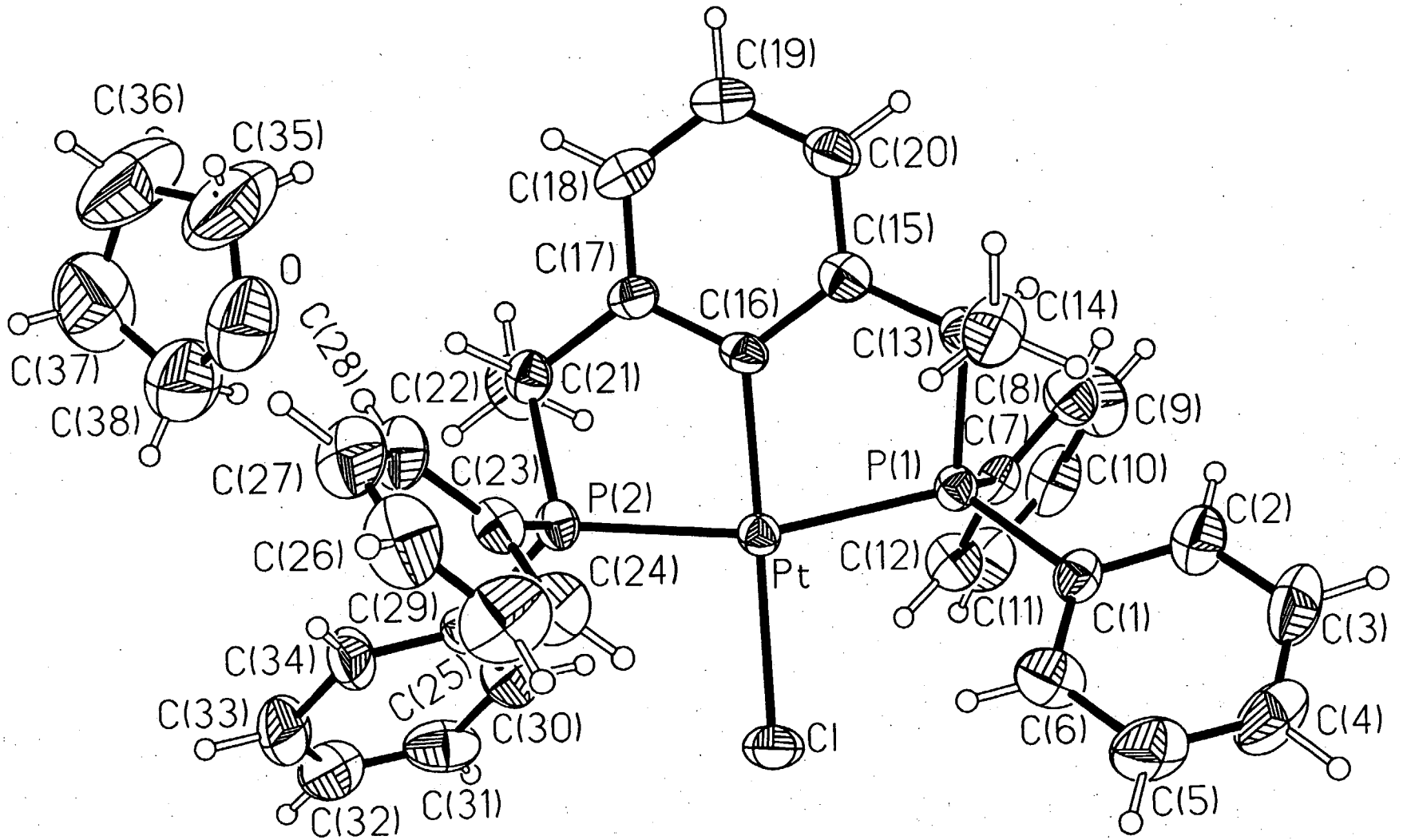
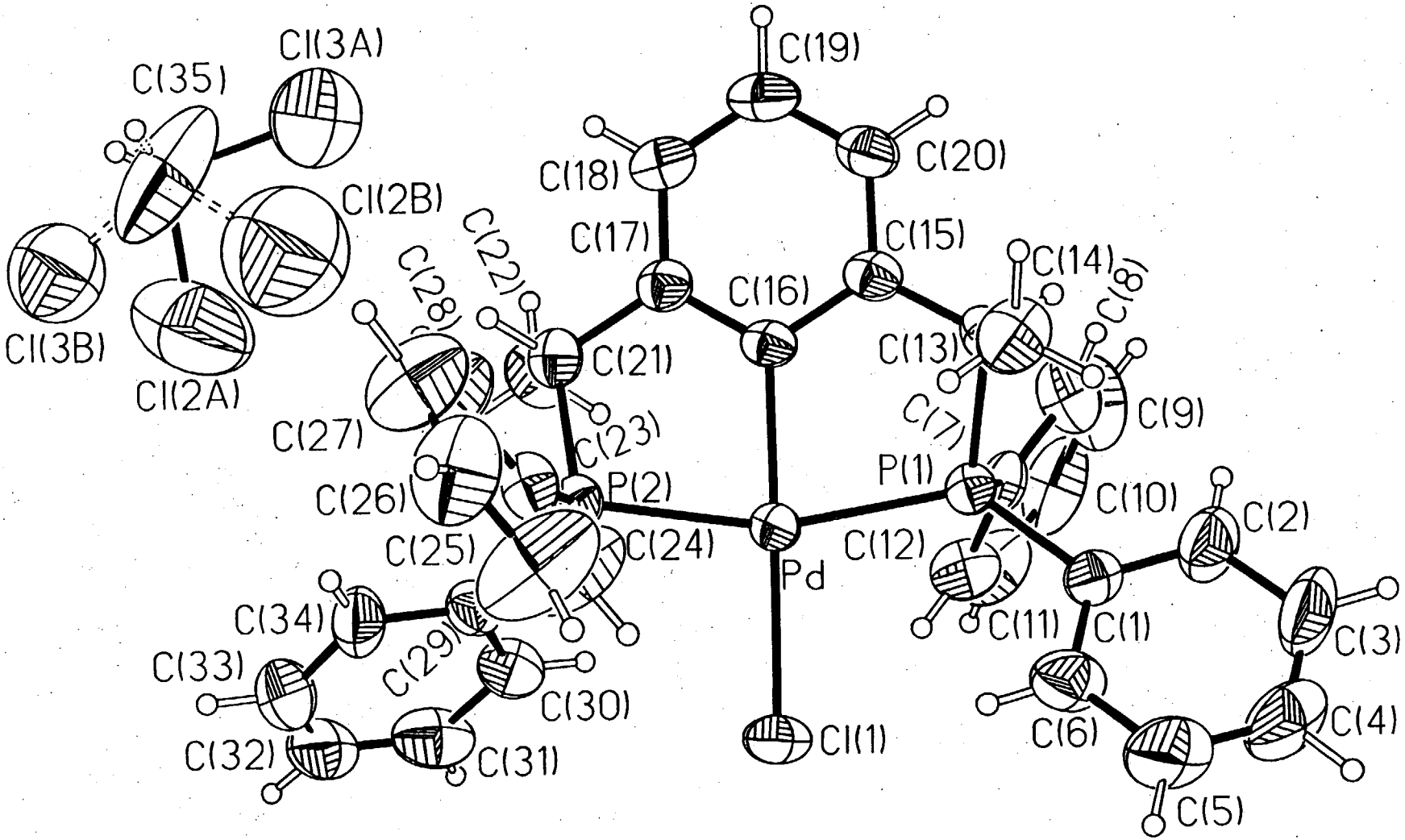
