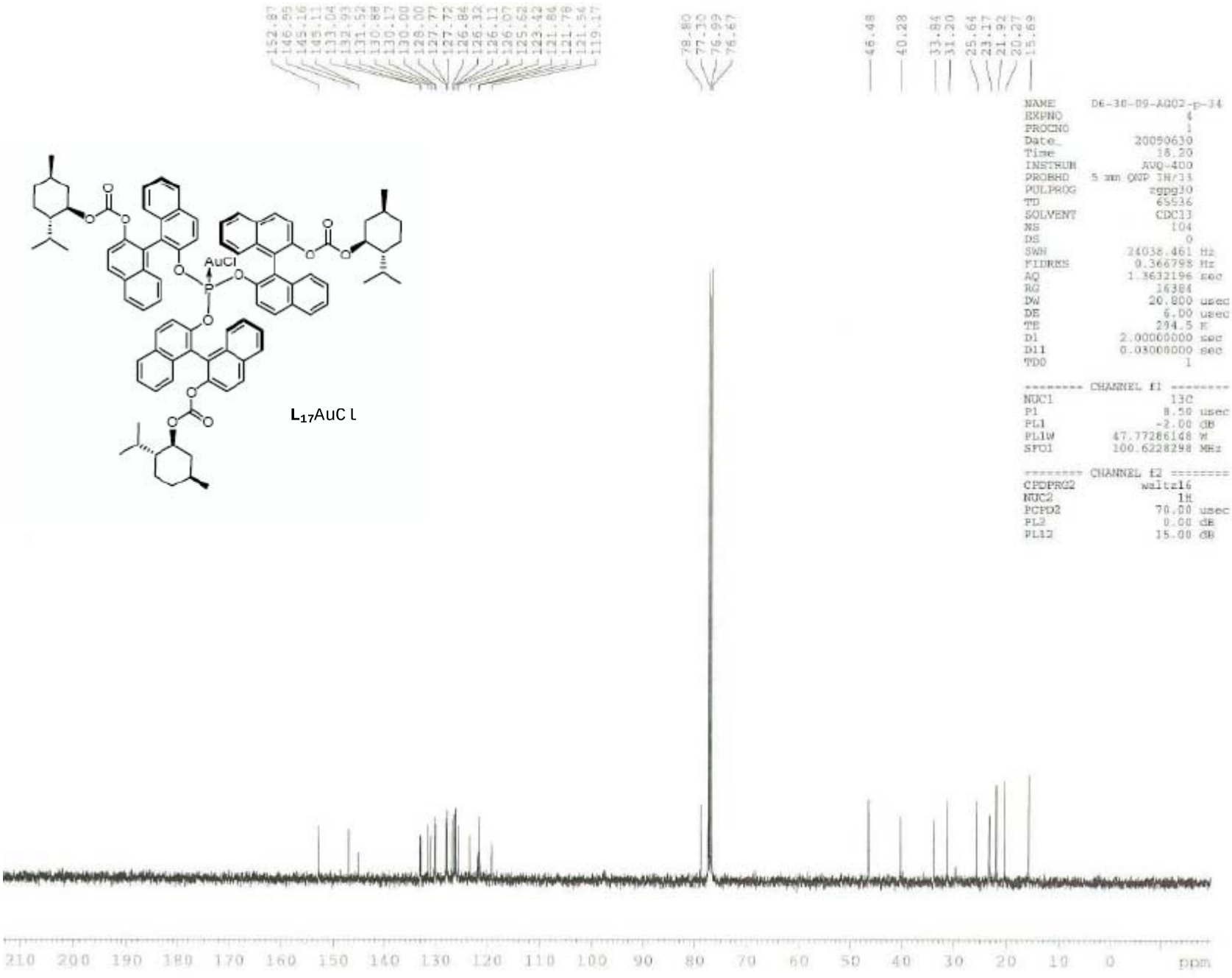
```
NAME          06-22-09-AG02-p31-col
EXPNO                 2
PROCNO                1
DU                   /u
USER              user
Date_          20090622
Time              14.25
INSTRUM        AVQ-400
PROBHD  5 mm QNP 1H/13
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                   19
DS                    0
SWH           97087.375 Hz
FIDRES        1.481436 Hz
AQ            0.3375655 sec
RG                 8192
DW               5.150 usec
DE               6.00 usec
TE              293.7 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 31P
P1                7.70 usec
PL1              -2.00 dB
PL1W       26.27507401 W
SFO1       161.9814041 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2            70.00 usec
PL2               0.00 dB
PL12             15.00 dB
PL13             17.00 dB
PL2W        9.54516888 W
PL12W       0.10184472 W
PL13W       0.19045115 W
SFO2       400.1316005 MHz
SI                65536
SF         161.9755989 MHz
WDW                  EM
SSB                   0
LB                1.00 Hz
GB                    0
PC                1.40
```

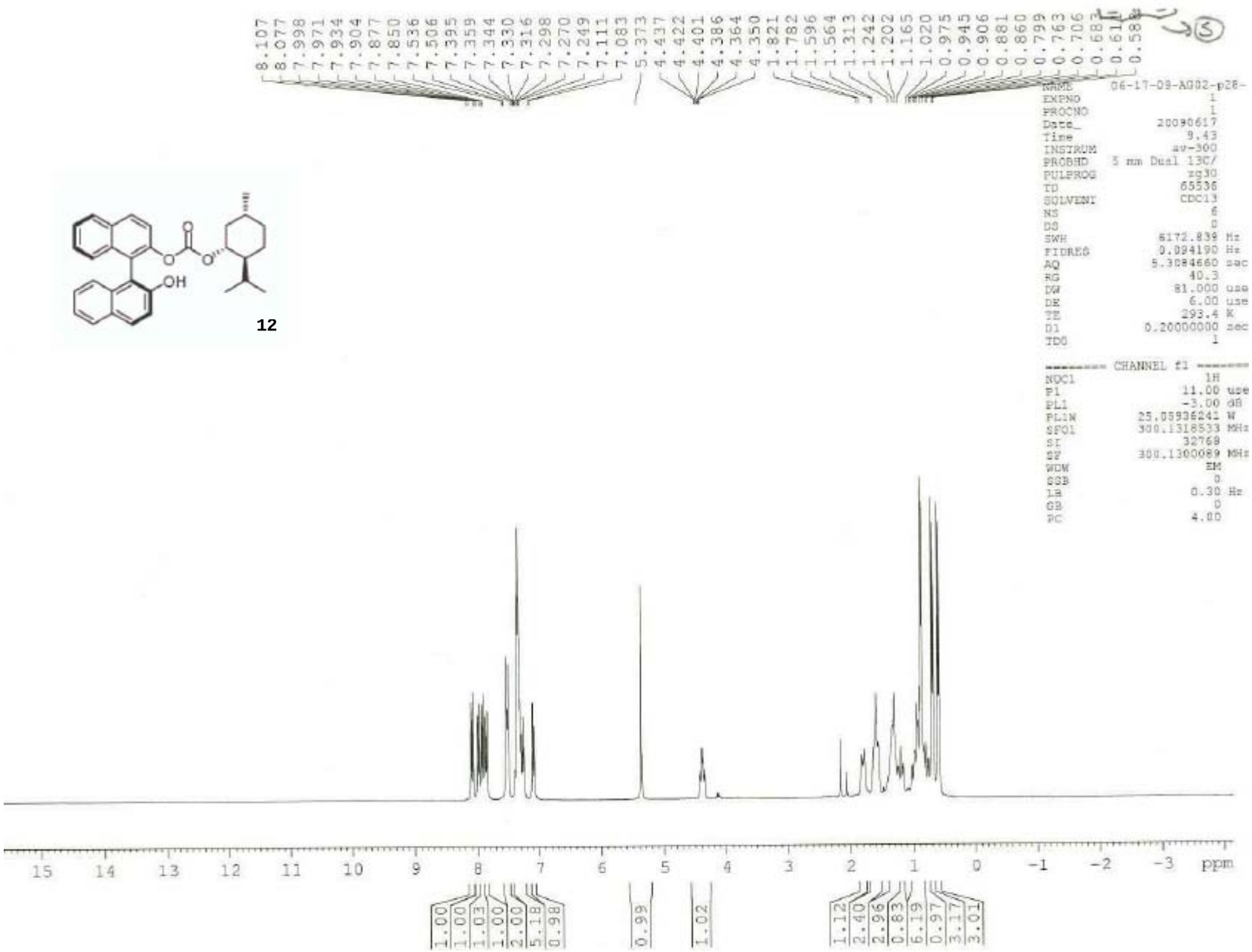


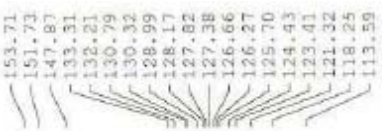


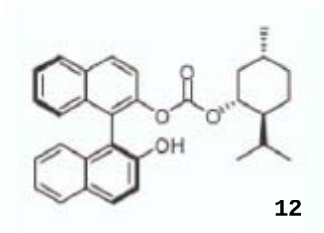
$L_{17}AuCl$

NAME	06-22-09-AGO2-pt4
EXPNO	4
PROCNO	1
DU	/u
USER	GonzalezA
Date_	20090622
Time	18.15
INSTRUM	AVQ-400
PROBHD	5 mm QNP 1H/13
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	0
SWH	97087.375 Hz
FIDRES	1.481436 Hz
AQ	0.3375655 sec
RG	8192
DW	5.150 usec
DE	6.00 usec
TE	292.8 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	31P
P1	7.70 usec
PL1	-2.00 dB
PL1W	26.27507401 W
SFO1	161.9814041 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	70.00 usec
PL2	0.00 dB
PL12	15.00 dB
PL13	17.00 dB
PL2W	9.54516888 W
PL12W	0.30184472 W
PL13W	0.19045115 W
SFO2	400.1316005 MHz
SI	65536
SF	161.9755989 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

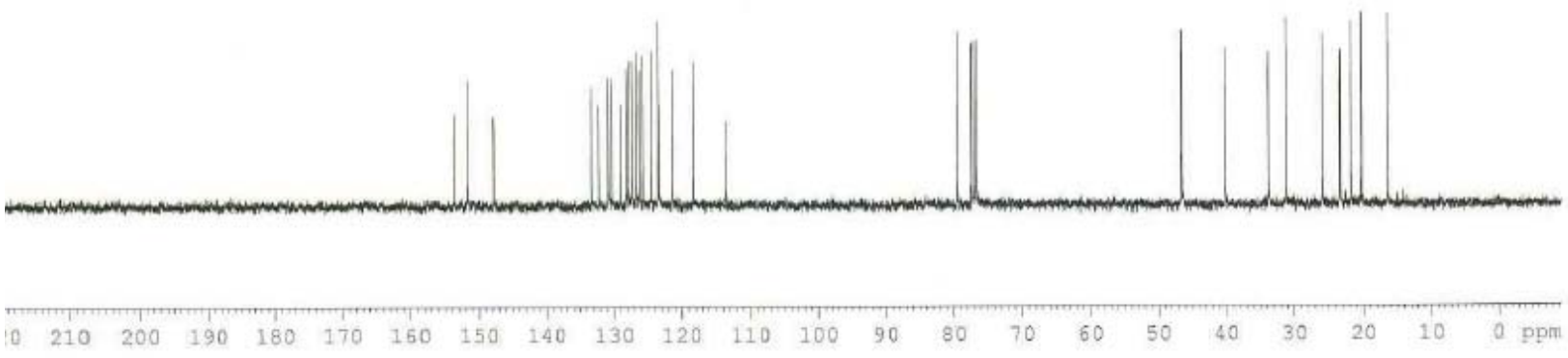

152.87
146.85
145.16
145.11
133.04
132.93
131.52
130.88
130.47
130.00
128.00
127.77
127.72
126.84
126.32
126.11
126.07
125.62
123.43
121.84
121.78
121.54
119.17
78.80
77.30
76.99
76.67
46.48
40.28
33.86
31.20
25.64
23.17
21.92
20.27
15.69
AuCl
L17AuCl
NAME D6-30-09-AG02-p-34
EXPNO 4
PROCNO 1
Date_ 20090630
Time 18.20
INSTRUM AVQ-400
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 104
DS 0
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3632196 sec
RG 16384
DW 20.800 usec
DE 6.00 usec
TE 294.5 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
CHANNEL f1
NUC1 13C
P1 8.50 usec
PL1 -2.00 dB
PL1W 47.77286148 W
SFO1 100.6228298 MHz
CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
PCPD2 70.00 usec
PL2 0.00 dB
PL12 15.00 dB
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm


8.107
8.077
7.998
7.971
7.934
7.904
7.877
7.850
7.536
7.506
7.395
7.359
7.344
7.330
7.316
7.298
7.270
7.249
7.111
7.083
5.373
4.437
4.422
4.401
4.386
4.364
4.350
1.821
1.782
1.596
1.564
1.313
1.242
1.202
1.165
1.020
0.975
0.945
0.906
0.881
0.860
0.799
0.763
0.706
0.683
0.614
0.588
OH
12
NAME 06-17-09-AG02-p28-
EXPNO 1
PROCNO 1
Date_ 20090617
Time 9.43
INSTRUM av-300
PROBHD 5 mm Dual 13C/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 6
DS 0
SWH 6172.839 Hz
FIDRES 0.094190 Hz
AQ 5.3084660 sec
RG 40.3
DW 81.000 use
DE 6.00 use
TE 293.4 K
D1 0.20000000 sec
TD0 1
CHANNEL f1
NUC1 1H
P1 11.00 use
PL1 -3.00 dB
PL1N 25.05936241 W
SFO1 300.1318533 MHz
SI 32768
SF 300.1300089 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 4.00
15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3 ppm
1.00 1.00 1.03 1.00 2.00 5.18 0.98
0.99
1.02
1.12 2.40 2.96 0.83 6.19 0.97 3.17 3.01

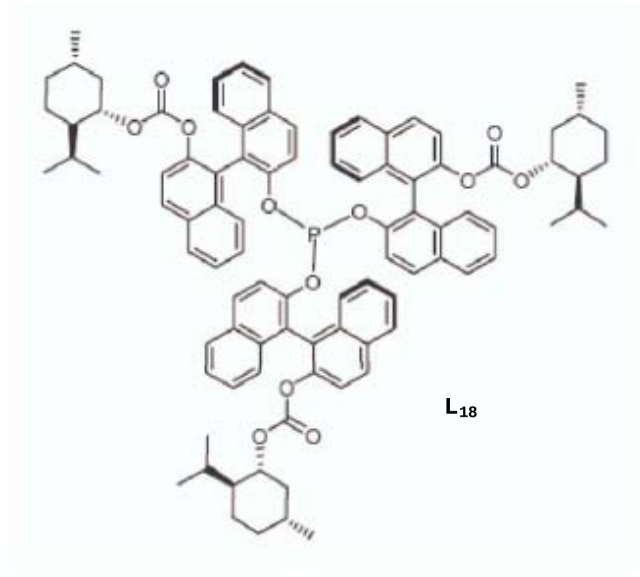




NAME	06-17-09-AG02-p28-col1
EXPNO	2
PROCNO	1
Date_	20090617
Time	9.44
INSTRUM	av-300
PROBHD	5 mm Dual 13C/
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	71
DS	0
SWH	17985.611 Hz
FIDRES	0.274439 Hz
AQ	1.8219508 sec
RG	32768
DW	27.800 usec
DE	6.00 usec
TE	293.4 K
D1	1.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	10.50 usec
PL1	0.00 dB
PL1W	32.65452194 W
SFO1	75.4760505 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	120.00 usec
PL2	-3.00 dB
PL12	17.76 dB

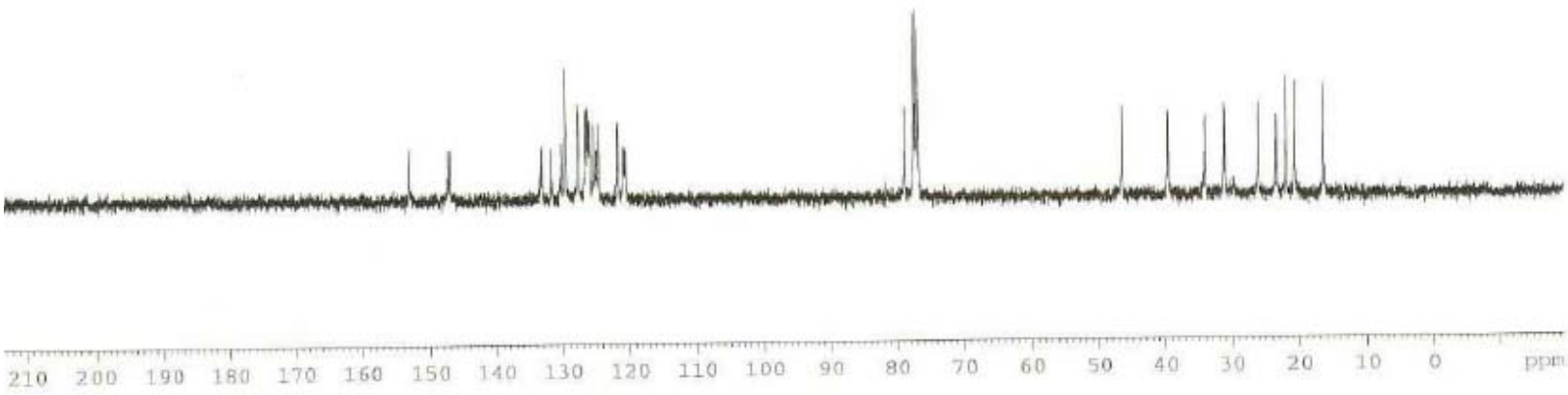


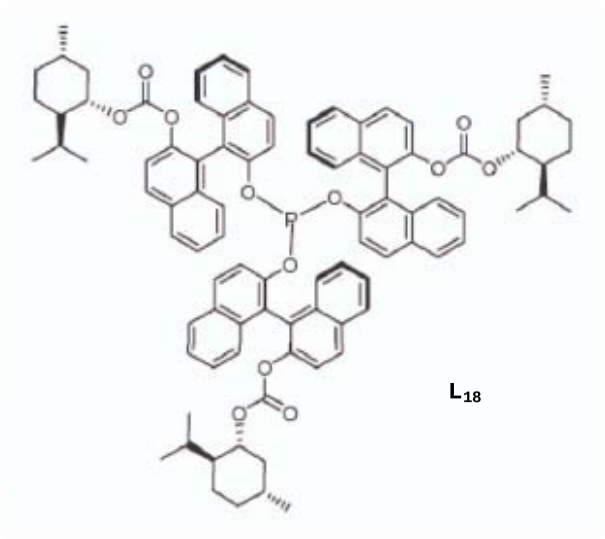
7.898
7.779
7.348
7.054
6.706
4.260
1.777
1.608
1.245
0.829
0.715
0.470
9.10
15.12
4.67
4.36
2.68
10.34
10.77
32.67
3.28
ppm



L_{18}

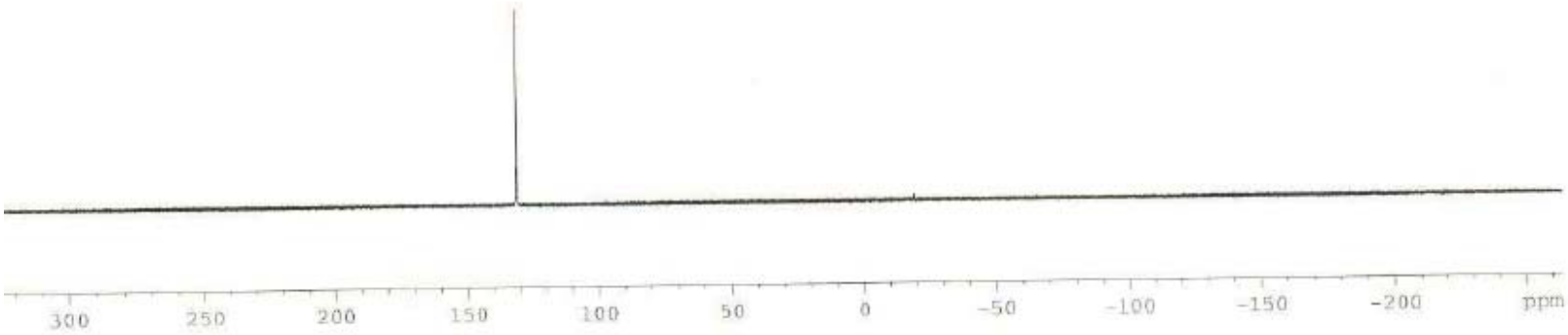
NAME	06-22-09-AG02-p32-co1
EXPNO	3
PROCNO	1
DU	/u
USER	GonsalesA
Date_	20090622
Time	18.06
INSTRUM	AVQ-400
PROBHD	5 mm QNP 1H/13
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	82
DS	0
SWH	24038.461 Hz
FIDRES	0.366798 Hz
AQ	1.3632196 sec
RG	16384
DW	20.800 usec
DE	6.00 usec
TE	293.1 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	8.50 usec
PL1	-2.00 dB
PL1W	47.77286148 W
SFO1	100.6228298 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	70.00 usec
PL2	0.00 dB
PL12	15.00 dB
PL13	17.00 dB
PL2W	9.54516888 W
PL12W	0.30184472 W
PL13W	0.19045115 W
SFO2	400.1316000 MHz
SI	32768
SF	100.6127851 MHz
WDW	EM
SSB	0
LB	1.50 Hz
GB	0
PC	1.40

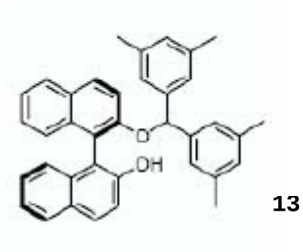




L_{18}

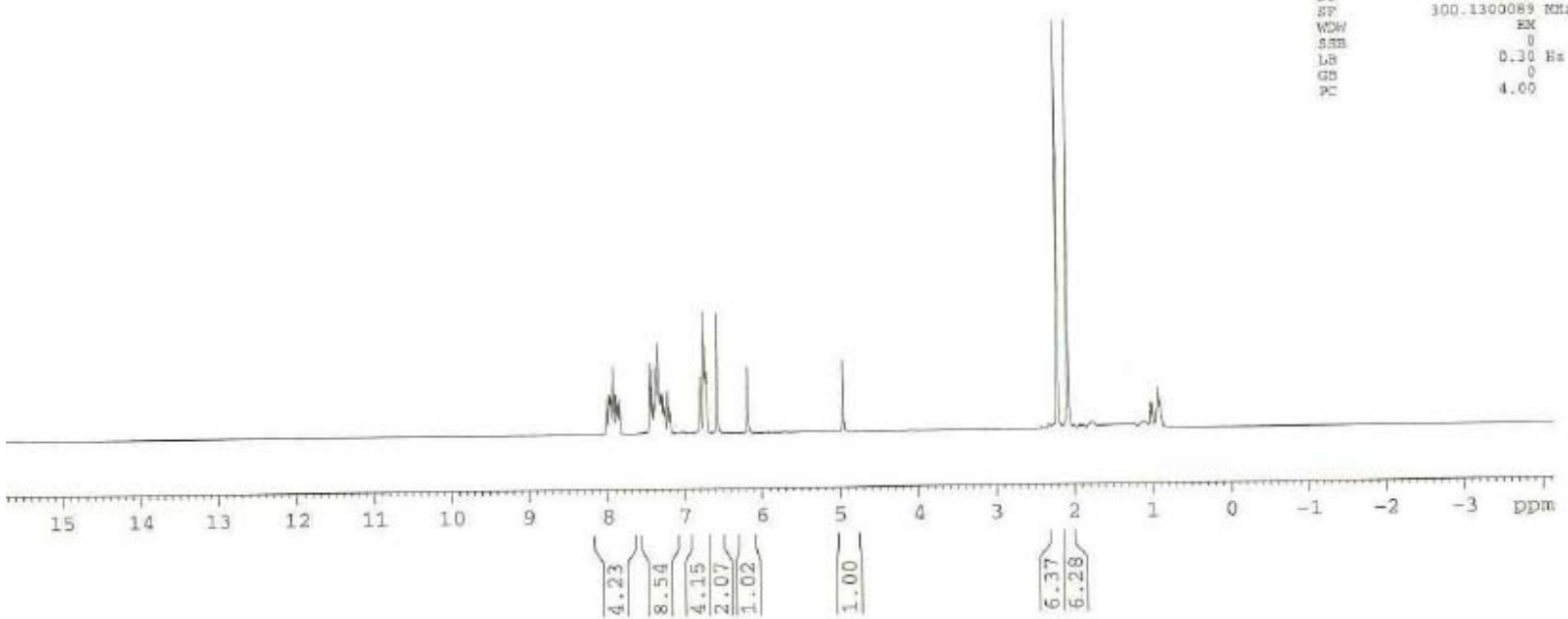
NAME	06-22-09-A003-p32-col
EXPNO	2
PROCNO	1
DU	/u
USER	GonzalezA
Date_	20090622
Time	16.01
INSTRUM	AVQ-400
PROBHD	5 mm QNP 1H/13
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	12
DS	0
SWH	97087.375 Hz
FIDRES	1.481436 Hz
AQ	0.3375655 sec
RG	8192
DW	5.150 usec
DE	6.00 usec
TE	292.8 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
========	CHANNEL f1 ========
NUC1	31P
P1	7.70 usec
PL1	-2.00 dB
PL1W	26.27507401 W
SFO1	161.9814041 MHz
========	CHANNEL f2 ========
CPDPRG2	waltz16
NUC2	1H
PCPD2	70.00 usec
PL2	0.00 dB
PL12	15.00 dB
PL13	17.00 dB
PL2W	9.54516888 W
PL12W	0.30184472 W
PL13W	0.19045115 W
SFO2	400.1316005 MHz
SI	65536
SF	161.9755989 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

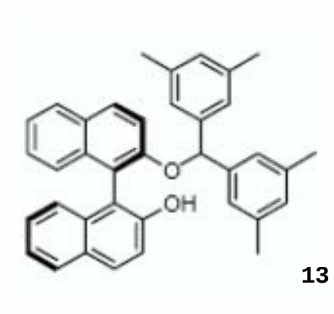




13

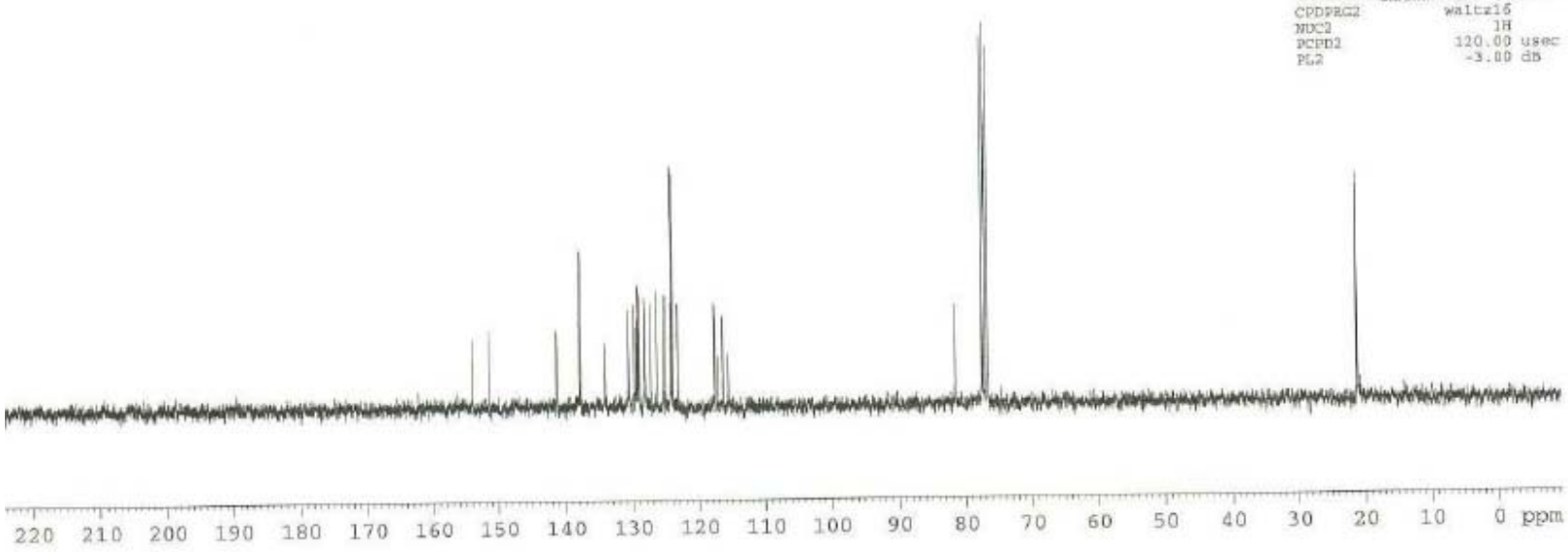
```
NAME            04-30-09-Ether-col
EXPNO                            1
PROCNO                           1
Date_                     20090430
Time                         18.31
INSTRUM                      av-300
PROBHD     5 mm Dual 13C/
PULPROG                       zg30
TD                           65536
SOLVENT                      CDCl3
NS                               7
DS                               0
SWH                    6172.839 Hz
FIDRES                 0.094190 Hz
AQ                     5.3084660 sec
RG                           101.6
DW                      81.000 usec
DE                       6.00 usec
TE                       300.0 K
D1                    0.20000000 sec
MCREST                0.00000000 sec
MCWRK                 0.01500000 sec

-------- CHANNEL f1 --------
NUC1                         1H
P1                      11.00 usec
PL1                      -3.00 dB
SFO1           300.1318533 MHz
SI                       32768
SF             300.1300089 MHz
WDW                         EM
SSB                          0
LB                      0.30 Hz
GB                           0
PC                        4.00
```

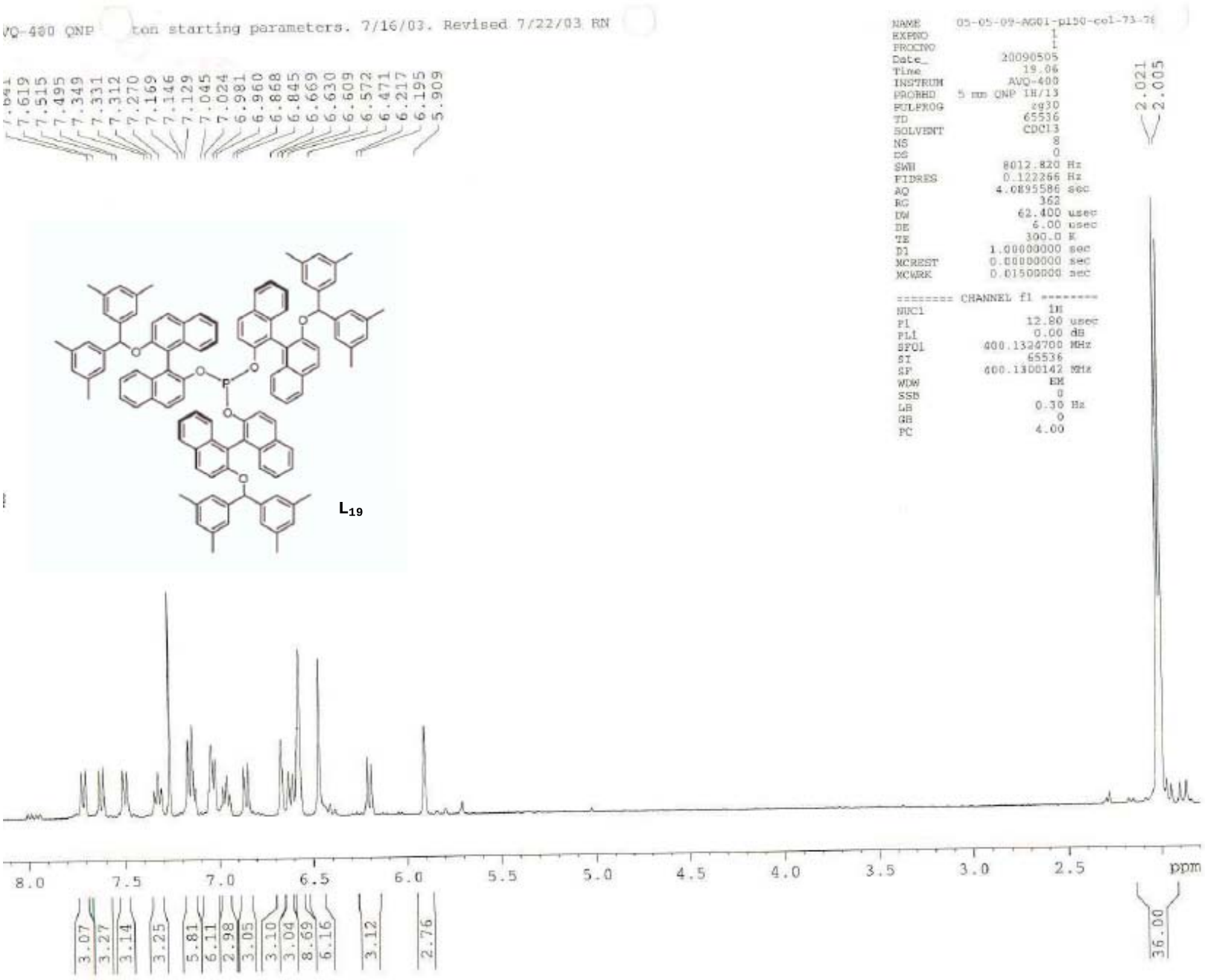




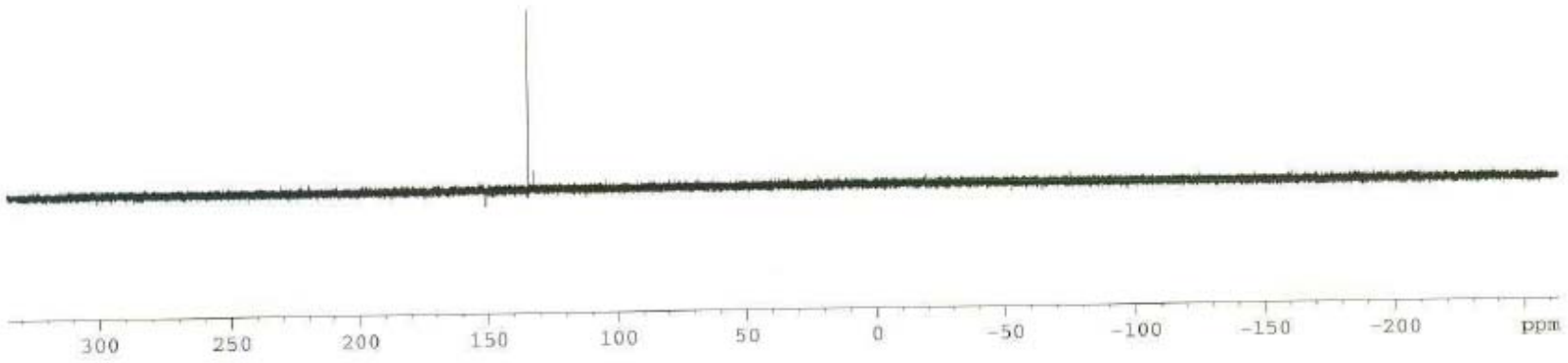
13

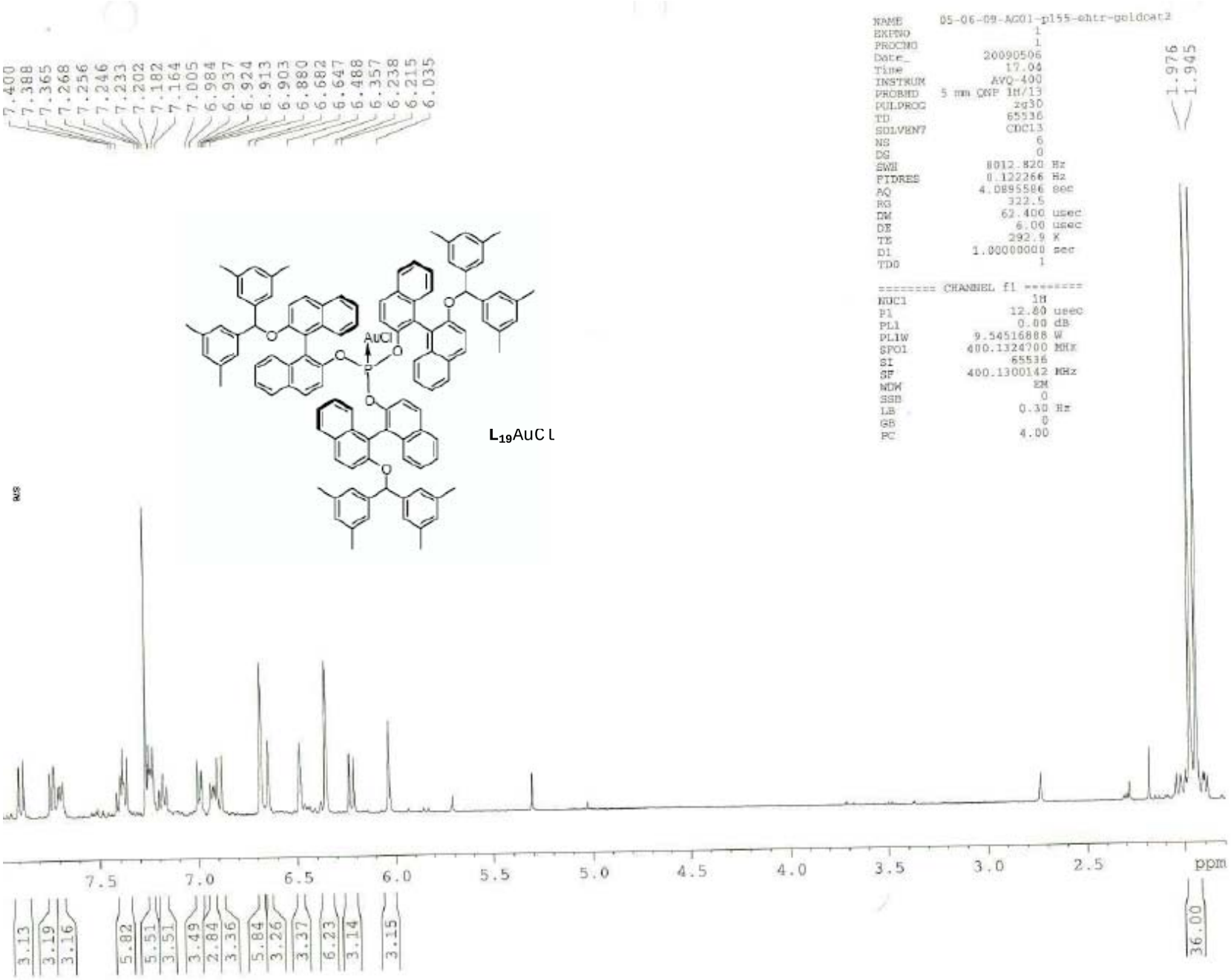
NAME	04-30-09-Ether-col
EXPNO	2
PROCNO	1
Date_	20090430
Time	18.32
INSTRUM	av-300
PROBHD	5 mm Dual 13C/
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	148
DS	0
SWH	17985.611 Hz
FIDRES	0.274439 Hz
AQ	1.8219508 sec
RG	32768
DW	27.800 usec
DE	6.00 usec
TE	300.0 K
D1	1.00000000 sec
d11	0.03000000 sec
DELTA	0.89999998 sec
MCREST	0.00000000 sec
MCWRK	0.01500000 sec
======== CHANNEL f1 ========	
NUC1	13C
P1	10.50 usec
PL1	0.00 dB
SFO1	75.4760505 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	120.00 usec
PL2	-3.00 dB

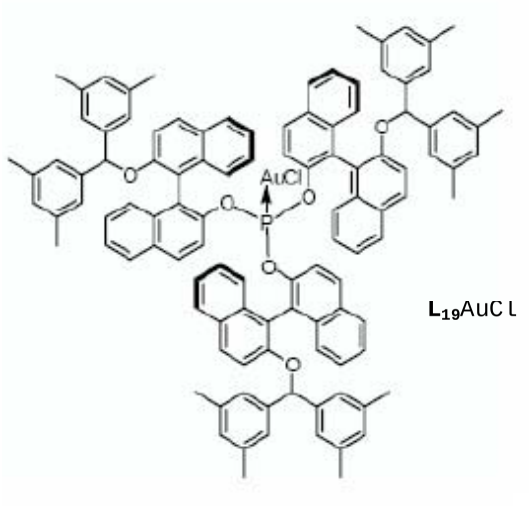



VQ-400 QNP ton starting parameters. 7/16/03. Revised 7/22/03 RN
7.619
7.515
7.495
7.349
7.331
7.312
7.270
7.169
7.146
7.129
7.045
7.024
6.981
6.960
6.868
6.845
6.669
6.630
6.609
6.572
6.471
6.217
6.195
5.909
NAME 05-05-09-AG01-p150-col-73-78
EXPNO 1
PROCNO 1
Date_ 20090505
Time 19.06
INSTRUM AVQ-400
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0895586 sec
RG 362
DW 62.400 usec
DE 6.00 usec
TE 300.0 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 12.80 usec
PL1 0.00 dB
SFO1 400.1324700 MHz
SI 65536
SF 400.1300142 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 4.00
2.021
2.005
L19
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
ppm
3.07
3.27
3.14
3.25
5.81
6.11
2.98
3.05
3.10
3.04
8.69
6.16
3.12
2.76
36.00

NAME	05-05-09-AG01-p150-r
EXPNO	2
PROCNO	1
Date_	20090505
Time	19.08
INSTRUM	AVQ-400
PROBHD	5 mm QNP 1H/13
PULPROG	zgpg30
TD	65536
SOLVENT	C6D6
NS	32
DS	0
SWH	97087.375 Hz
FIDRES	1.481436 Hz
AQ	0.3375655 sec
RG	8192
DW	5.150 usec
DE	6.00 usec
TE	300.6 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
MCREST	0.00000000 sec
MCWRK	0.01500000 sec
======== CHANNEL f1 ========	
NUC1	31P
P1	7.70 usec
PL1	-2.00 dB
SFO1	161.9814041 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	70.00 usec
PL2	0.00 dB



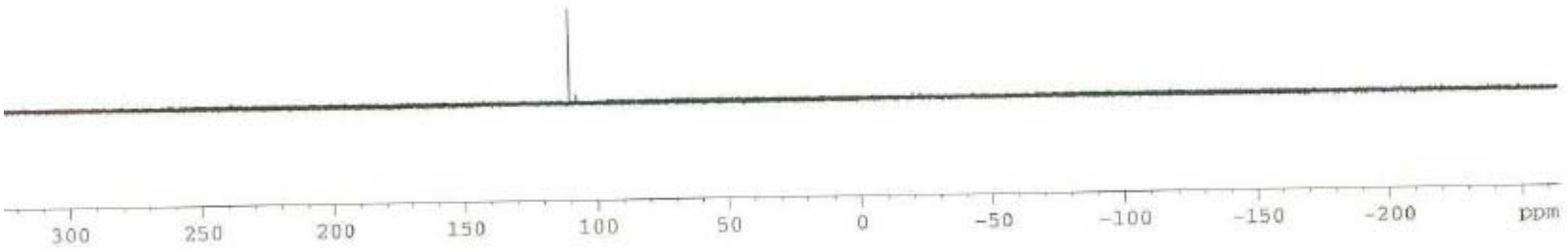

7.400
7.388
7.365
7.268
7.256
7.246
7.233
7.202
7.182
7.164
7.005
6.984
6.937
6.924
6.913
6.903
6.880
6.682
6.647
6.488
6.357
6.238
6.215
6.035
AuCl
L19AuCl
NAME 05-06-09-AG01-pl55-ehtr-goldcat2
EXPNO 1
PROCNO 1
Date_ 20090506
Time 17.04
INSTRUM AVQ-400
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 6
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0895586 sec
RG 322.5
DW 62.400 usec
DE 6.00 usec
TE 292.9 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 12.80 usec
PL1 0.00 dB
PL1W 9.54516888 W
SFO1 400.1324700 MHz
SI 65536
SF 400.1300142 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 4.00
1.976
1.945
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
ppm
3.13
3.19
3.16
5.82
5.51
3.51
3.49
2.84
3.36
5.84
3.26
3.37
6.23
3.14
3.15
36.00

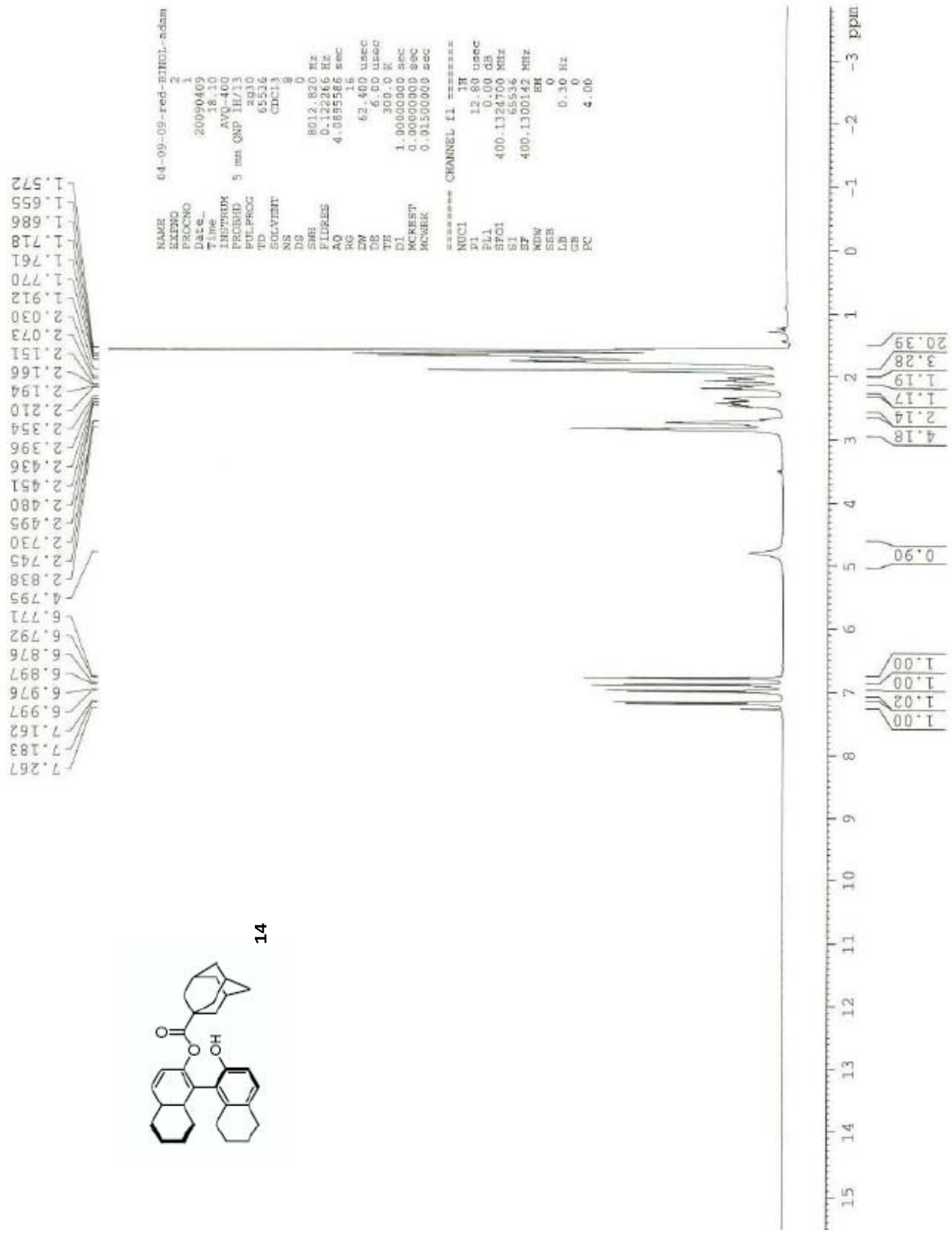


$L_{19}AuCl$

110.56

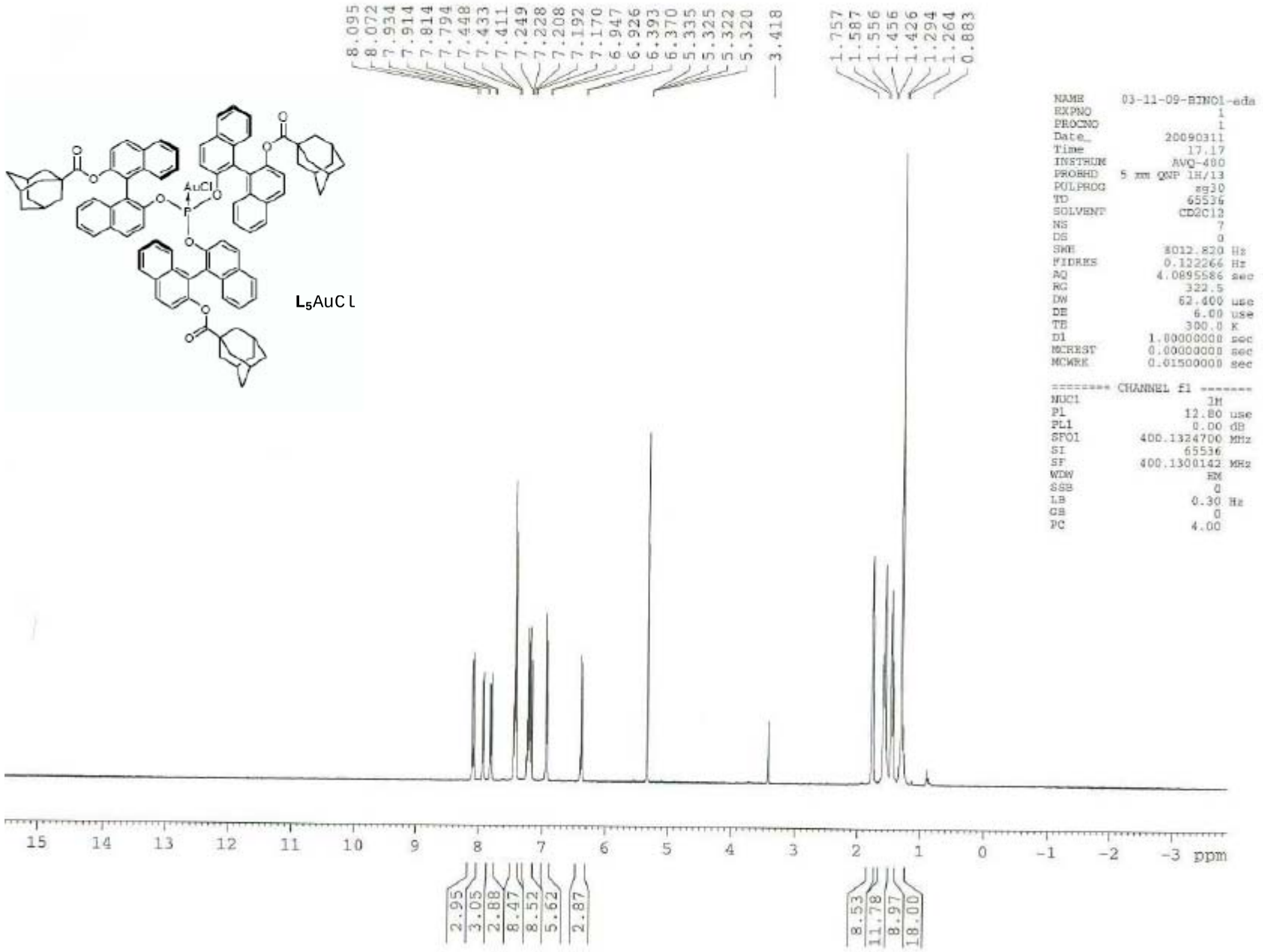
```
NAME          05-06-09-AG01-pl55-ehtr-gold
EXPNO                    2
PROCNO                   1
Date_             20090506
Time                 17.05
INSTRUM           AVQ-400
PROBHD  5 mm QNP 1H/13
PULPROG           zgpg30
TD                  65536
SOLVENT             CDCl3
NS                     27
DS                      0
SWH           97087.375 Hz
FIDRES        1.481436 Hz
AQ            0.3375655 sec
RG                   8192
DW                5.150 usec
DE                6.00 usec
TE                292.9 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                   31P
P1                    7.70 usec
PL1                  -2.00 dB
PL1W        26.27507401 W
SFO1        161.9814041 MHz

======== CHANNEL f2 ========
CPDPRG2             waltz16
NUC2                    1H
PCPD2                 70.00 usec
PL2                   0.00 dB
PL12                 15.00 dB
```

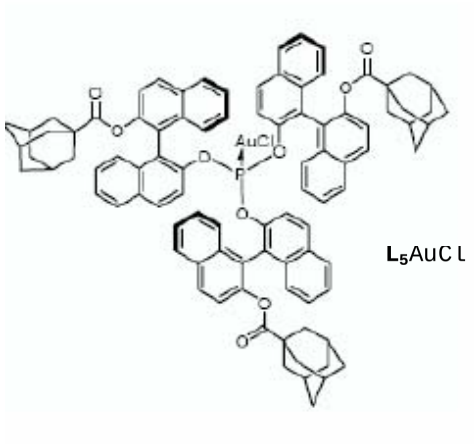



64-09-09-red-BINOL-adam
NAME
EXPNO
PROCNO
Date_
Time
INSTRUM
PROBHD
PULPROG
TD
SOLVENT
NS
DS
SWH
FIDRES
AQ
RG
DW
DB
TE
D1
MCREST
MCWREK
======== CHANNEL f1 ========
NUC1
P1
PL1
SFO1
SI
SF
WDW
SSB
LB
GB
PC
1H
12.80 usec
0.00 dB
400.1324700 MHz
65536
400.1300142 MHz
EM
0
0.30 Hz
0
4.00
8012.820 Hz
0.122266 Hz
4.0895586 sec
16
62.400 usec
6.00 usec
300.0 K
1.00000000 sec
0.00000000 sec
0.01500000 sec
5 mm QNP 1H/13
2930
65536
CDCl3
8
0
7.267
7.183
7.162
6.997
6.976
6.897
6.876
6.792
6.771
4.795
2.838
2.745
2.730
2.495
2.480
2.451
2.436
2.396
2.354
2.210
2.194
2.166
2.151
2.073
2.030
1.912
1.770
1.761
1.718
1.686
1.655
1.572
0.90
4.18
2.14
1.17
1.19
3.28
20.39
1.00
1.00
1.02
1.00
ppm

14


14
OH
O
O
177.20
150.66
147.09
138.16
135.81
135.68
130.18
129.64
129.36
127.88
122.49
119.28
114.00
77.32
77.00
76.68
40.51
38.13
36.28
29.58
29.31
27.69
27.18
26.78
23.21
23.14
22.76
22.62
ppm


8.095
8.072
7.934
7.914
7.814
7.794
7.448
7.433
7.411
7.249
7.228
7.208
7.192
7.170
6.947
6.926
6.393
6.370
5.335
5.325
5.322
5.320
3.418
1.757
1.587
1.556
1.456
1.426
1.294
1.264
0.883
AuCl
P
L5AuCl
NAME 03-11-09-BINOl-eda
EXPNO 1
PROCNO 1
Date_ 20090311
Time 17.17
INSTRUM AVQ-400
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 65536
SOLVENT CD2Cl2
NS 7
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0895586 sec
RG 322.5
DW 62.400 use
DE 6.00 use
TE 300.0 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 =======
NUC1 1H
P1 12.80 use
PL1 0.00 dB
SFO1 400.1324700 MHz
SI 65536
SF 400.1300142 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 4.00
15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3 ppm
2.95
3.05
2.88
8.47
8.52
5.62
2.87
8.53
11.78
8.97
18.00

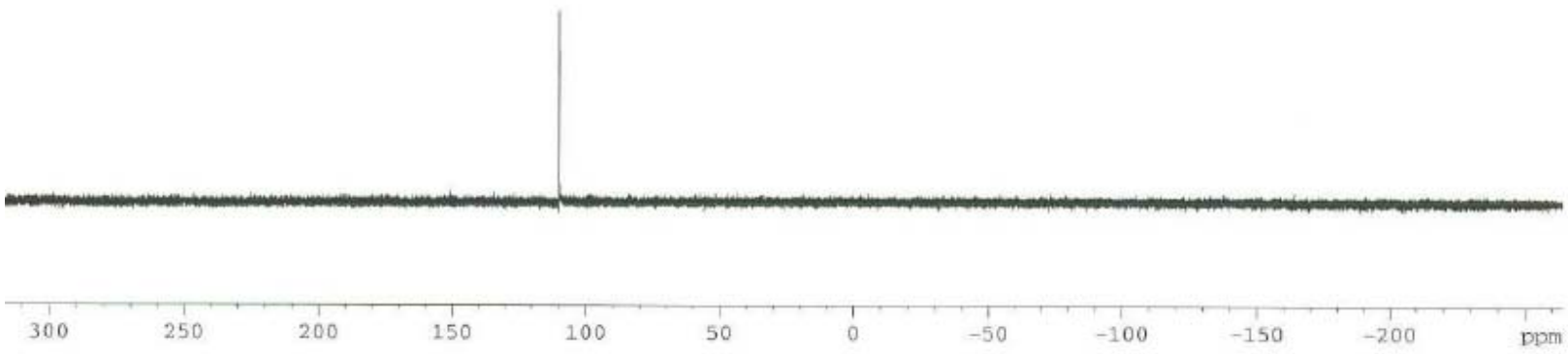


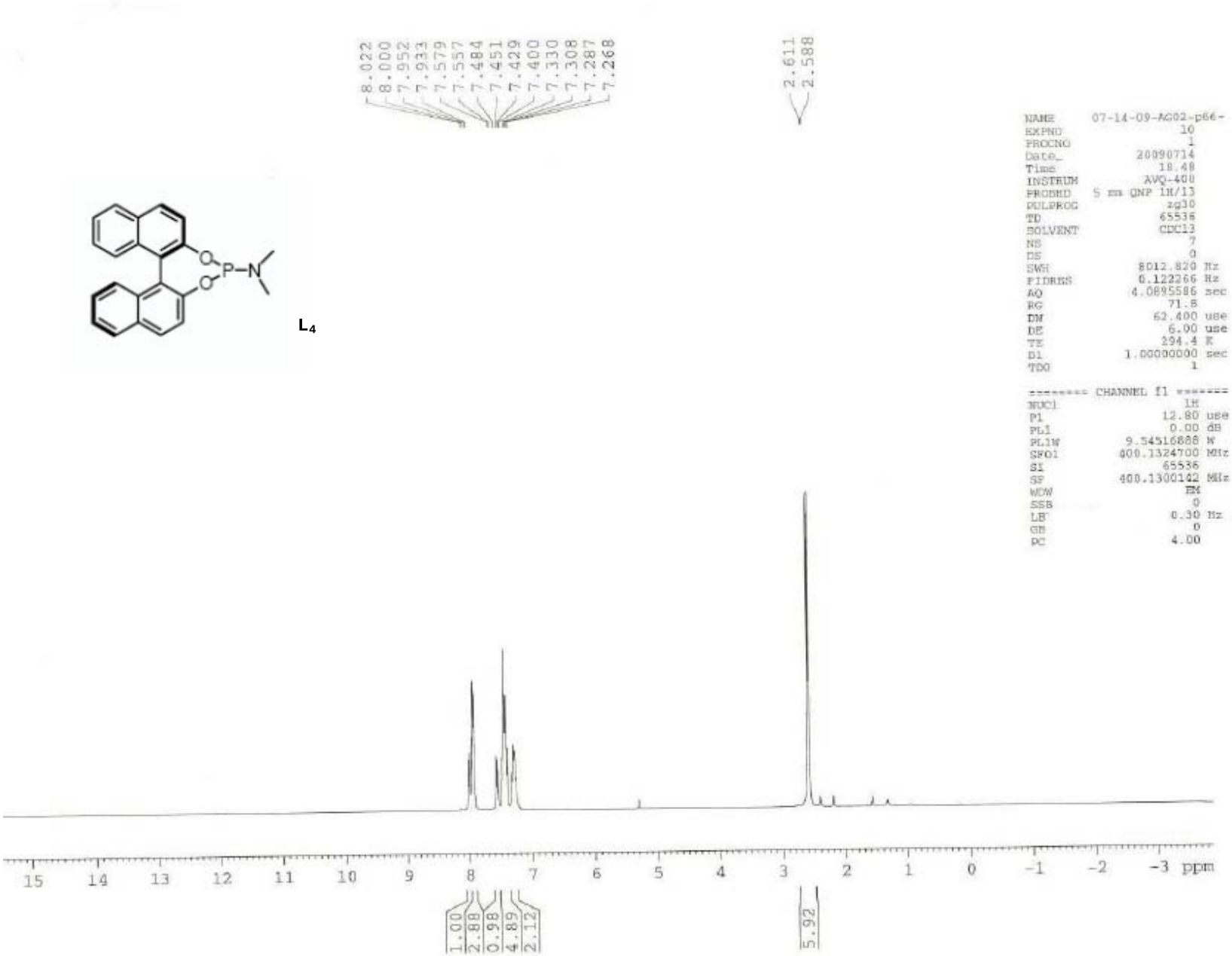
L_5AuCl

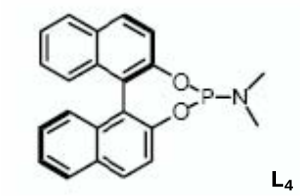
150.64

109.70

NAME	03-11-09-BINO1-adam-
EXPNO	3
PROCNO	1
Date_	20090311
Time	17.18
INSTRUM	AVQ-400
PROBHD	5 mm QNP 1H/13
PULPROG	zgpg30
TD	65536
SOLVENT	C6D6
NS	32
DS	0
SWH	97087.375 Hz
FIDRES	1.481436 Hz
AQ	0.3375655 sec
RG	8192
DW	5.150 usec
DE	6.00 usec
TE	300.0 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
MCREST	0.00000000 sec
MCWRK	0.01500000 sec
======== CHANNEL f1 ========	
NUC1	31P
P1	7.70 usec
PL1	-2.00 dB
SFO1	161.9814041 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	70.00 usec
PL2	0.00 dB



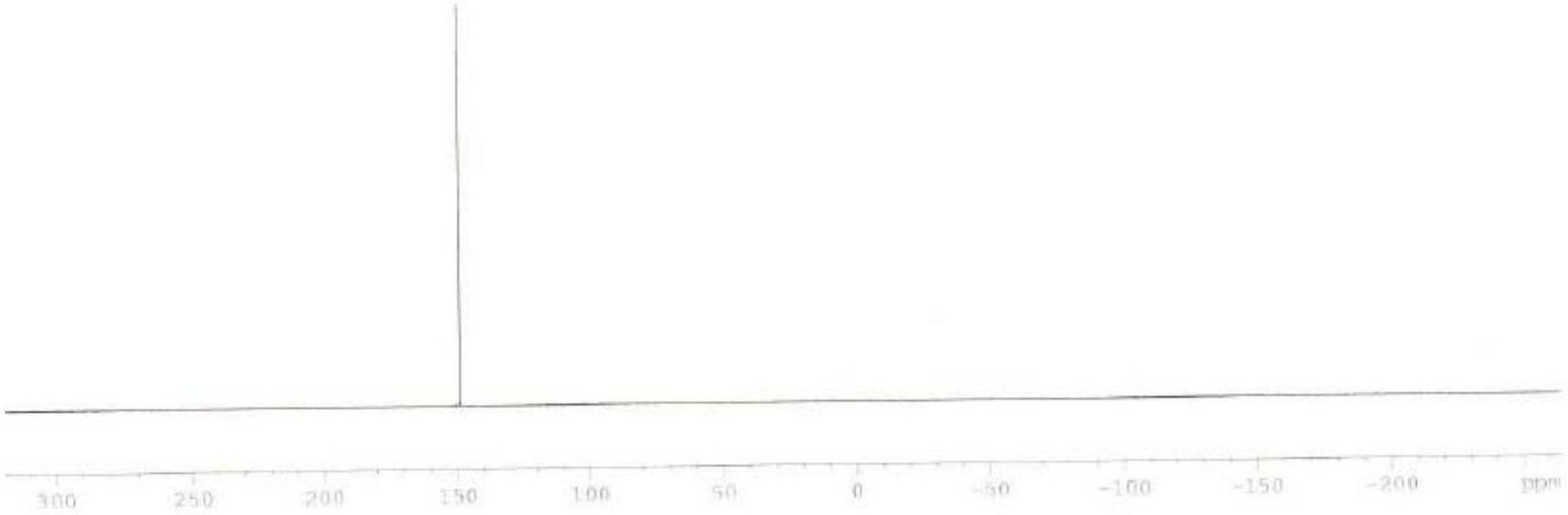

8.022
8.000
7.952
7.933
7.579
7.557
7.484
7.451
7.429
7.400
7.330
7.308
7.287
7.268
2.611
2.588
L4
NAME 07-14-09-AC02-p66-
EXPNO 10
PROCNO 1
Date_ 20090714
Time 18.48
INSTRUM AVQ-400
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 7
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0895586 sec
RG 71.5
DW 62.400 use
DE 6.00 use
TE 294.4 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 =======
NUC1 1H
P1 12.80 use
PL1 0.00 dB
PL1W 9.54516888 W
SFO1 400.1324700 MHz
SI 65536
SF 400.1300142 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 4.00
15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3 ppm
1.00
2.88
0.98
4.89
2.12
5.92

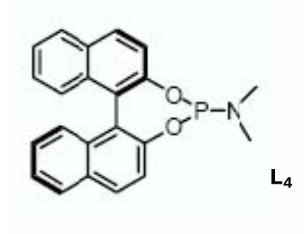


L_4

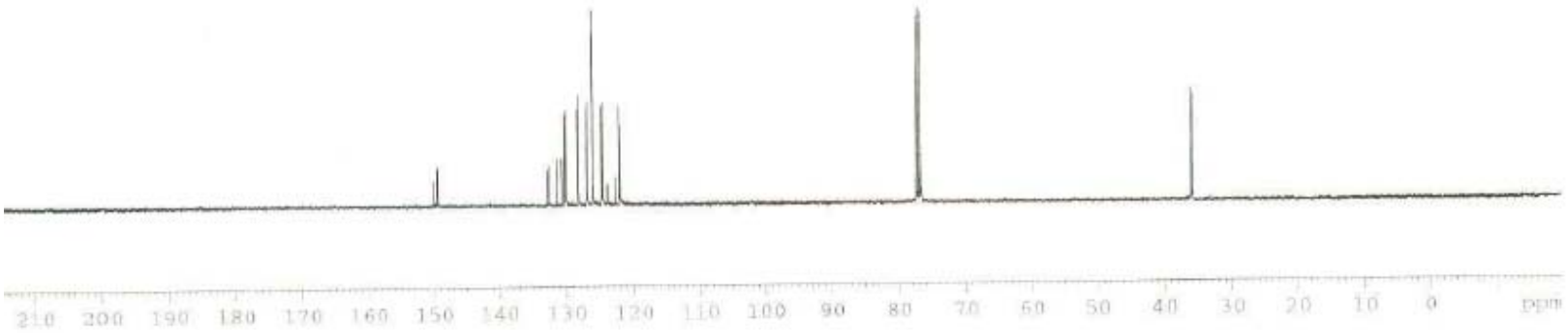
148.75

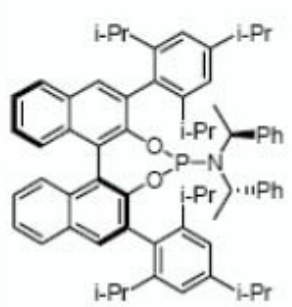
NAME	07-14-09-AG02-p66-cc
EXPNO	11
PROCNO	1
Date_	20090714
Time	18.49
INSTRUM	AVQ-400
PROBHD	5 mm QNP 1H/13
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	10
DS	0
SWH	97087.375 Hz
FIDRES	1.481436 Hz
AQ	0.3375655 sec
RG	8192
DW	5.150 usec
DE	6.00 usec
TE	294.4 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	31P
P1	7.70 usec
PL1	-2.00 dB
PL1W	26.27507401 W
SFO1	161.9814041 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	70.00 usec
PL2	0.00 dB
PL12	15.00 dB



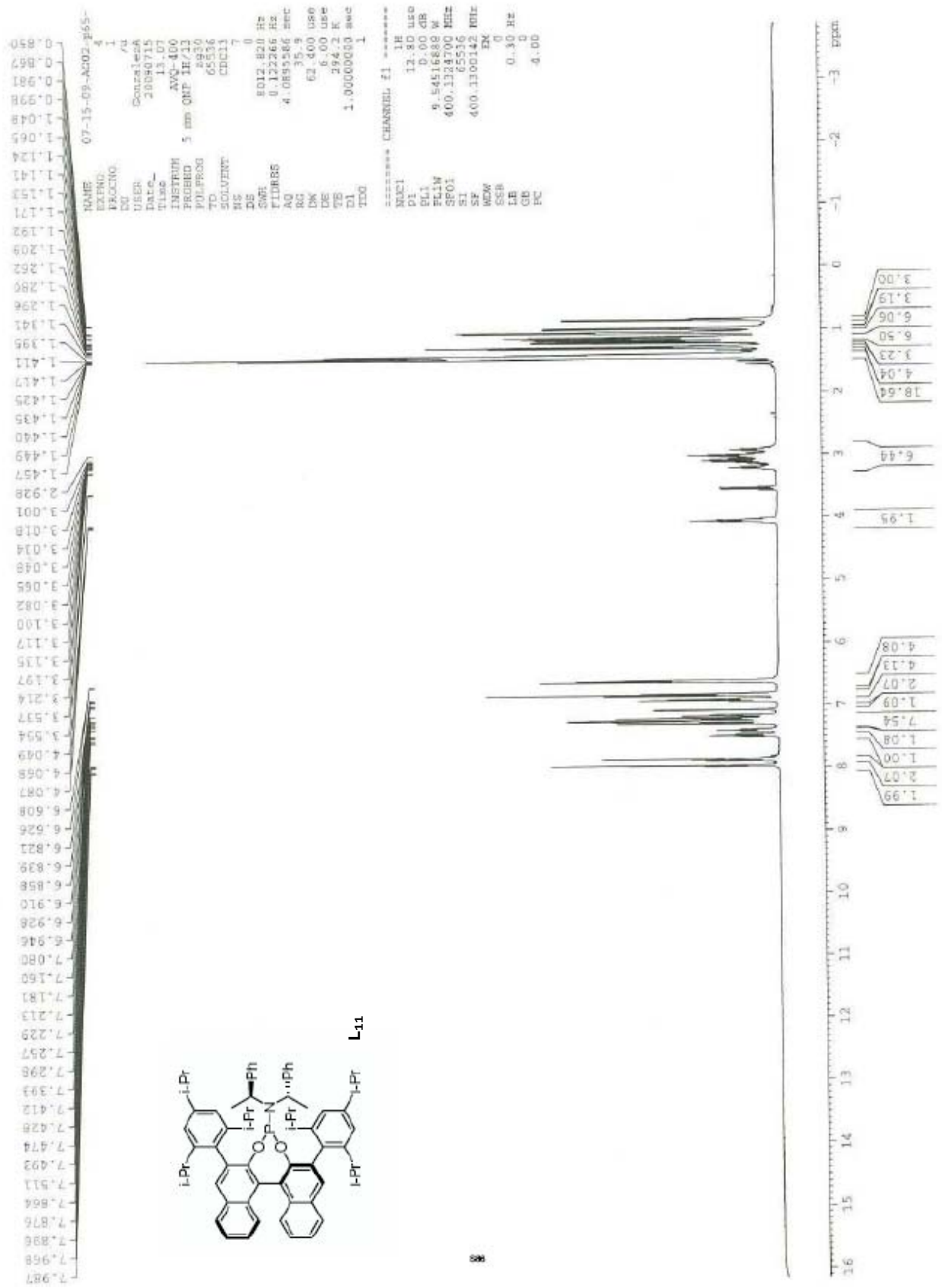


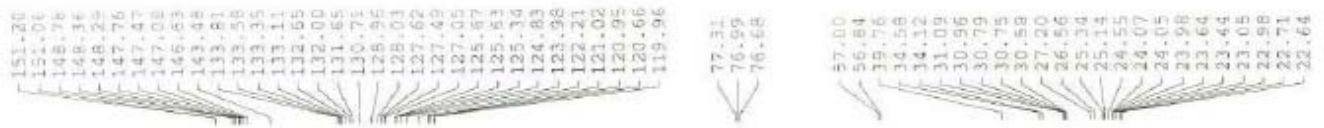

```
NAME          07-14-09-AG02-p66-c
EXPNO                      12
PROCNO                      1
Date_                20090714
Time                    18.50
INSTRUM                AVQ-400
PROBHD    5 mm QNP 1H/13
PULPROG                zgpg30
TD                      65536
SOLVENT                 CDCl3
NS                        127
DS                          0
SWH                24038.461 Hz
FIDRES             0.366798 Hz
AQ                 1.3632196 sec
RG                      16384
DW                   20.800 usec
DE                    6.00 usec
TE                   294.5 K
D1                2.00000000 sec
D11               0.03000000 sec
TD0                         1

======== CHANNEL f1 ========
NUC1                      13C
P1                     8.50 usec
PL1                   -2.00 dB
PL1W          47.77286148 W
SFO1          100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2                waltz16
NUC2                       1H
PCPD2                 70.00 usec
PL2                    0.00 dB
PL12                  15.00 dB
```

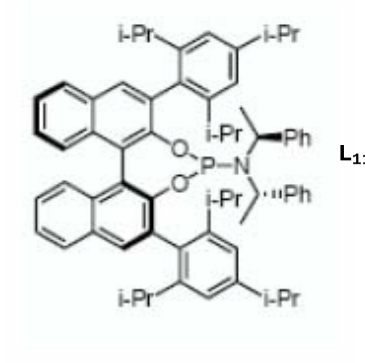




L_{11}

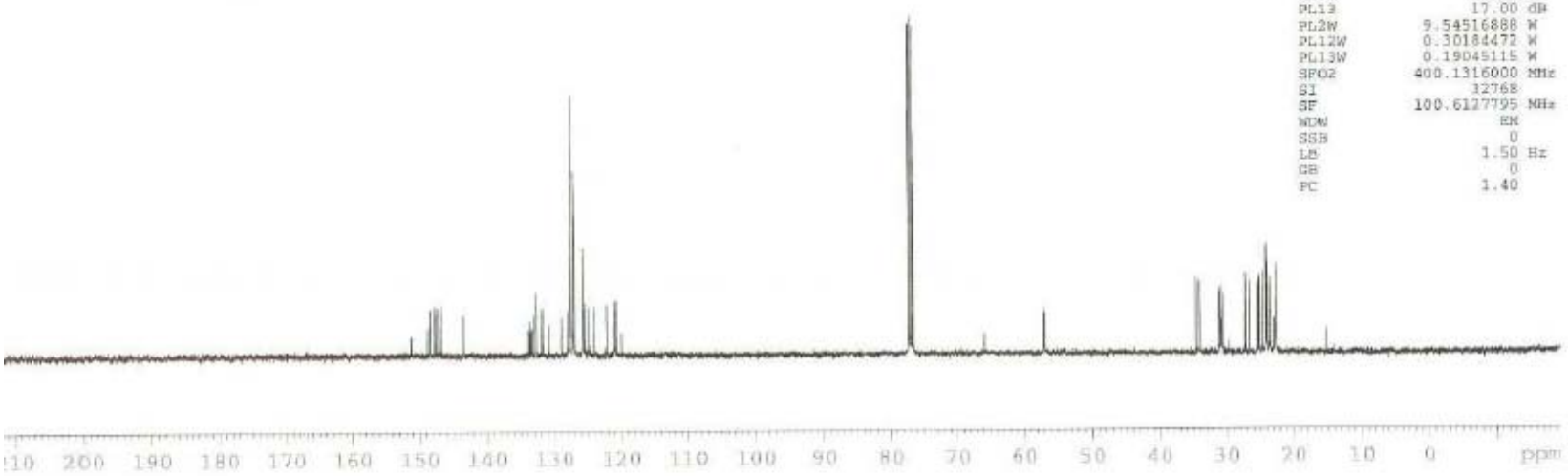

L11
i-Pr
i-Ph
i-Pr
i-Ph
i-Pr
i-Pr
i-Pr
i-Pr
ppm

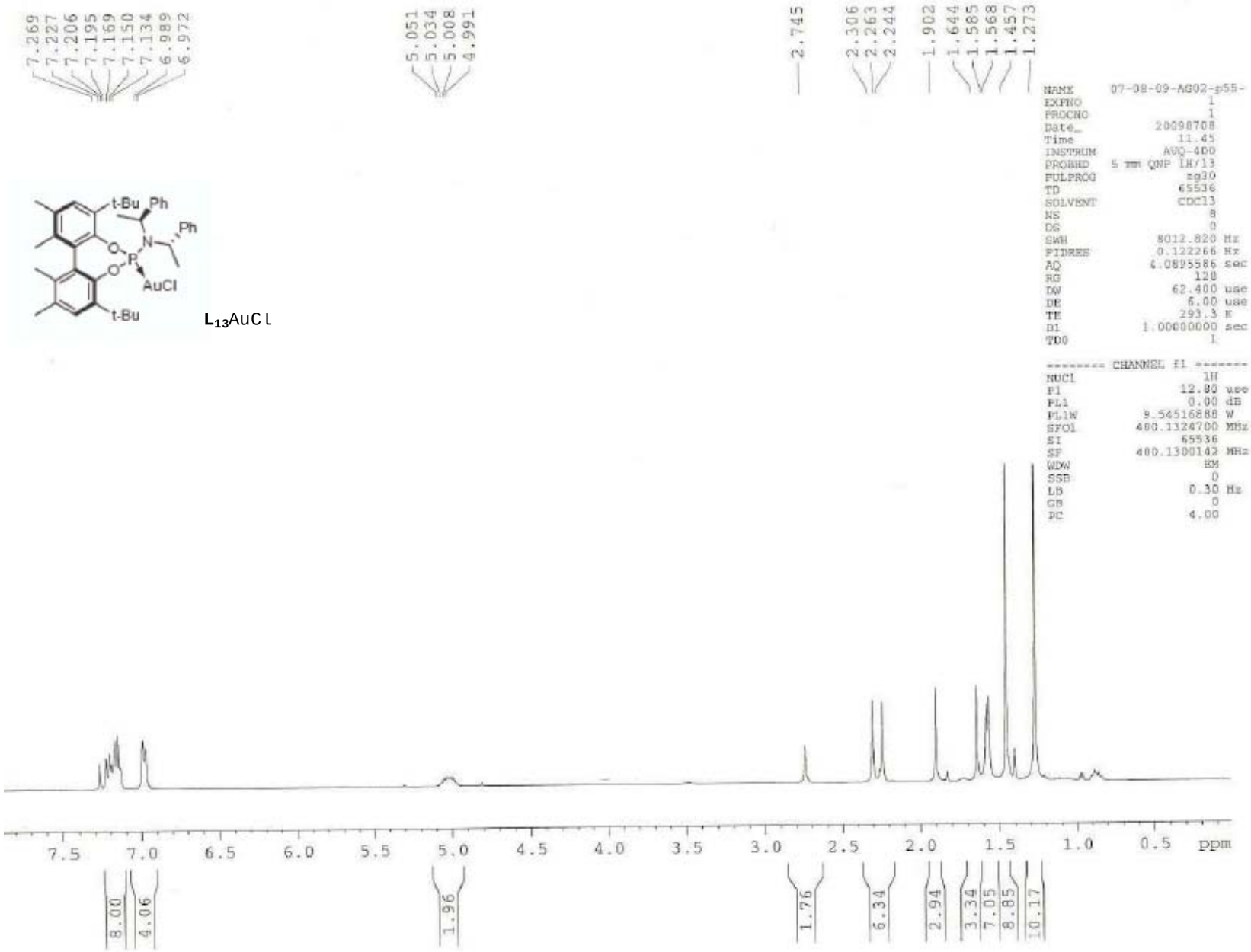


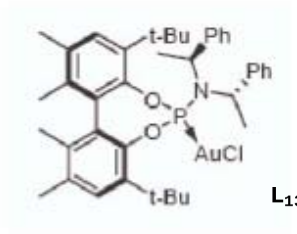


L_{11}

```
NAME            07-15-09-AG02-p65-co
EXPNO                              5
PROCNO                             1
DU                                 /u
USER                      GonzalezA
Date_                      20090715
Time                          13.13
INSTRUM                    AVQ-400
PROBHD     5 mm QNP 1H/13
PULPROG                    zgpg30
TD                             65536
SOLVENT                      CDCl3
NS                               126
DS                                 0
SWH                    24038.461 Hz
FIDRES                  0.366798 Hz
AQ                     1.3632196 sec
RG                             16384
DW                        20.800 usec
DE                         6.00 usec
TE                           294.6 K
D1                     2.00000000 sec
D11                    0.03000000 sec
TD0                                1

======== CHANNEL f1 ========
NUC1                           13C
P1                            8.50 usec
PL1                          -2.00 dB
PL1W                47.77286148 W
SFO1               100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2                    waltz16
NUC2                           1H
PCPD2                        70.00 usec
PL2                           0.00 dB
PL12                         15.00 dB
PL13                         17.00 dB
PL2W                 9.54516888 W
PL12W                0.30184472 W
PL13W                0.19045115 W
SFO2               400.1316000 MHz
SI                         32768
SF                 100.6127795 MHz
WDW                           EM
SSB                            0
LB                          1.50 Hz
GB                             0
PC                          1.40
```



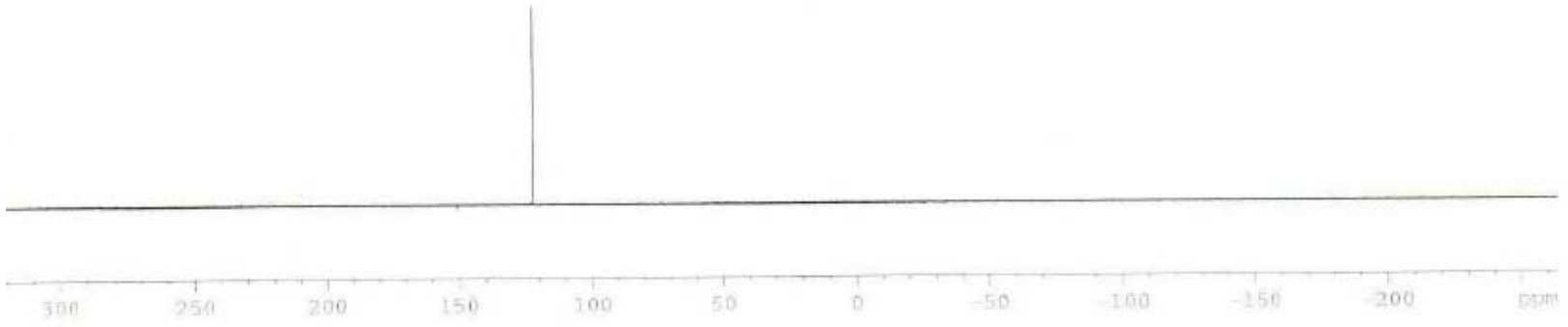

7.269
7.227
7.206
7.195
7.169
7.150
7.134
6.989
6.972
5.051
5.034
5.008
4.991
2.745
2.306
2.263
2.244
1.902
1.644
1.585
1.568
1.457
1.273
t-Bu
Ph
Ph
N
O
O
P
AuCl
t-Bu
L13AuCl
NAME 07-08-09-AG02-p55-
EXPNO 1
PROCNO 1
Date_ 20090708
Time 11.45
INSTRUM AVQ-400
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0895586 sec
RG 128
DW 62.400 usec
DE 6.00 usec
TE 293.3 K
D1 1.00000000 sec
TD0 1
CHANNEL f1
NUC1 1H
P1 12.80 usec
PL1 0.00 dB
PL1W 9.54516888 W
SFO1 400.1324700 MHz
SI 65536
SF 400.1300142 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 4.00
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm
8.00
4.06
1.96
1.76
6.34
2.94
3.34
7.05
8.85
10.17

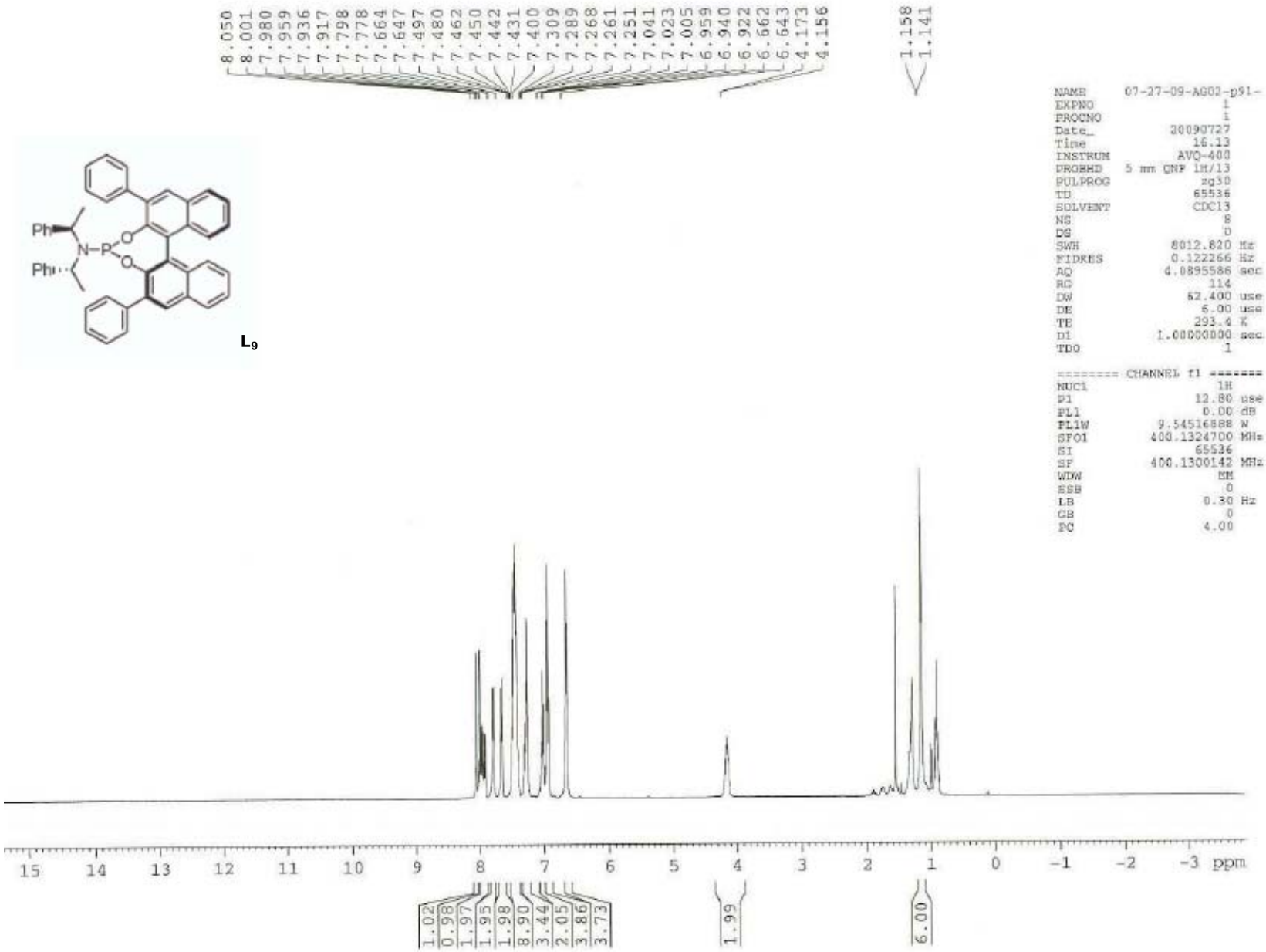


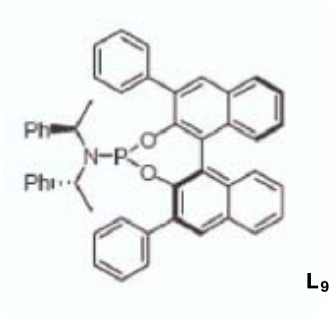
$L_{13}AuCl$

122.34

NAME	07-08-09-AG02-p65-01
EXPNO	2
PROCNO	1
Date_	20090708
Time	11.46
INSTRUM	AVQ-400
PROBHD	5 mm QNP 1H/13
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	13
DS	0
SWH	97087.375 Hz
FIDRES	1.481436 Hz
AQ	0.3375655 sec
RG	8192
DW	5.150 usec
DE	6.00 usec
TE	293.3 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	31P
P1	7.70 usec
PL1	-2.00 dB
PL1W	26.27507401 W
SFO1	161.9814041 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	70.00 usec
PL2	0.00 dB
PL12	15.00 dB



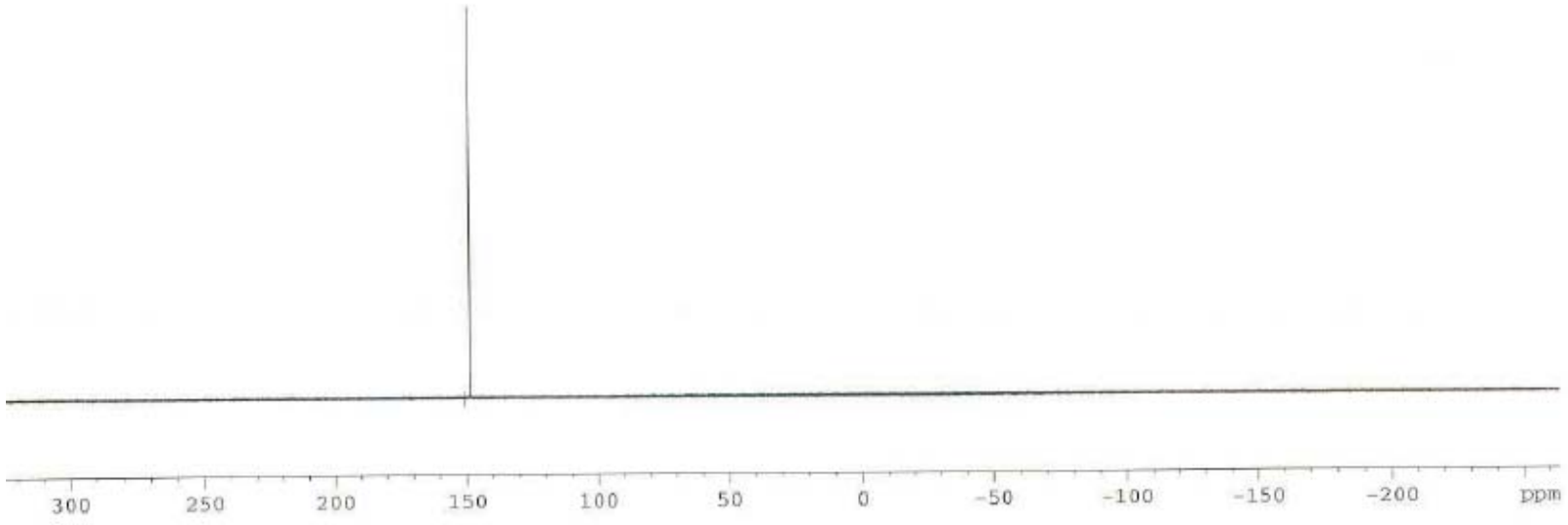

8.050
8.001
7.980
7.959
7.936
7.917
7.798
7.778
7.664
7.647
7.497
7.480
7.462
7.450
7.442
7.431
7.400
7.309
7.289
7.268
7.261
7.251
7.041
7.023
7.005
6.959
6.940
6.922
6.662
6.643
4.173
4.156
1.158
1.141
Ph
N
P
O
O
Ph
L9
NAME 07-27-09-AG02-p91-
EXPNO 1
PROCNO 1
Date_ 20090727
Time 16.13
INSTRUM AVQ-400
PROBHD 5 mm CNP 1H/13
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0895586 sec
RG 114
DW 62.400 use
DE 6.00 use
TE 293.4 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 =======
NUC1 1H
P1 12.80 use
PL1 0.00 dB
PL1W 9.54516888 W
SFO1 400.1324700 MHz
SI 65536
SF 400.1300142 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 4.00
15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3 ppm
1.02
0.98
1.97
1.95
1.98
8.90
3.44
2.05
3.86
3.73
1.99
6.00

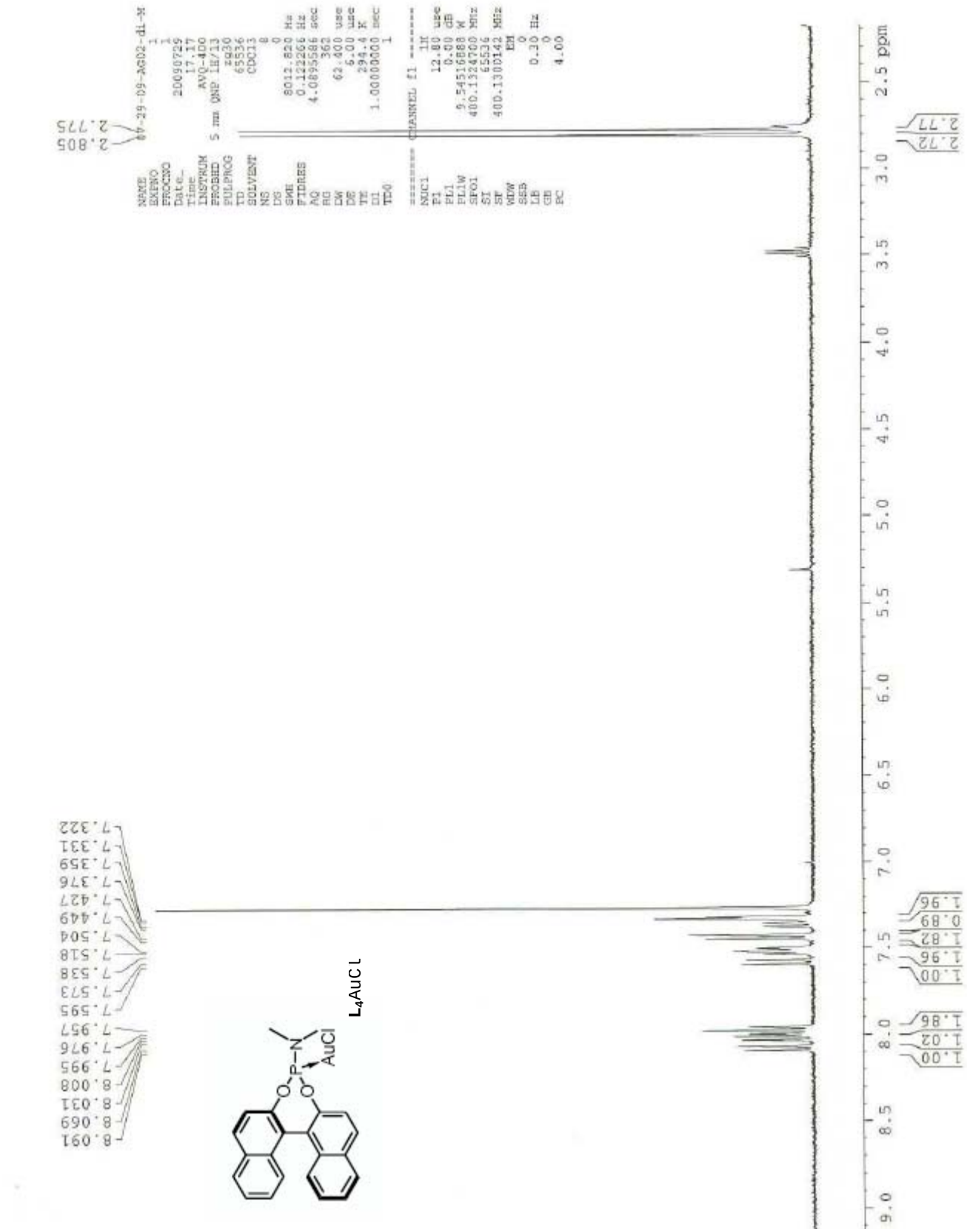


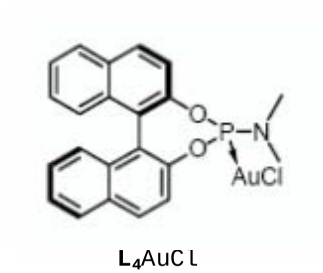
L_9

146.87

NAME	07-27-09-AG02-p91-cc
EXPNO	2
PROCNO	1
Date_	20090727
Time	16.14
INSTRUM	AVQ-400
PROBHD	5 mm QNP 1H/13
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	14
DS	0
SWH	97087.375 Hz
FIDRES	1.481436 Hz
AQ	0.3375655 sec
RG	8192
DW	5.150 usec
DE	6.00 usec
TE	293.4 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	31P
P1	7.70 usec
PL1	-2.00 dB
PL1W	26.27507401 W
SFO1	161.9814041 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	70.00 usec
PL2	0.00 dB
PL12	15.00 dB



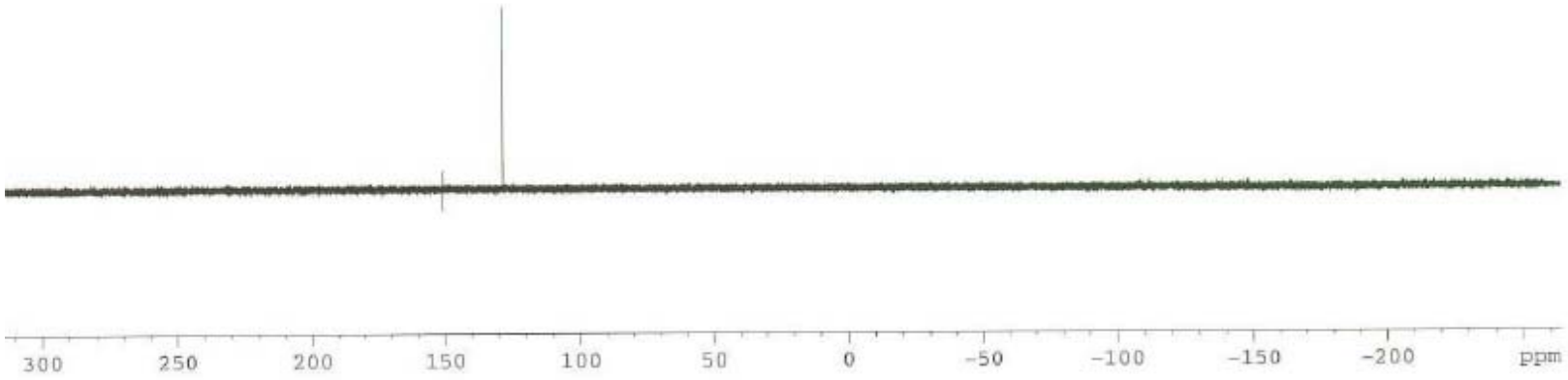

L4AuCl
AuCl
2.775
2.805
7.322
7.331
7.359
7.376
7.427
7.449
7.504
7.518
7.538
7.573
7.595
7.957
7.976
7.995
8.008
8.031
8.069
8.091
2.72
2.77
1.00
1.96
1.82
0.89
1.96
1.00
1.02
1.86
2.5 ppm

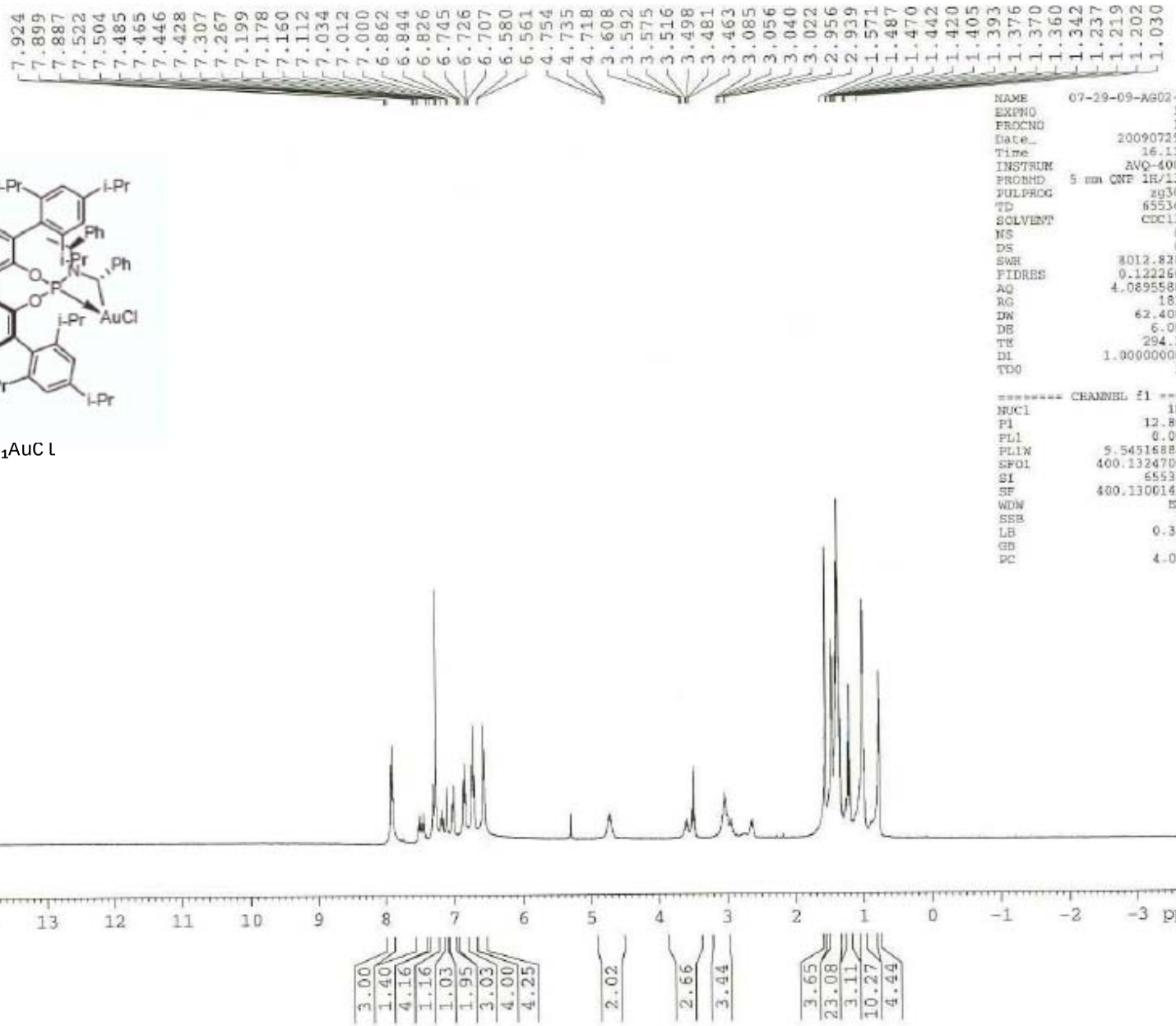


L_4AuCl

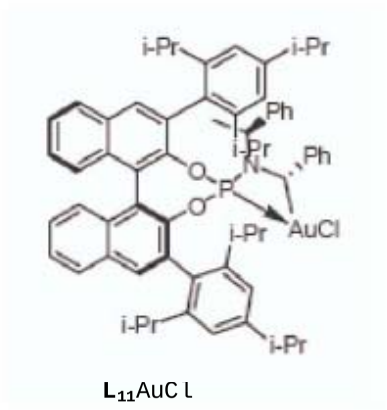
128.18

NAME	07-29-09-AG02-di-Me-
EXPNO	2
PROCNO	1
Date_	20090729
Time	17.18
INSTRUM	AVQ-400
PROBHD	5 mm QNP 1H/13
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	30
DS	0
SWH	97087.375 Hz
FIDRES	1.481436 Hz
AQ	0.3375655 sec
RG	8192
DW	5.150 usec
DE	6.00 usec
TE	294.4 K
D1	1.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	31P
P1	7.70 usec
PL1	-2.00 dB
PL1W	26.27507401 W
SFO1	161.9814041 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	70.00 usec
PL2	0.00 dB
PL12	15.00 dB




7.924
7.899
7.887
7.522
7.504
7.485
7.465
7.446
7.428
7.307
7.267
7.199
7.178
7.160
7.112
7.034
7.012
7.000
6.862
6.844
6.826
6.745
6.726
6.707
6.580
6.561
4.754
4.735
4.718
3.608
3.592
3.575
3.516
3.498
3.481
3.463
3.085
3.056
3.040
3.022
2.956
2.939
1.571
1.487
1.470
1.442
1.420
1.405
1.393
1.376
1.370
1.360
1.342
1.237
1.219
1.202
1.030
i-Pr
i-Pr
Ph
i-Pr
Ph
AuCl
i-Pr
i-Pr
i-Pr
NAME 07-29-09-AG02-TRIP
EXPNO 1
PROCNO 1
Date_ 20090729
Time 16.13
INSTRUM AVQ-400
PROBHD 5 mm CNP 1H/13
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0895586 sec
RG 181
DW 62.400 use
DE 6.00 use
TE 294.2 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 =======
NUC1 1H
P1 12.80 use
PL1 0.00 dB
PL1W 9.54516888 W
SFO1 400.1324700 MHz
SI 65536
SF 400.1300142 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 4.00
15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3 ppm
3.00
1.40
4.16
1.16
1.03
1.95
3.03
4.00
4.25
2.02
2.66
3.44
3.65
23.08
3.11
10.27
4.44

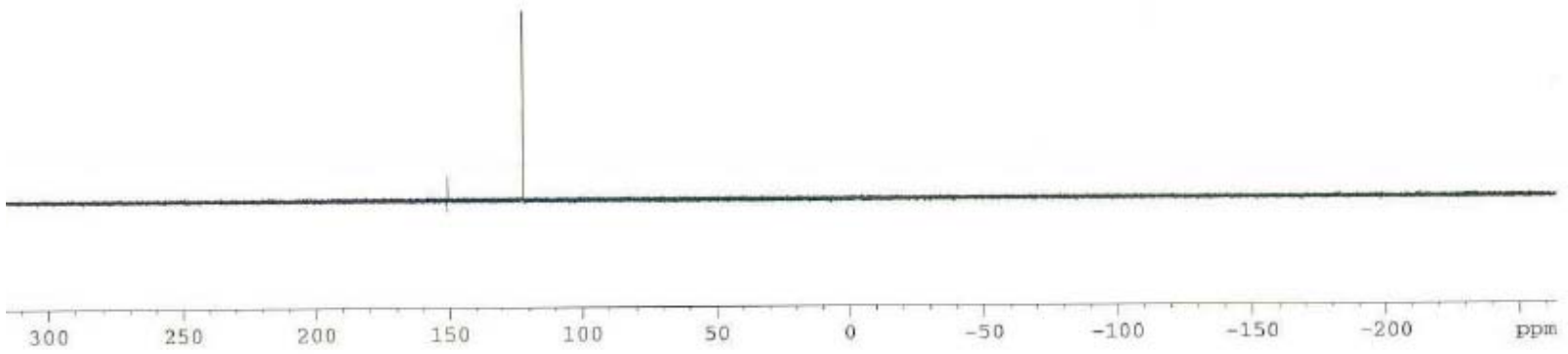
$L_{11}AuCl$

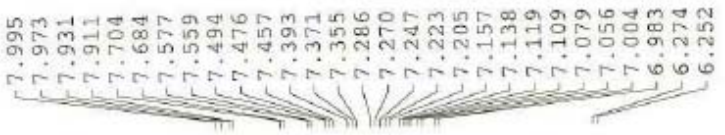


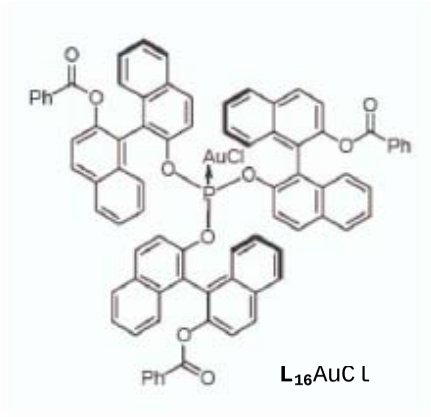
$L_{11}AuCl$

122.08

NAME	07-29-09-AG02-TRIP-A
EXPNO	2
PROCNO	1
Date_	20090729
Time	16.15
INSTRUM	AVQ-400
PROBHD	5 mm QNP 1H/13
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	25
DS	0
SWH	97087.375 Hz
FIDRES	1.481436 Hz
AQ	0.3375655 sec
RG	8192
DW	5.150 usec
DE	6.00 usec
TE	294.3 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	31P
P1	7.70 usec
PL1	-2.00 dB
PL1W	26.27507401 W
SFO1	161.9814041 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	70.00 usec
PL2	0.00 dB
PL12	15.00 dB

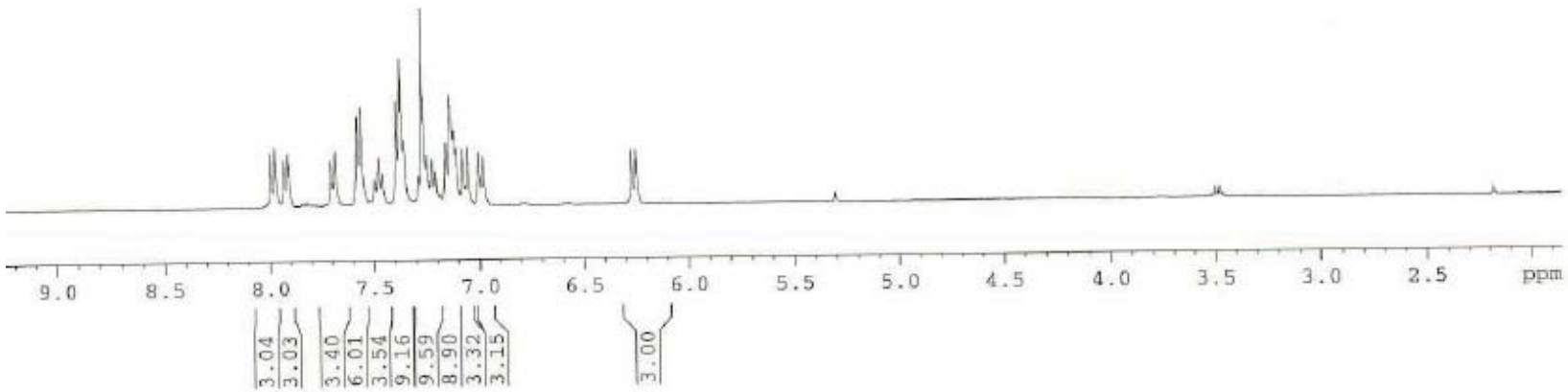


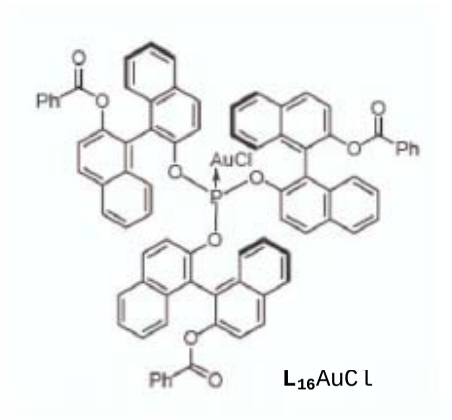




$L_{16}AuCl$

NAME	07-29-09-AGO2-Bn-B
EXPNO	2
PROCNO	1
Date_	20090729
Time	15.46
INSTRUM	AVQ-400
PROBHD	5 mm QNP 1H/13
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	8
DS	0
SWH	8012.820 Hz
FIDRES	0.122266 Hz
AQ	4.0895586 sec
RG	362
DW	62.400 use
DE	6.00 use
TE	294.4 K
D1	1.00000000 sec
TD0	1
========	CHANNEL f1 =======
NUC1	1H
P1	12.80 use
PL1	0.00 dB
PL1W	9.54516888 W
SFO1	400.1324700 MHz
SI	65536
SF	400.1300142 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	4.00

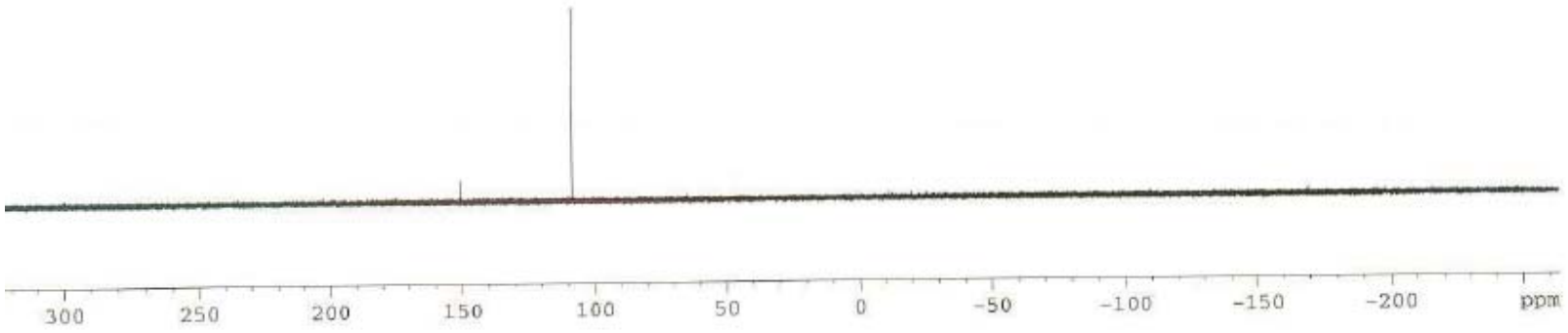


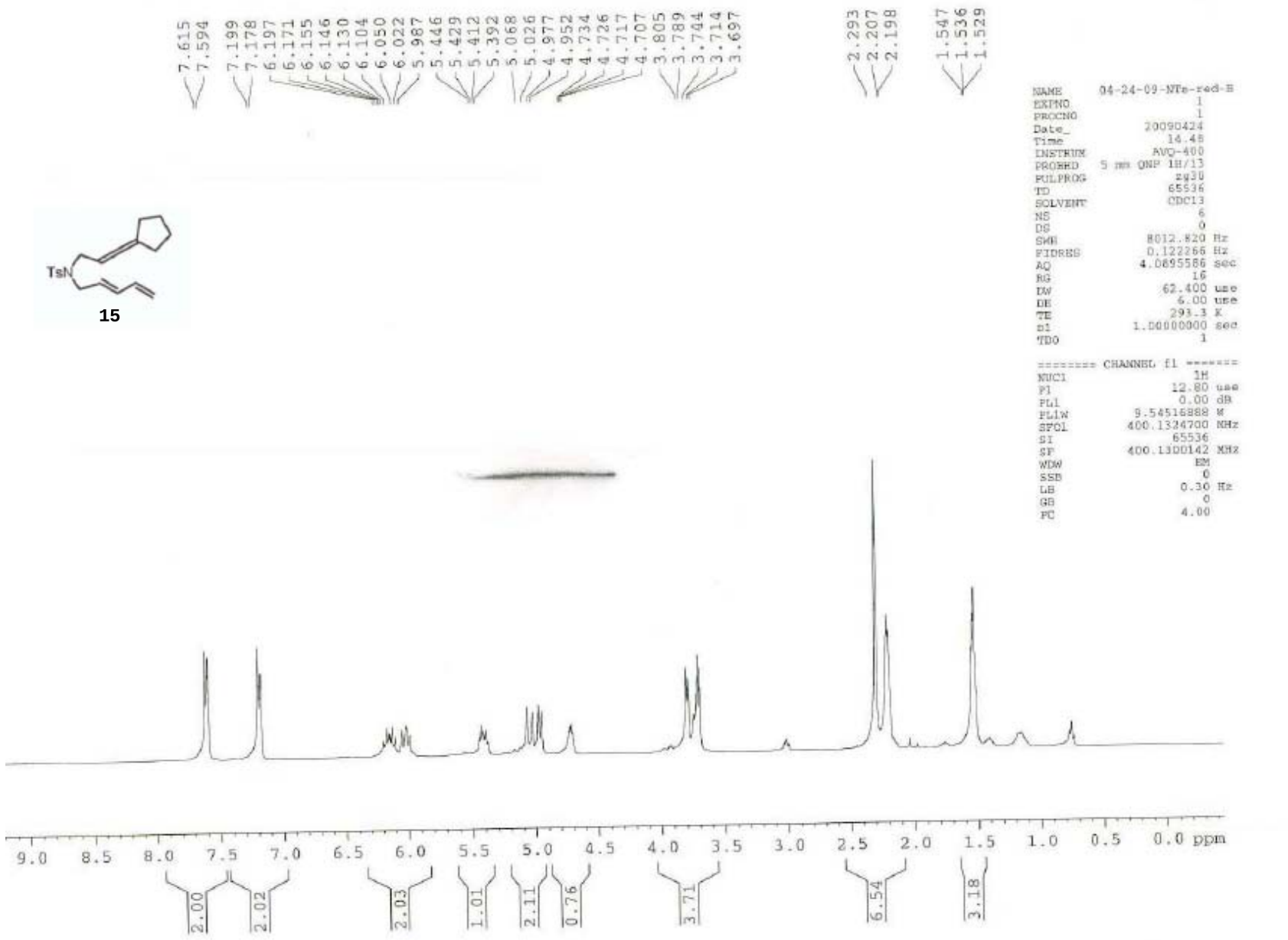


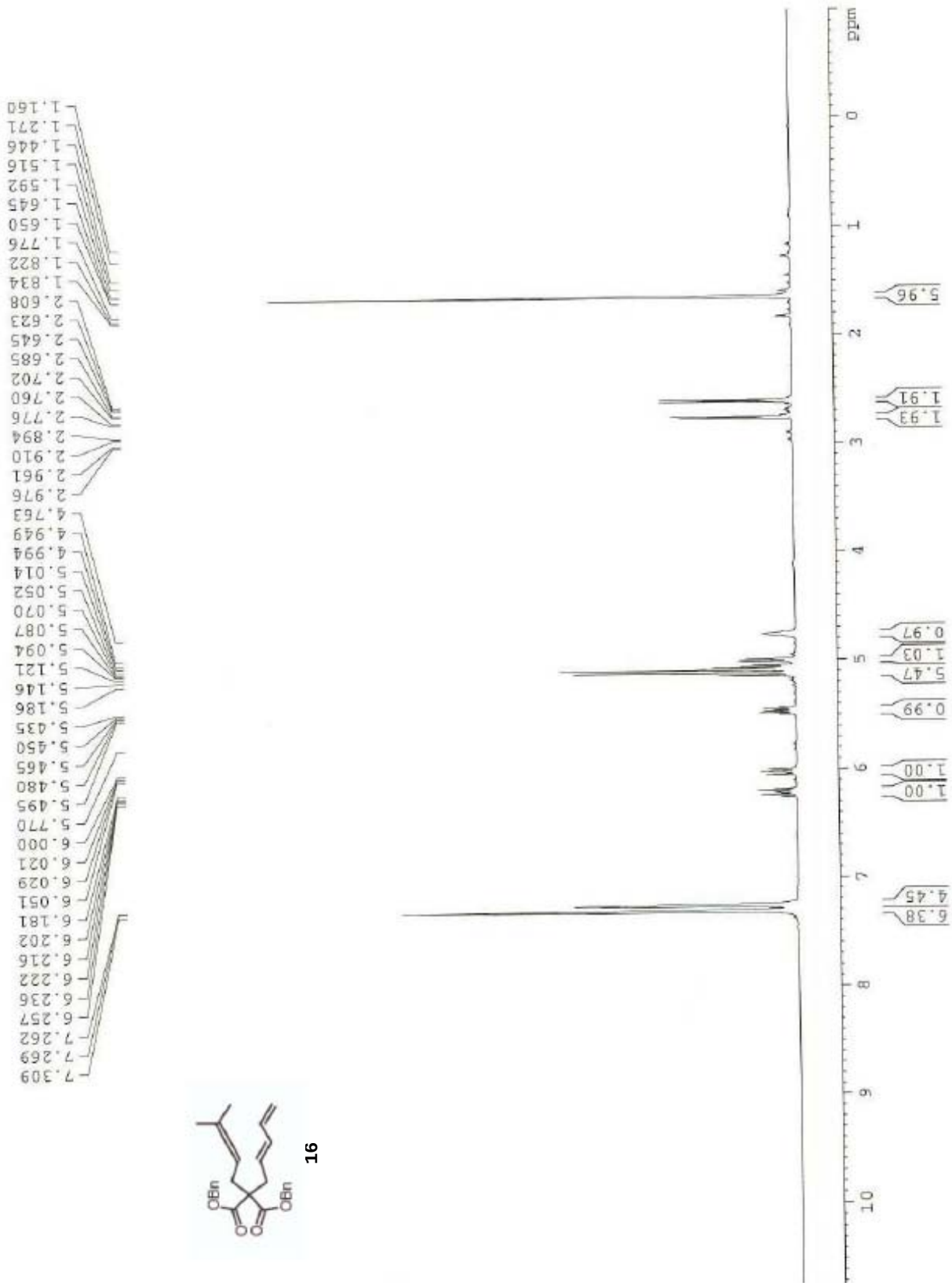
$L_{16}AuCl$

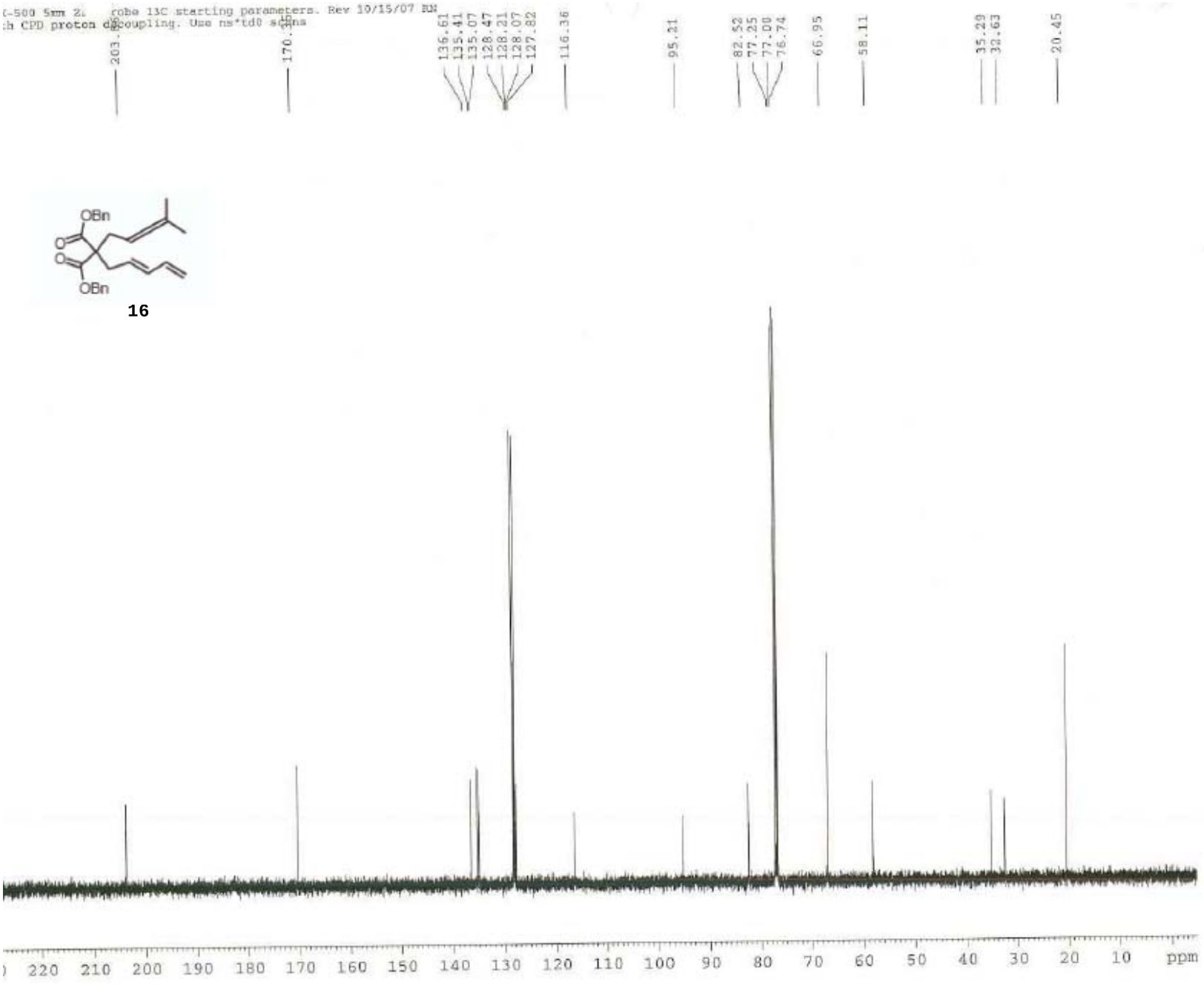
108.43

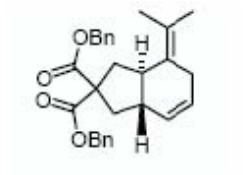
NAME	07-29-09-AG02-Bn-SI3
EXPNO	3
PROCNO	1
Date_	20090729
Time	15.48
INSTRUM	AVQ-400
PROBHD	5 mm QNP 1H/13
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	30
DS	0
SWH	97087.375 Hz
FIDRES	1.481436 Hz
AQ	0.3375655 sec
RG	8192
DW	5.150 usec
DE	6.00 usec
TE	294.4 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	31P
P1	7.70 usec
PL1	-2.00 dB
PL1W	26.27507401 W
SFO1	161.9814041 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	70.00 usec
PL2	0.00 dB
PL12	15.00 dB




7.615
7.594
7.199
7.178
6.197
6.171
6.155
6.146
6.130
6.104
6.050
6.022
5.987
5.446
5.429
5.412
5.392
5.068
5.026
4.977
4.952
4.734
4.726
4.717
4.707
3.805
3.789
3.744
3.714
3.697
2.293
2.207
2.198
1.547
1.536
1.529
TsN
15
NAME 04-24-09-NTs-red-S
EXPNO 1
PROCNO 1
Date_ 20090424
Time 14.48
INSTRUM AVQ-400
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 6
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0895586 sec
RG 16
DW 62.400 use
DE 6.00 use
TE 293.3 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 =======
NUC1 1H
P1 12.80 use
PL1 0.00 dB
PL1W 9.54516888 W
SFO1 400.1324700 MHz
SI 65536
SF 400.1300142 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 4.00
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm
2.00
2.02
2.03
1.01
2.11
0.76
3.71
6.54
3.18

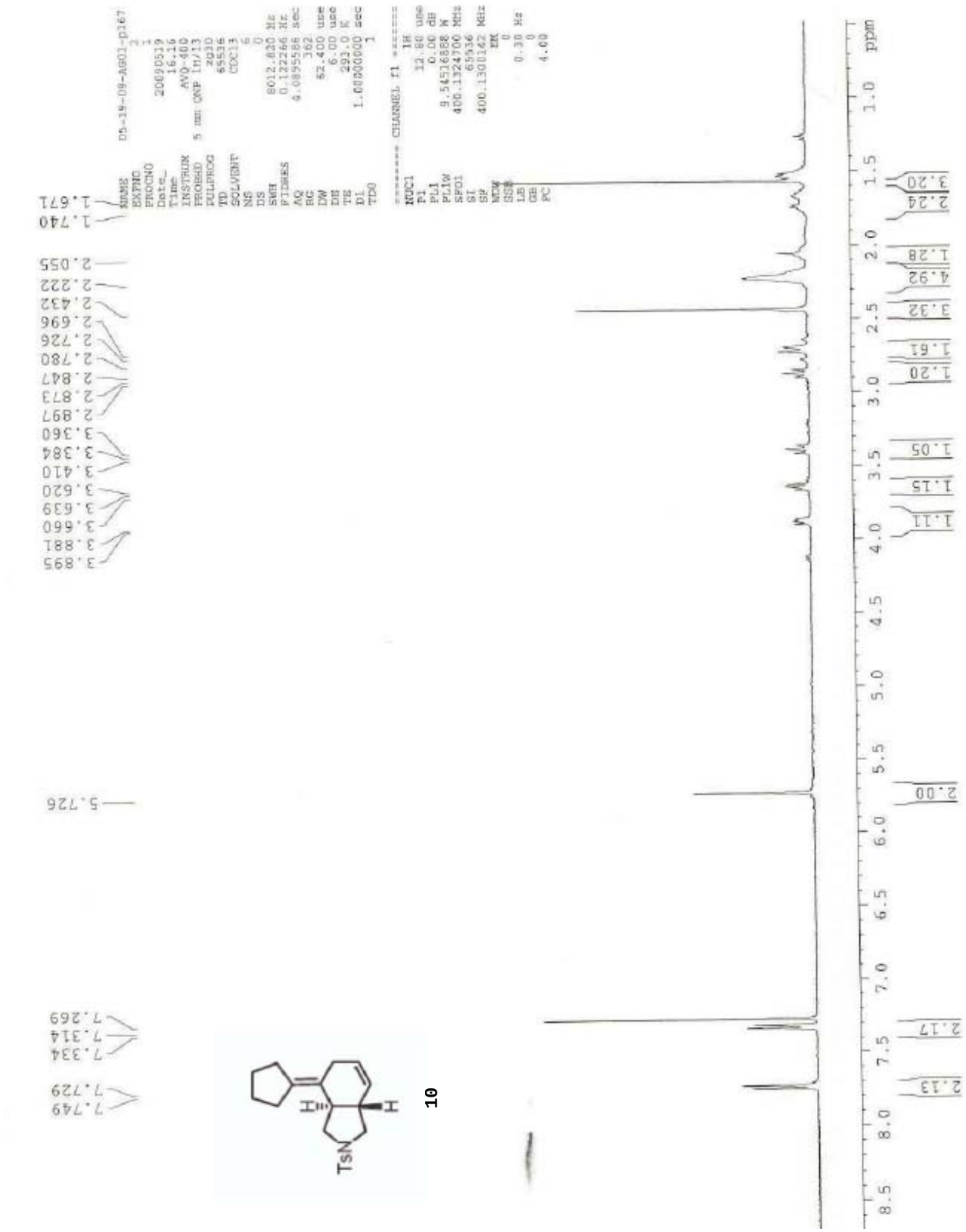

ppm
0
1
2
3
4
5
6
7
8
9
10
5.96
1.93
1.91
0.97
1.03
5.47
0.99
1.00
1.00
6.38
4.45
OBn
OBn
O
O
16
7.309
7.269
7.262
6.257
6.236
6.222
6.216
6.202
6.181
6.051
6.029
6.021
6.000
5.770
5.495
5.480
5.465
5.450
5.435
5.186
5.146
5.121
5.094
5.087
5.070
5.052
5.014
4.994
4.949
4.763
2.976
2.961
2.910
2.894
2.776
2.760
2.702
2.685
2.645
2.623
2.608
1.834
1.822
1.776
1.650
1.645
1.592
1.516
1.446
1.271
1.160

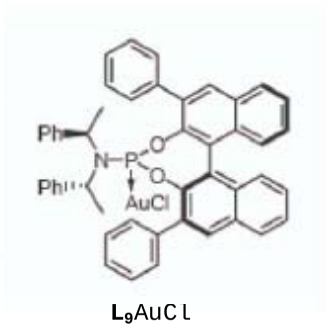

203.82
170.15
136.61
135.41
135.07
128.47
128.21
128.07
127.82
116.36
95.21
82.52
77.25
77.00
76.74
66.95
58.11
35.29
32.63
20.45
OBn
OBn
16
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm


OBn
O
O
OBn
H
H

9

7.304
7.269
7.254
5.854
5.831
5.736
5.118
5.088
3.026
3.008
2.873
2.825
2.764
2.700
2.668
2.653
2.195
1.759
1.732
1.646
1.565
1.441
1.263
NAME 04-28-09-AG01-p142
EXPNO 1
PROCNO 1
Date_ 20090428
Time 18.48
INSTRUM AVQ-400
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0895586 sec
RG 362
DW 62.400 use
DE 6.00 use
TE 300.0 K
D1 1.00000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 1H
P1 12.80 use
PL1 0.00 dB
SFO1 400.1324700 MHz
SI 65536
SF 400.1300142 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 4.00
15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3 ppm
10.70
1.89
4.00
0.93
2.93
2.69
3.42
4.85

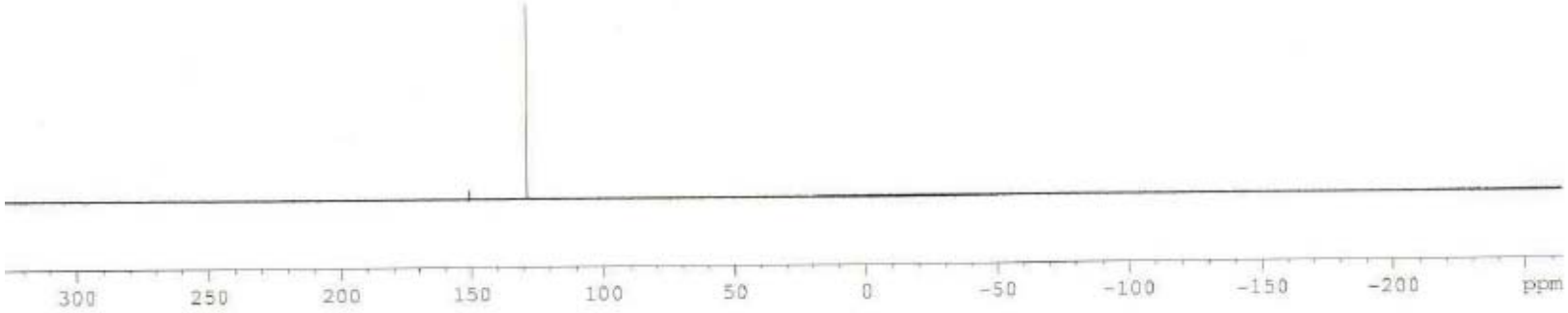

10
TsN
H
H
1.671
1.740
2.055
2.222
2.432
2.696
2.726
2.780
2.847
2.873
2.897
3.360
3.384
3.410
3.620
3.639
3.660
3.881
3.895
5.726
7.269
7.314
7.334
7.729
7.749
ppm

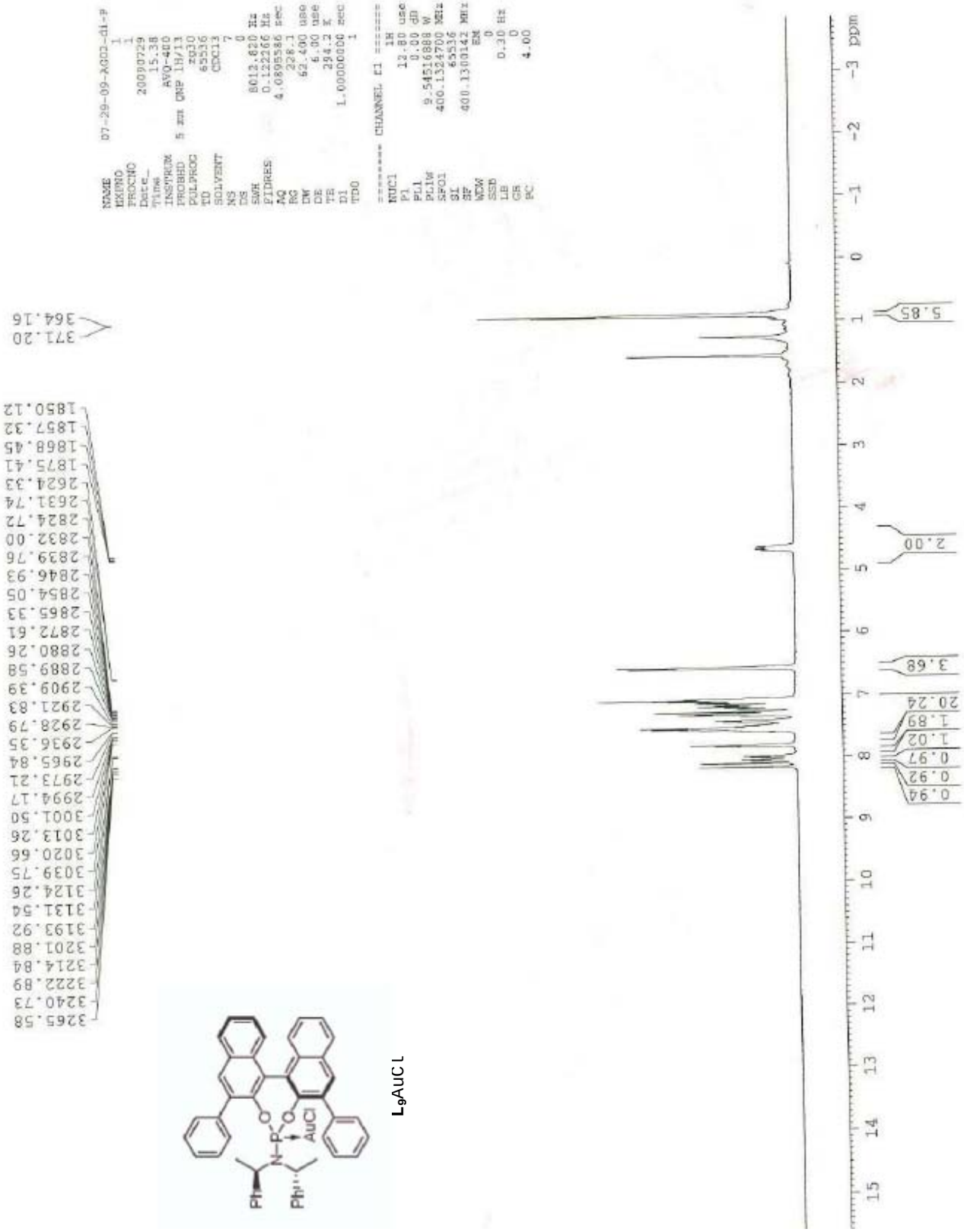


L_9AuCl

128.24

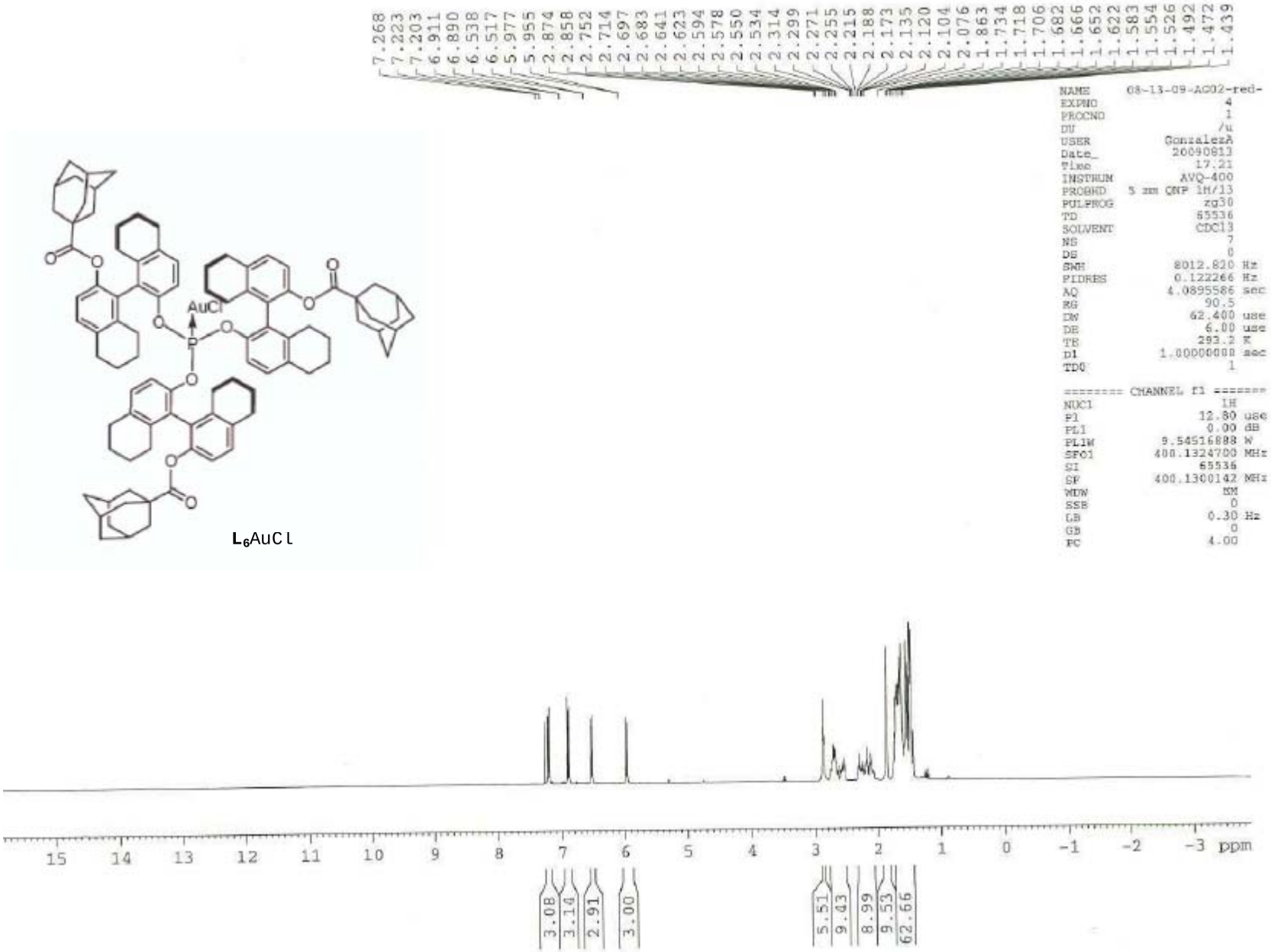
```
NAME          07-29-09-AG02-di-Ph-
EXPNO                            2
PROCNO                           1
Date_                     20090729
Time                         15.39
INSTRUM                  AVQ-400
PROBHD     5 mm QNP 1H/13
PULPROG                  zgpg30
TD                           65536
SOLVENT                  CDCl3
NS                              23
DS                               0
SWH                   97087.375 Hz
FIDRES                 1.481436 Hz
AQ                    0.3375655 sec
RG                            8192
DW                        5.150 usec
DE                        6.00 usec
TE                        294.2 K
D1                    2.00000000 sec
D11                   0.03000000 sec
TD0                              1

======== CHANNEL f1 ========
NUC1                         31P
P1                         7.70 usec
PL1                       -2.00 dB
PL1W          26.27507401 W
SFO1          161.9814041 MHz

======== CHANNEL f2 ========
CPDPRG2                  waltz16
NUC2                         1H
PCPD2                     70.00 usec
PL2                        0.00 dB
PL12                      15.00 dB
```

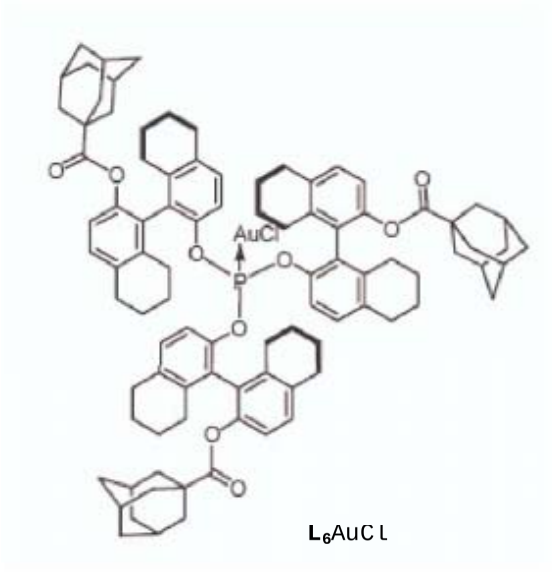



NAME 07-29-09-A303-d1-p
EXPNO 1
PROCNO 1
Date_ 20090729
Time 15.38
INSTRUM AVQ-400
PROBHD 5 mm DUP 1H/13
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 7
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0895586 sec
RG 228.1
DW 62.400 usec
DE 6.00 usec
TE 294.2 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 12.80 usec
PL1 0.00 dB
PL1W 9.54516888 W
SFO1 400.1324700 MHz
SI 65536
SF 400.1300142 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 4.00
5.85
2.00
3.68
0.94
0.92
0.97
1.02
1.89
20.24
ppm
364.16
371.20
1850.12
1857.32
1868.45
1875.41
2624.33
2631.74
2824.72
2832.00
2839.76
2846.93
2854.05
2865.33
2872.61
2880.26
2889.58
2909.39
2921.83
2928.79
2936.35
2965.84
2973.21
2994.17
3001.50
3013.26
3020.66
3039.75
3124.26
3131.54
3193.92
3201.88
3214.84
3222.89
3240.73
3265.58

O
O
P
N
AuCl
Ph
Ph

L9AuCl

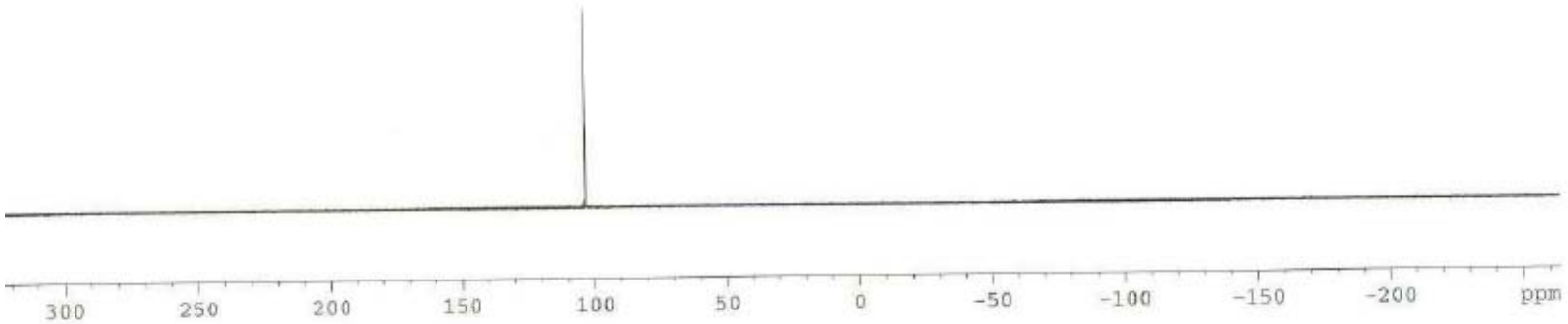

7.268
7.223
7.203
6.911
6.890
6.538
6.517
5.977
5.955
2.874
2.858
2.752
2.714
2.697
2.683
2.641
2.623
2.594
2.578
2.550
2.534
2.314
2.299
2.271
2.255
2.215
2.188
2.173
2.135
2.120
2.104
2.076
1.863
1.734
1.718
1.706
1.682
1.666
1.652
1.622
1.583
1.554
1.526
1.492
1.472
1.439
AuCl
P
O
L6AuCl
NAME 08-13-09-AG02-red-
EXPNO 4
PROCNO 1
DU /u
USER GonzalezA
Date_ 20090813
Time 17.21
INSTRUM AVQ-400
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 7
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0895586 sec
RG 90.5
DW 62.400 use
DE 6.00 use
TE 293.2 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 12.80 use
PL1 0.00 dB
PL1W 9.54516888 W
SFO1 400.1324700 MHz
SI 65536
SF 400.1300142 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 4.00
15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3 ppm
3.08
3.14
2.91
3.00
5.51
9.43
8.99
9.53
62.66

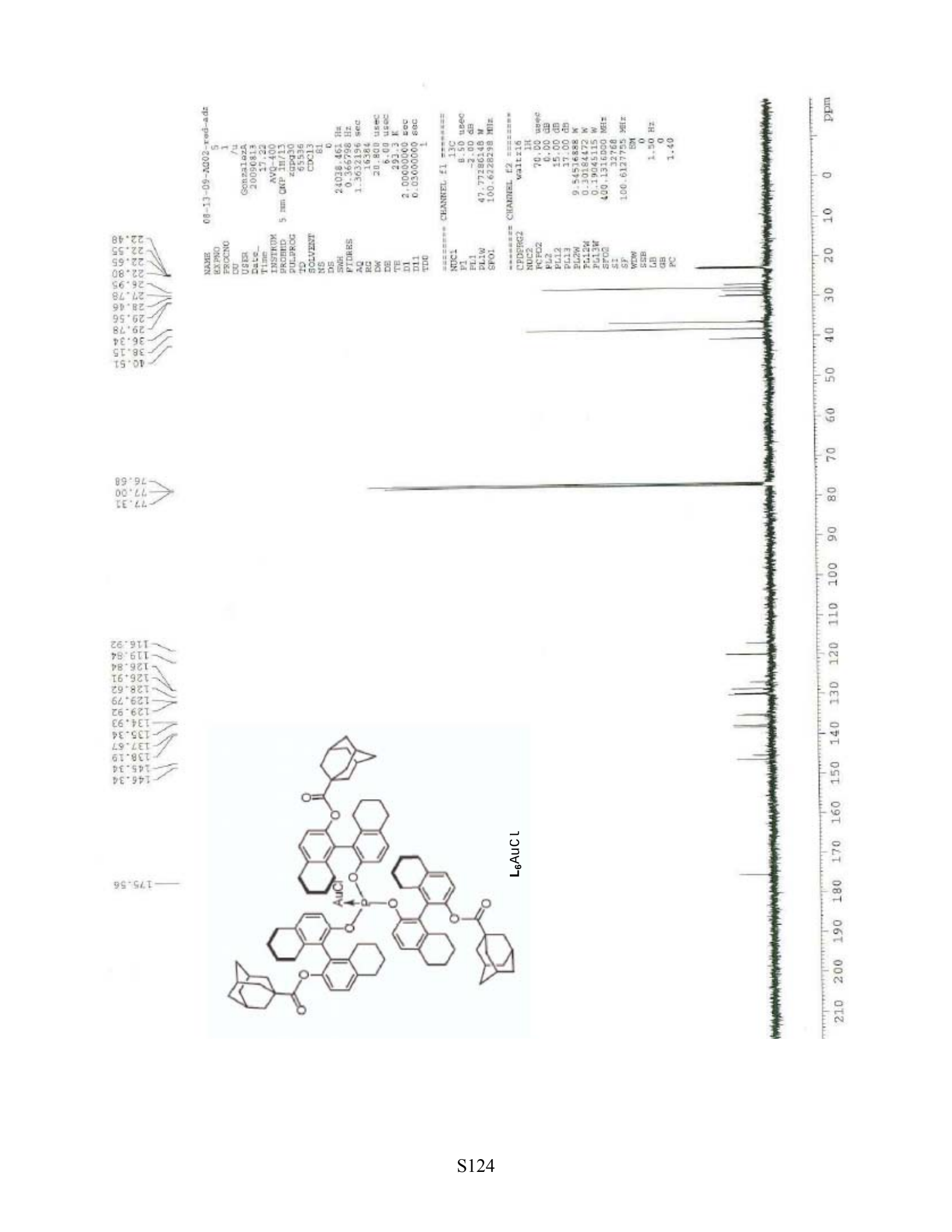


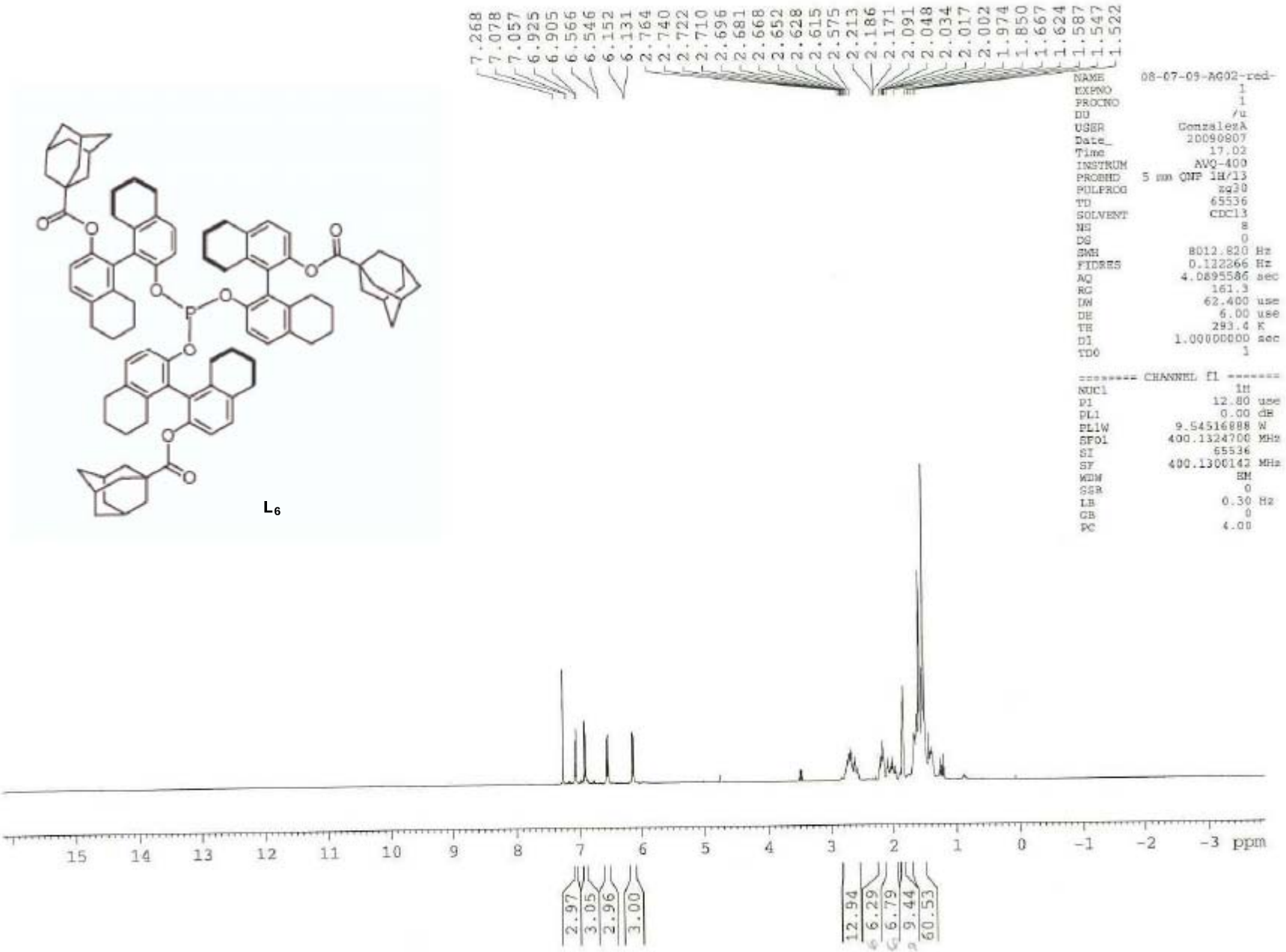
L_6AuCl

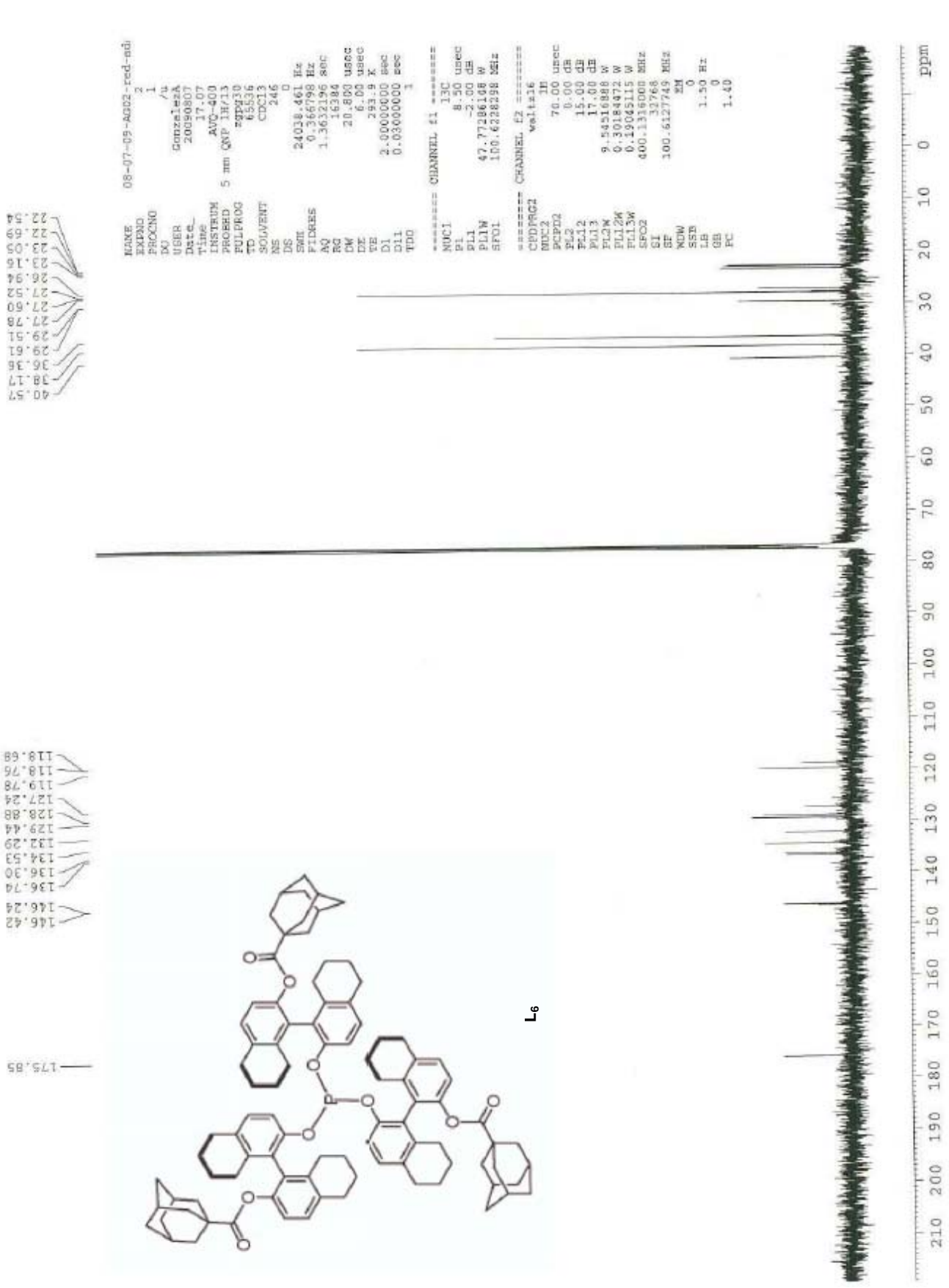
103.79

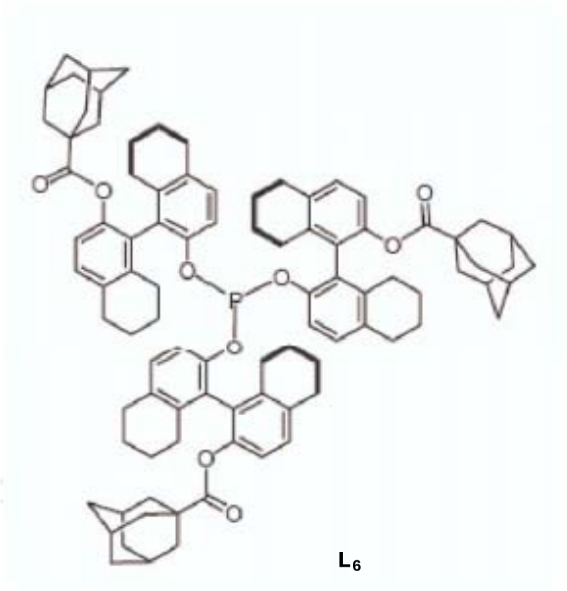
NAME	08-13-09-AG02-red-ac
EXPNO	2
PROCNO	1
Date_	20090813
Time	9.50
INSTRUM	AVQ-400
PROBHD	5 mm QNP 1H/13
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	9
DS	0
SWH	97087.375 Hz
FIDRES	1.481436 Hz
AQ	0.3375655 sec
RG	8192
DW	5.150 usec
DE	6.00 usec
TE	293.4 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	31P
P1	7.70 usec
PL1	-2.00 dB
PL1W	26.27507401 W
SFO1	161.9814041 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	70.00 usec
PL2	0.00 dB
PL12	15.00 dB




22.48
22.55
22.65
22.80
26.95
27.78
28.46
29.56
29.78
36.34
38.15
40.51
77.31
77.00
76.68
116.92
119.84
126.84
126.91
128.62
129.79
129.92
134.93
135.34
137.67
138.19
145.34
146.34
175.56
AuCl
L6AuCl
NAME 08-13-09-AG02-red-adz
EXPNO 5
PROCNO 1
CU /u
USER Gonzaleza
Date_ 20090813
Time 17.22
INSTRUM AVQ-400
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 81
DS 0
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3632196 sec
RG 16384
DW 20.800 usec
DE 6.00 usec
TE 291.3 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 8.50 usec
PL1 -2.00 dB
PL1W 47.77286148 W
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 70.00 usec
PL2 0.00 dB
PL12 15.00 dB
PL13 17.00 dB
PL2W 9.54516888 W
PL12W 0.30184472 W
PL13W 0.19045115 W
SFO2 400.1316000 MHz
SI 32768
SF 100.6127755 MHz
WDW EM
SSB 0
LB 1.50 Hz
GB 0
PC 1.40
ppm

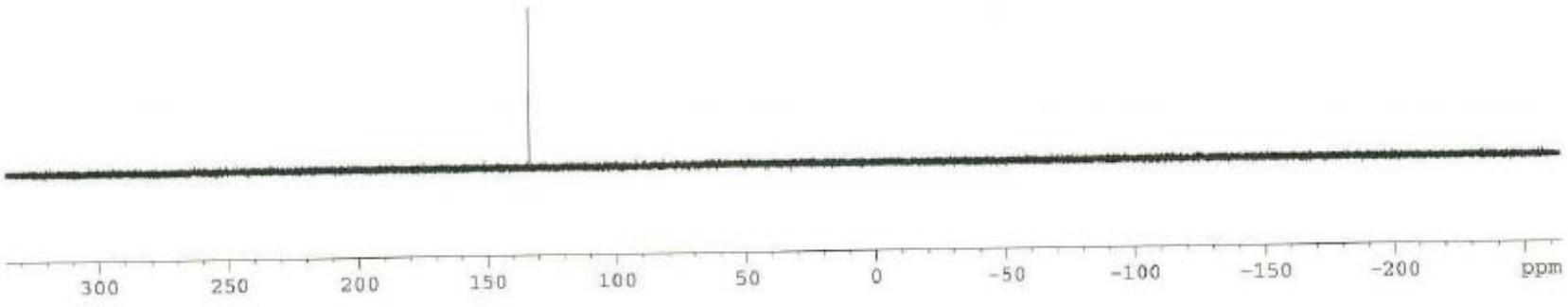

7.268
7.078
7.057
6.925
6.905
6.566
6.546
6.152
6.131
2.764
2.740
2.722
2.710
2.696
2.681
2.668
2.652
2.628
2.615
2.575
2.213
2.186
2.171
2.091
2.048
2.034
2.017
2.002
1.974
1.850
1.667
1.624
1.587
1.547
1.522
NAME 08-07-09-AG02-red-
EXPNO 1
PROCNO 1
DU /u
USER GonzalezA
Date_ 20090807
Time 17.02
INSTRUM AVQ-400
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0895586 sec
RG 161.3
DW 62.400 use
DE 6.00 use
TE 293.4 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 12.80 use
PL1 0.00 dB
PL1W 9.54516888 W
SFO1 400.1324700 MHz
SI 65536
SF 400.1300142 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 4.00
P
O
L6
15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3 ppm
2.97
3.05
2.96
3.00
12.94
6.29
6.79
9.44
60.53

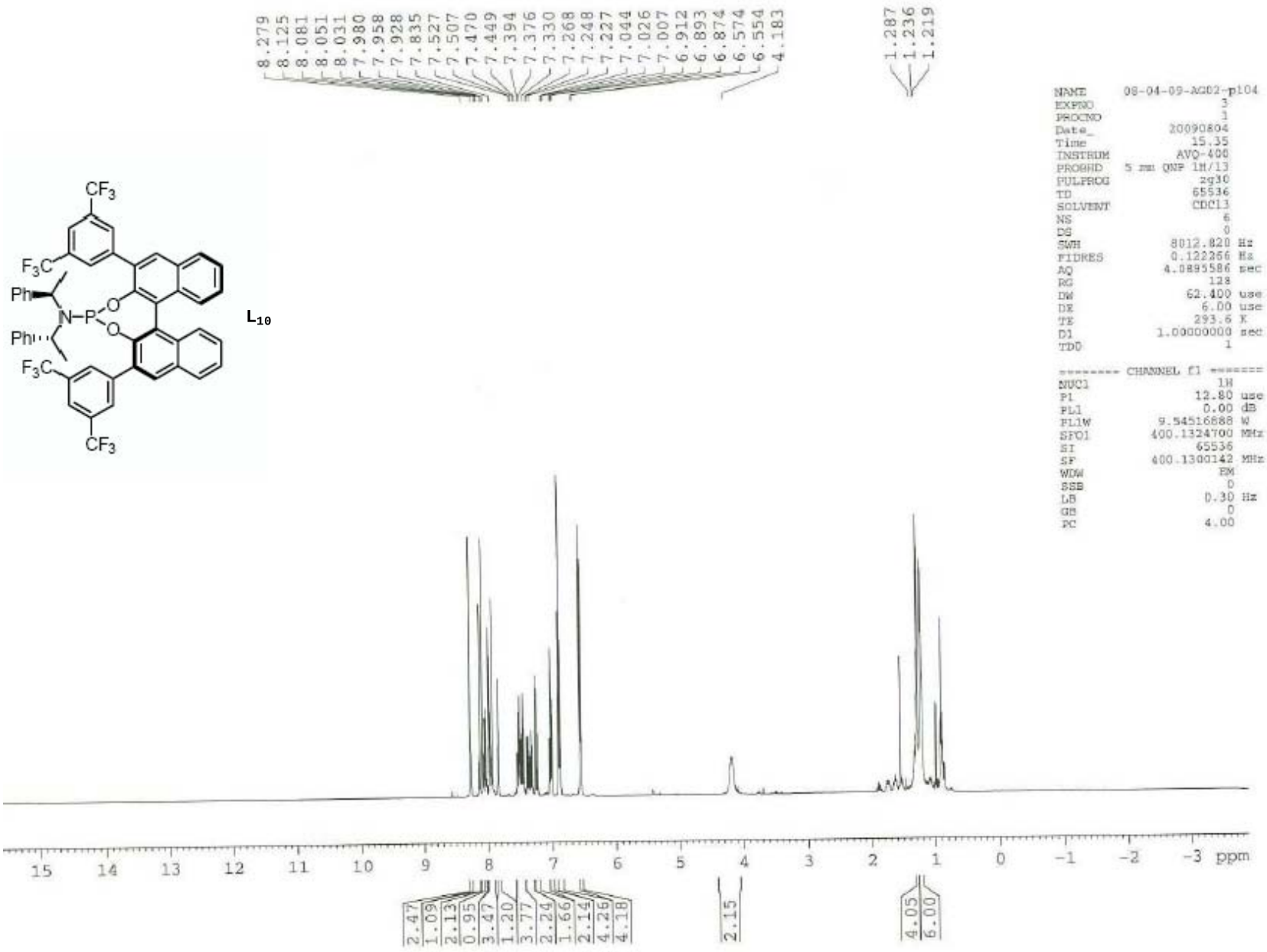

L6
ppm

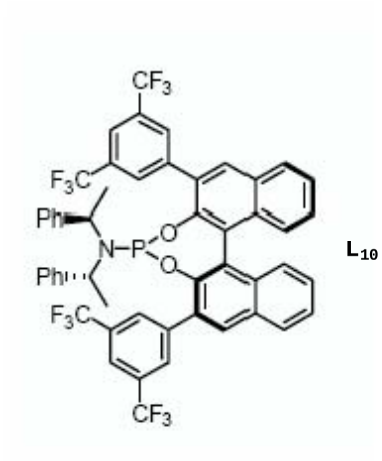


L_6

NAME	08-07-09-AG02-red-ads
EXPNO	3
PROCNO	1
DU	/u
USER	GonzalezA
Date_	20090807
Time	17.19
INSTRUM	AVQ-400
PROBHD	5 mm QNP 1H/13
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	3
DS	0
SWH	97087.375 Hz
FIDRES	1.481436 Hz
AQ	0.3375655 sec
RG	8192
DW	5.150 usec
DE	6.00 usec
TE	294.0 K
D1	1.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	31P
P1	7.70 usec
PL1	-2.00 dB
PL1W	26.27507401 W
SFO1	161.9814041 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	70.00 usec
PL2	0.00 dB
PL12	15.00 dB
PL13	17.00 dB
PL2W	9.54516888 W
PL12W	0.30184472 W
PL13W	0.19045115 W
SFO2	400.1316005 MHz
SI	65536
SF	161.9755989 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40



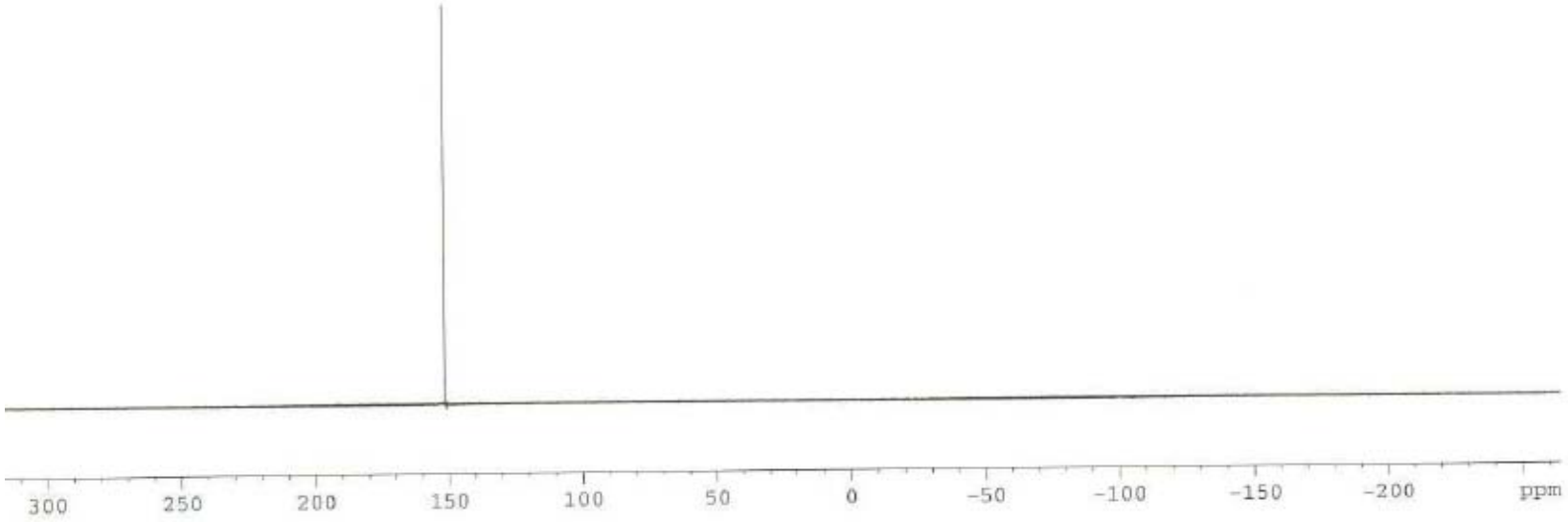

8.279
8.125
8.081
8.051
8.031
7.980
7.958
7.928
7.835
7.527
7.507
7.470
7.449
7.394
7.376
7.330
7.268
7.248
7.227
7.044
7.026
7.007
6.912
6.893
6.874
6.574
6.554
4.183
1.287
1.236
1.219
CF3
F3C
Ph
N
P
O
O
Ph
F3C
CF3
L10
NAME 08-04-09-AG02-p104
EXPNO 3
PROCNO 1
Date_ 20090804
Time 15.35
INSTRUM AVQ-400
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 6
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0895586 sec
RG 128
DW 62.400 use
DE 6.00 use
TE 293.6 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 12.80 use
PL1 0.00 dB
PL1W 9.54516688 W
SFO1 400.1324700 MHz
SI 65536
SF 400.1300142 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 4.00
15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3 ppm
2.47 1.09 2.13 0.95 3.47 1.20 3.77 2.24 1.66 2.14 4.26 4.18
2.15
4.05 6.00

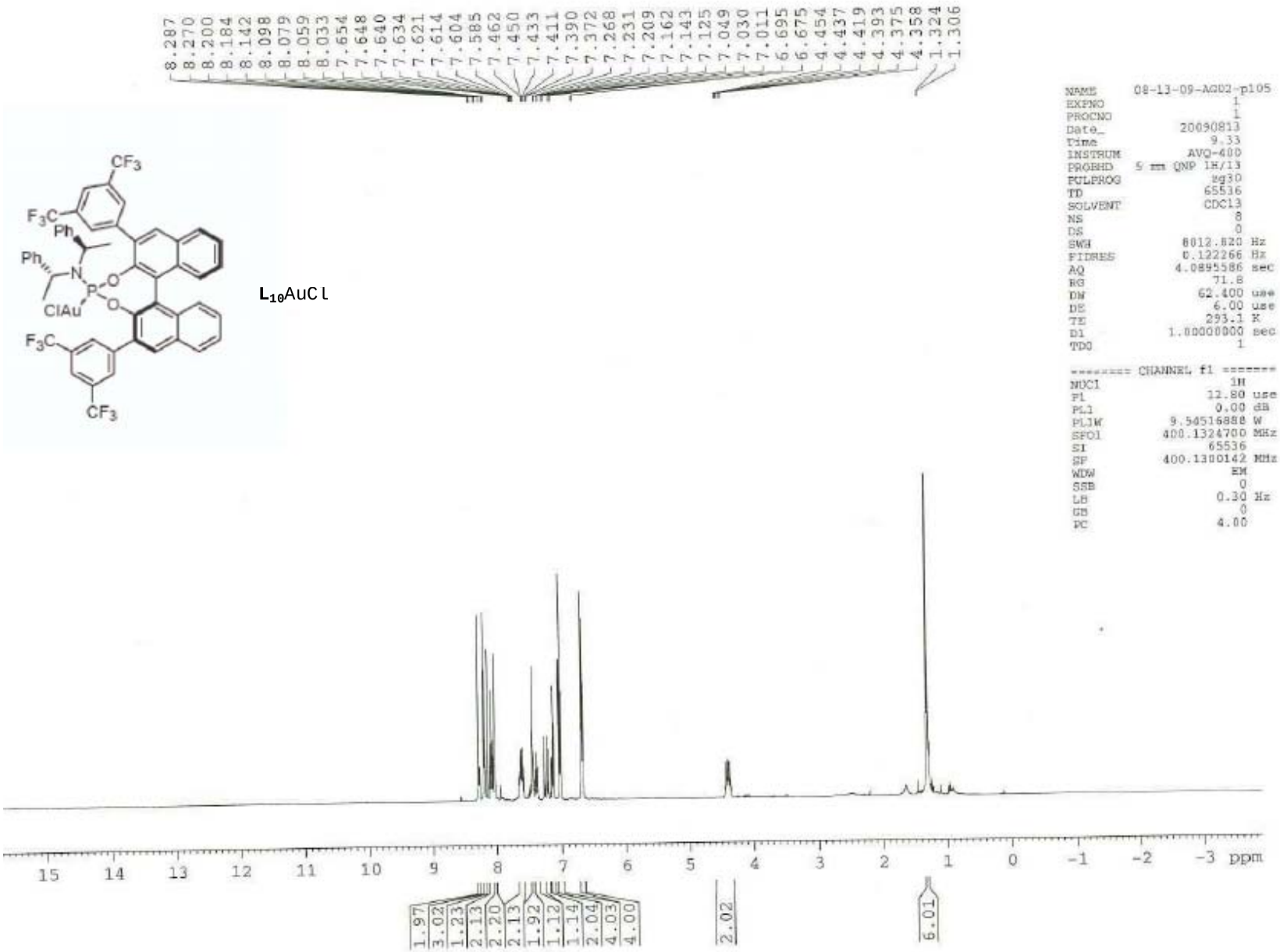


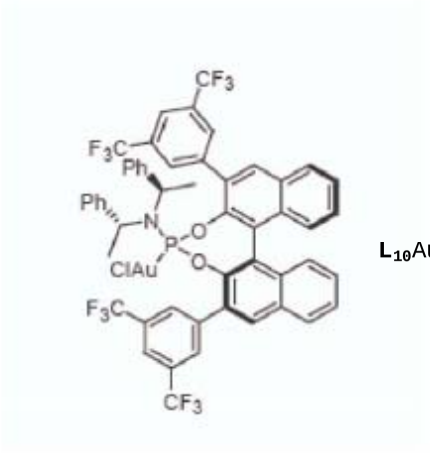
L_{10}

151.40

NAME	08-04-09-AG02-p104-c
EXPNO	4
PROCNO	1
Date_	20090804
Time	15.36
INSTRUM	AVQ-400
PROBHD	5 mm QNP 1H/13
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	17
DS	0
SWH	97087.375 Hz
FIDRES	1.481436 Hz
AQ	0.3375655 sec
RG	8192
DW	5.150 usec
DE	6.00 usec
TE	293.6 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	31P
P1	7.70 usec
PL1	-2.00 dB
PL1W	26.27507401 W
SFO1	161.9814041 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	70.00 usec
PL2	0.00 dB
PL12	15.00 dB



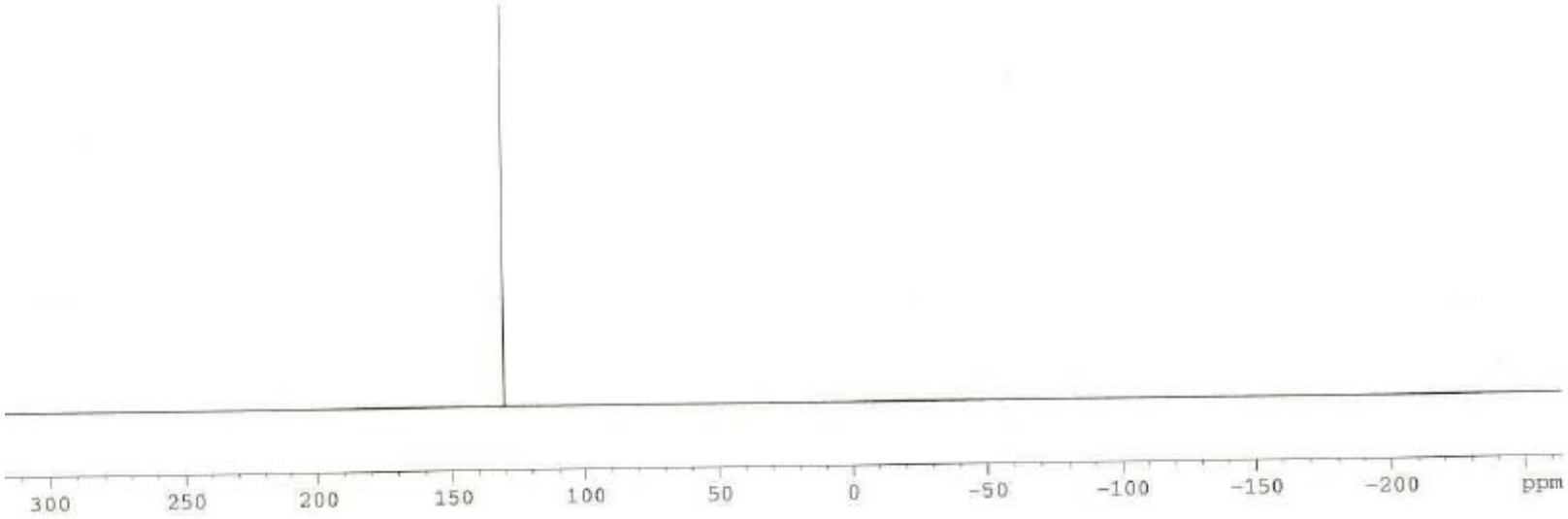

8.287
8.270
8.200
8.184
8.142
8.098
8.079
8.059
8.033
7.654
7.648
7.640
7.634
7.621
7.614
7.604
7.585
7.462
7.450
7.433
7.411
7.390
7.372
7.268
7.231
7.209
7.162
7.143
7.125
7.049
7.030
7.011
6.695
6.675
4.454
4.437
4.419
4.393
4.375
4.358
1.324
1.306
CF3
F3C
Ph
Ph
N
P
O
O
ClAu
F3C
CF3
L10AuCl
NAME 08-13-09-AG02-p105
EXPNO 1
PROCNO 1
Date_ 20090813
Time 9.33
INSTRUM AVQ-400
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0895586 sec
RG 71.8
DW 62.400 use
DE 6.00 use
TE 293.1 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 =======
NUC1 1H
P1 12.80 use
PL1 0.00 dB
PL1W 9.56516888 W
SFO1 400.1324700 MHz
SI 65536
SF 400.1300142 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 4.00
15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3 ppm
1.97
3.02
1.23
2.13
2.20
2.13
1.92
1.12
1.14
2.04
4.03
4.00
2.02
6.01

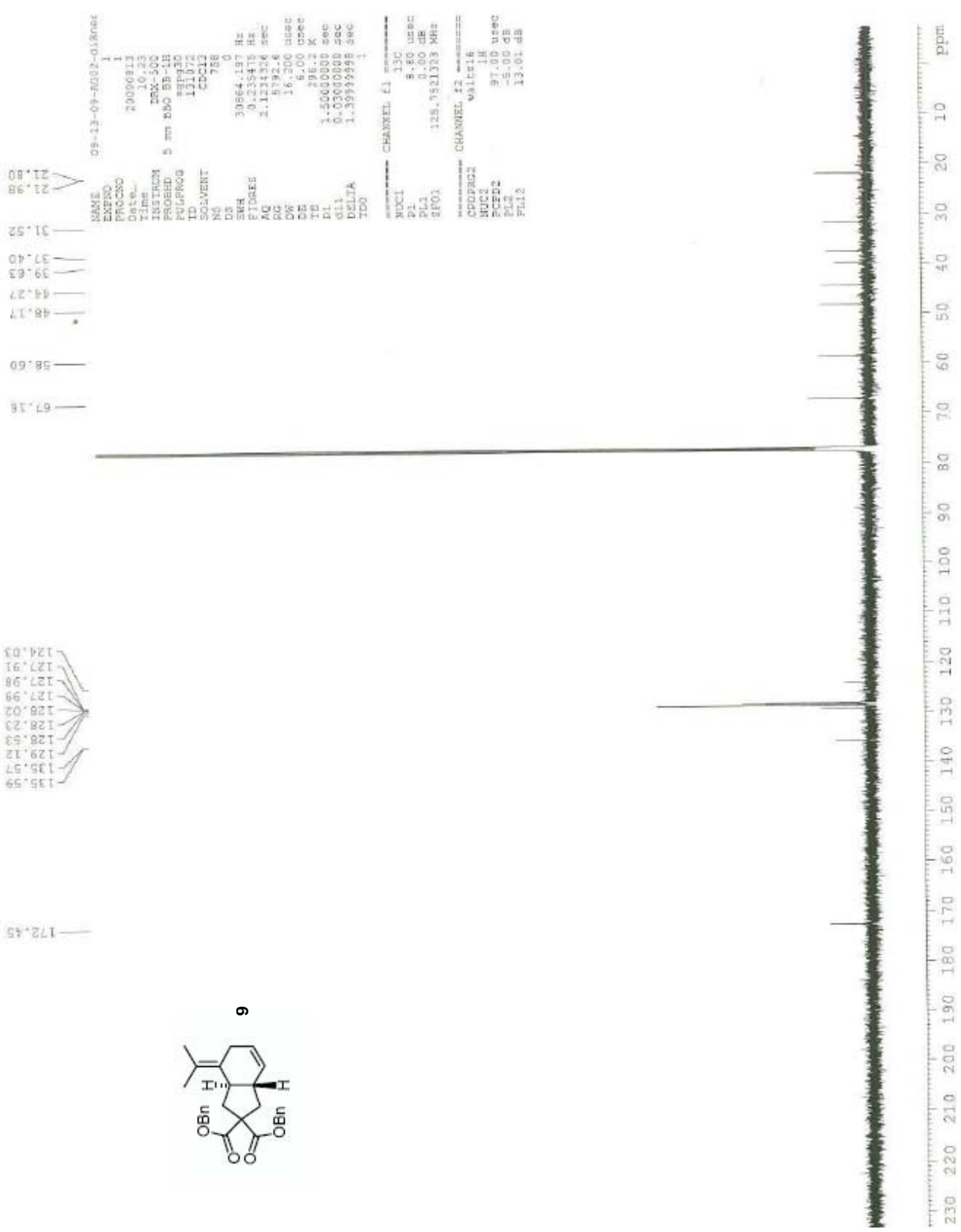


$L_{10}AuCl$

130.43

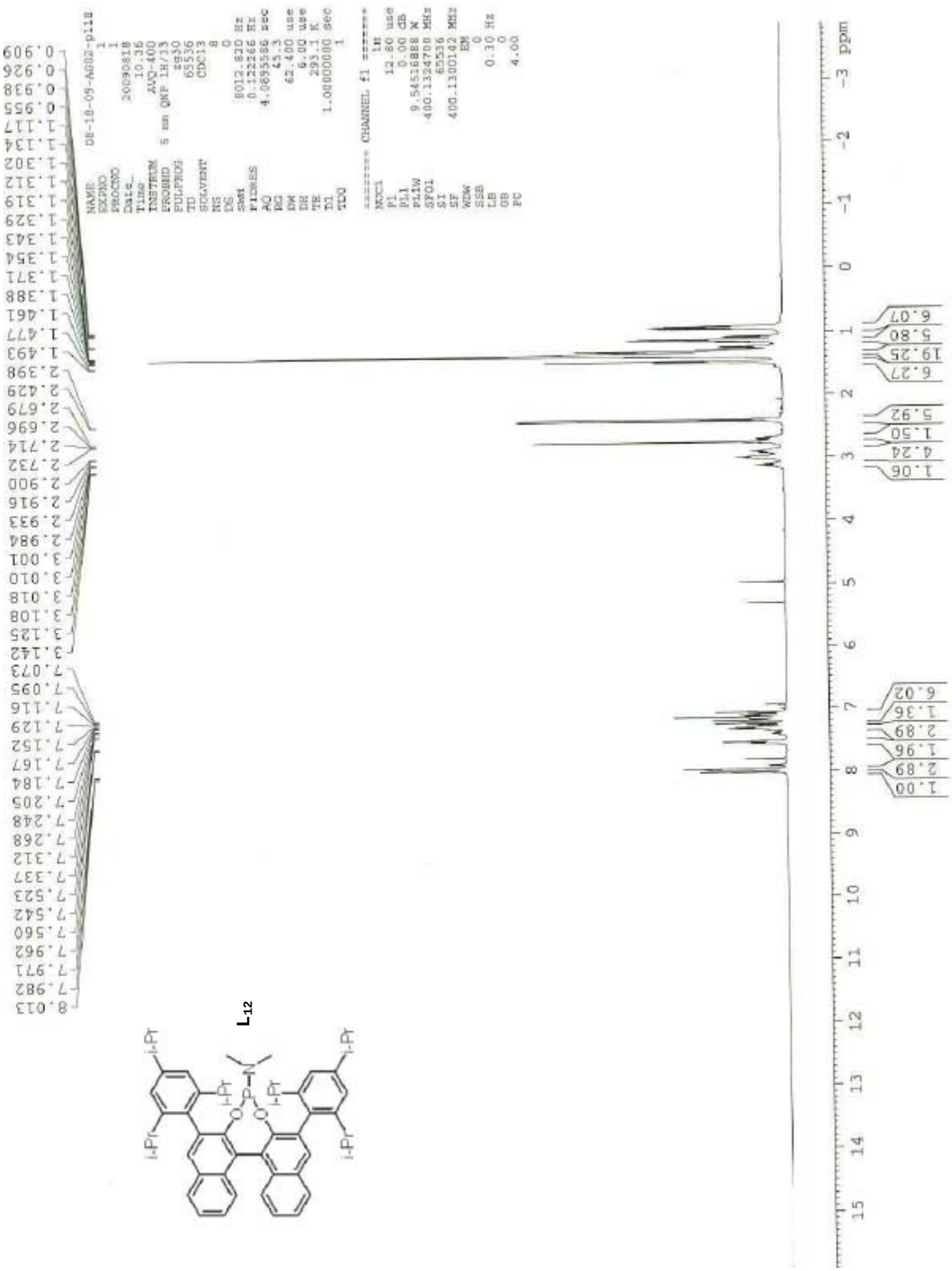
```
NAME          08-13-09-AG02-p105
EXPNO                          2
PROCNO                         1
Date_                   20090813
Time                        9.34
INSTRUM                  AVQ-400
PROBHD    5 mm QNP 1H/13
PULPROG                  zgpg30
TD                        65536
SOLVENT                    CDCl3
NS                            16
DS                             0
SWH                  97087.375 Hz
FIDRES               1.481436 Hz
AQ                   0.3375655 sec
RG                         8192
DW                      5.150 usec
DE                        6.00 usec
TE                       293.1 K
D1                  2.00000000 sec
D11                 0.03000000 sec
TD0                            1

======== CHANNEL f1 ========
NUC1                         31P
P1                          7.70 usec
PL1                        -2.00 dB
PL1W               26.27507401 W
SFO1               161.9814041 MHz

======== CHANNEL f2 ========
CPDPRG2                  waltz16
NUC2                         1H
PCPD2                      70.00 usec
PL2                         0.00 dB
PL12                       15.00 dB
```

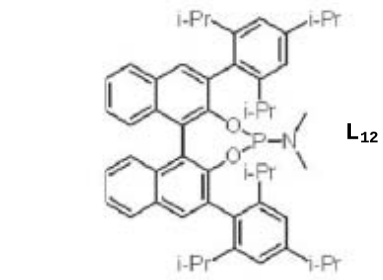



09-13-09-AG02-diAnet
NAME
EXPNO
PROCNO
Date_
Time
INSTRUM
PROBHD
PULPROG
TD
SOLVENT
NS
DS
SWH
FIDRES
AQ
RG
DW
DE
TE
D1
d11
DELTA
TD0
CHANNEL f1
NUC1
P1
PL1
SFO1
CHANNEL f2
CPDPRG2
NUC2
PCPD2
PL2
PL12
ppm
21.80
21.98
31.52
37.40
39.63
44.27
48.17
58.60
67.18
124.03
127.91
127.98
127.99
128.02
128.23
128.53
129.12
135.57
135.59
172.45

9

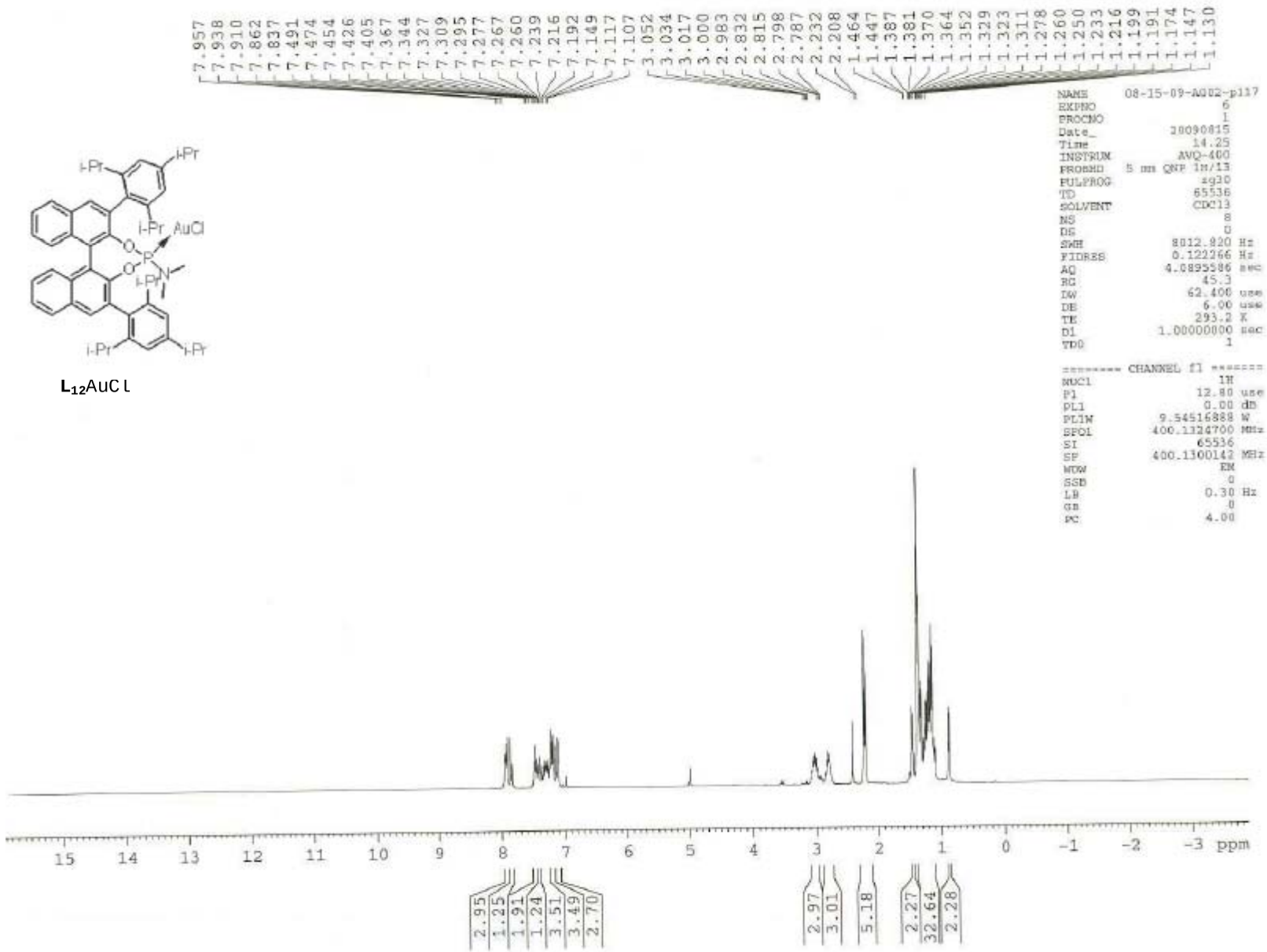
OBn
OBn
O
O
H
H


L12
i-Pr
i-Pr
i-Pr
i-Pr
i-Pr
i-Pr
ppm

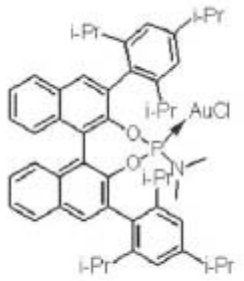


L_{12}

NAME	08-15-09-AG02-p117-c
EXPNO	7
PROCNO	1
Date_	20090815
Time	14.27
INSTRUM	AVD-400
PROBHD	5 mm QNP 1H/13
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	32
DS	0
SWH	97087.375 Hz
FIDRES	1.481436 Hz
AQ	0.3375655 sec
RG	8192
DW	5.150 usec
DE	6.00 usec
TE	293.4 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	31P
P1	7.70 usec
PL1	-2.00 dB
PL1W	26.27507401 W
SFO1	161.9814041 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	70.00 usec
PL2	0.00 dB
PL12	15.00 dB


7.957
7.938
7.910
7.862
7.837
7.491
7.474
7.454
7.426
7.405
7.367
7.344
7.327
7.309
7.295
7.277
7.267
7.260
7.239
7.216
7.192
7.149
7.117
7.107
3.052
3.034
3.017
3.000
2.983
2.832
2.815
2.798
2.787
2.232
2.208
1.464
1.447
1.387
1.381
1.370
1.364
1.352
1.329
1.323
1.311
1.278
1.260
1.250
1.233
1.216
1.199
1.191
1.174
1.147
1.130
i-Pr
i-Pr
i-Pr
AuCl
i-Pr
i-Pr
i-Pr
i-Pr
NAME 08-15-09-AG02-p117
EXPNO 6
PROCNO 1
Date_ 20090815
Time 14.25
INSTRUM AVQ-400
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0895586 sec
RG 45.3
DW 62.400 usec
DE 6.00 usec
TE 293.2 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 12.80 usec
PL1 0.00 dB
PL1W 9.54516888 W
SFO1 400.1324700 MHz
SI 65536
SF 400.1300142 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 4.00
15
14
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
-2
-3 ppm
2.95
1.25
1.91
1.24
3.51
3.49
2.70
2.97
3.01
5.18
2.27
32.64
2.28

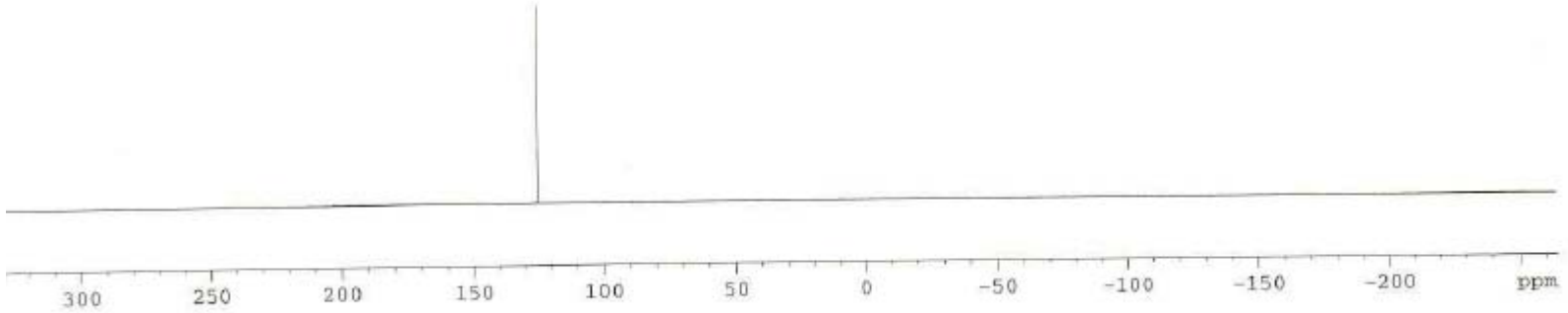
$L_{12}AuCl$

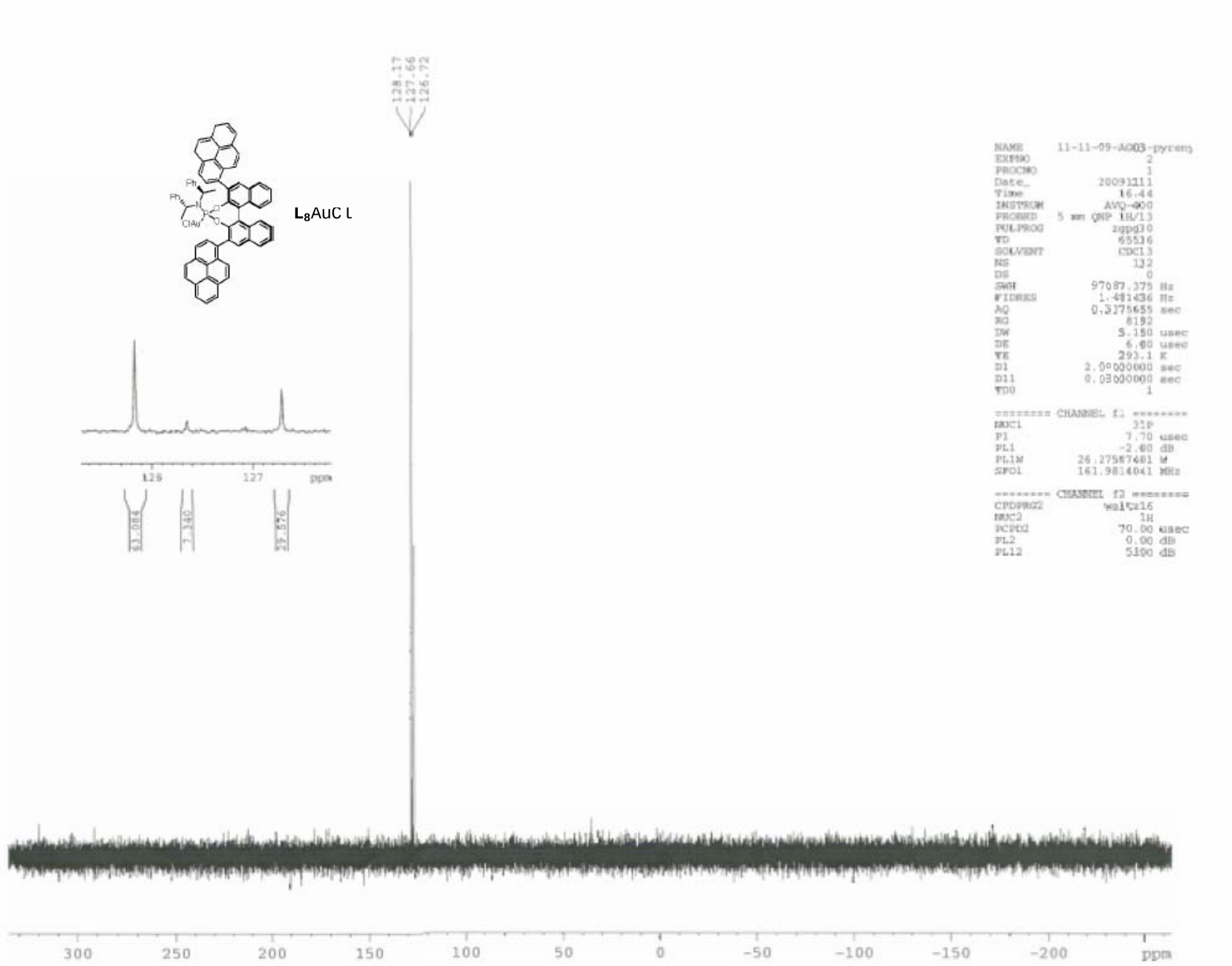


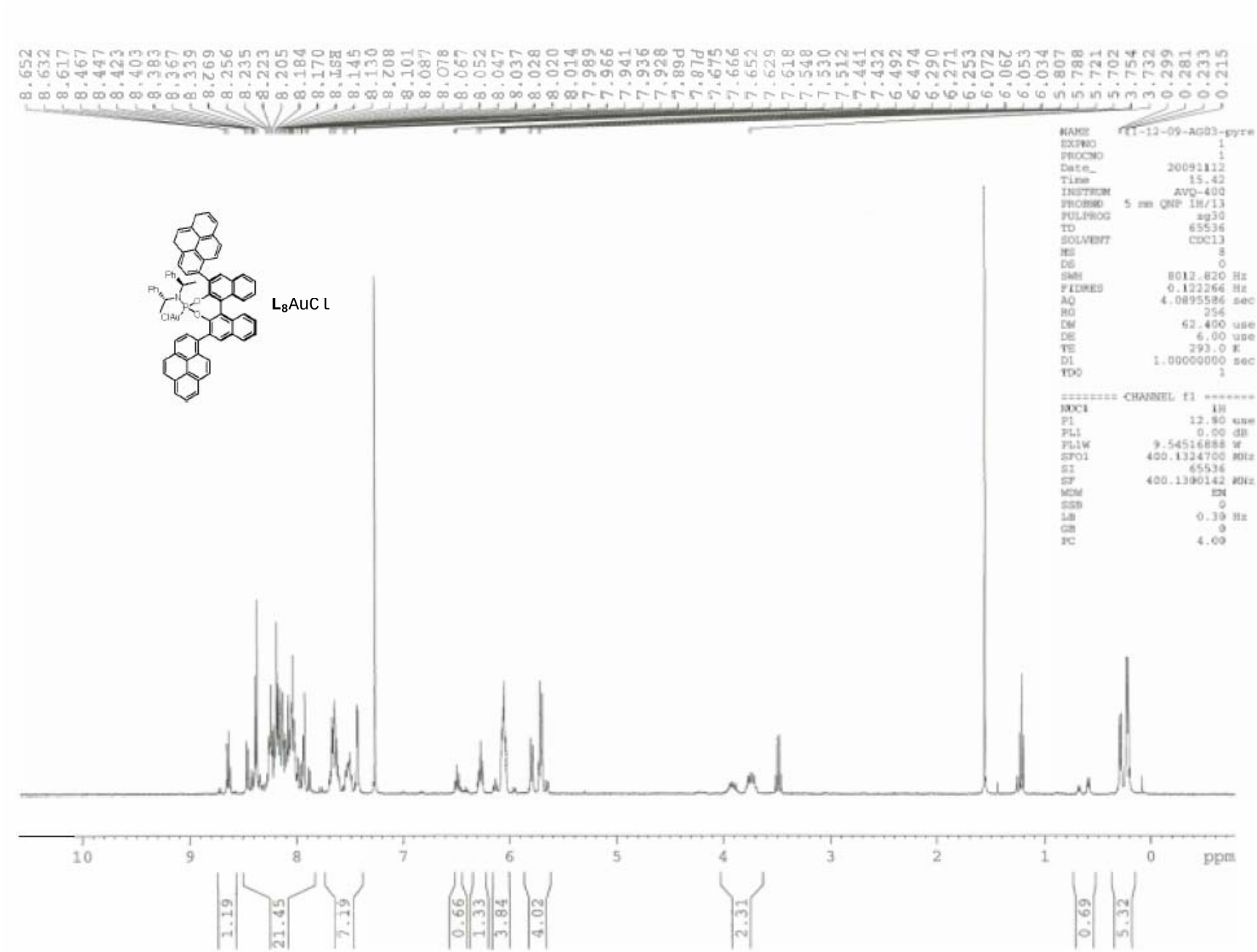
$L_{12}AuCl$

124.87

NAME	08-18-09-AG02-p118-P
EXPNO	2
PROCNO	1
Date_	20090818
Time	10.37
INSTRUM	AVQ-400
PROBHD	5 mm QNP 1H/13
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	13
DS	0
SWH	97087.375 Hz
FIDRES	1.481436 Hz
AQ	0.3375655 sec
RG	8192
DW	5.150 usec
DE	6.00 usec
TE	293.1 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	31P
P1	7.70 usec
PL1	-2.00 dB
PL1W	26.27507401 W
SFO1	161.9814041 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	70.00 usec
PL2	0.00 dB
PL12	15.00 dB




128.17
127.66
126.72
L8AuCl
126
127
ppm
1.000
7.340
29.576
NAME 11-11-09-AG03-pyrene
EXPNO 2
PROCNO 1
Date_ 20091111
Time 16.44
INSTRUM AVQ-400
PROBHD 5 mm QNP 1H/13
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 112
DS 0
SWH 97087.375 Hz
FIDRES 1.481436 Hz
AQ 0.3375655 sec
RG 8192
DW 5.150 usec
DE 6.00 usec
TE 293.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 31P
P1 7.70 usec
PL1 -2.00 dB
PL1W 26.27587401 W
SFO1 161.9814041 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 70.00 usec
PL2 0.00 dB
PL12 5300 dB
300
250
200
150
100
50
0
-50
-100
-150
-200
ppm


L8AuCl
NAME t1-12-09-AG03-pyre
EXPNO 1
PROCNO 1
Date_ 20091112
Time 15.42
INSTRUM AVQ-400
PROBHD 5 mm QNP 1H/13
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 0
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0895586 sec
RG 256
DW 62.400 use
DE 6.00 use
TE 293.0 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 12.90 use
PL1 0.00 dB
PL1W 9.54516888 W
SFO1 400.1324700 MHz
SI 65536
SF 400.1300142 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 4.00
10
9
8
7
6
5
4
3
2
1
0
ppm
1.19
21.45
7.19
0.66
1.33
3.84
4.02
2.31
0.69
5.32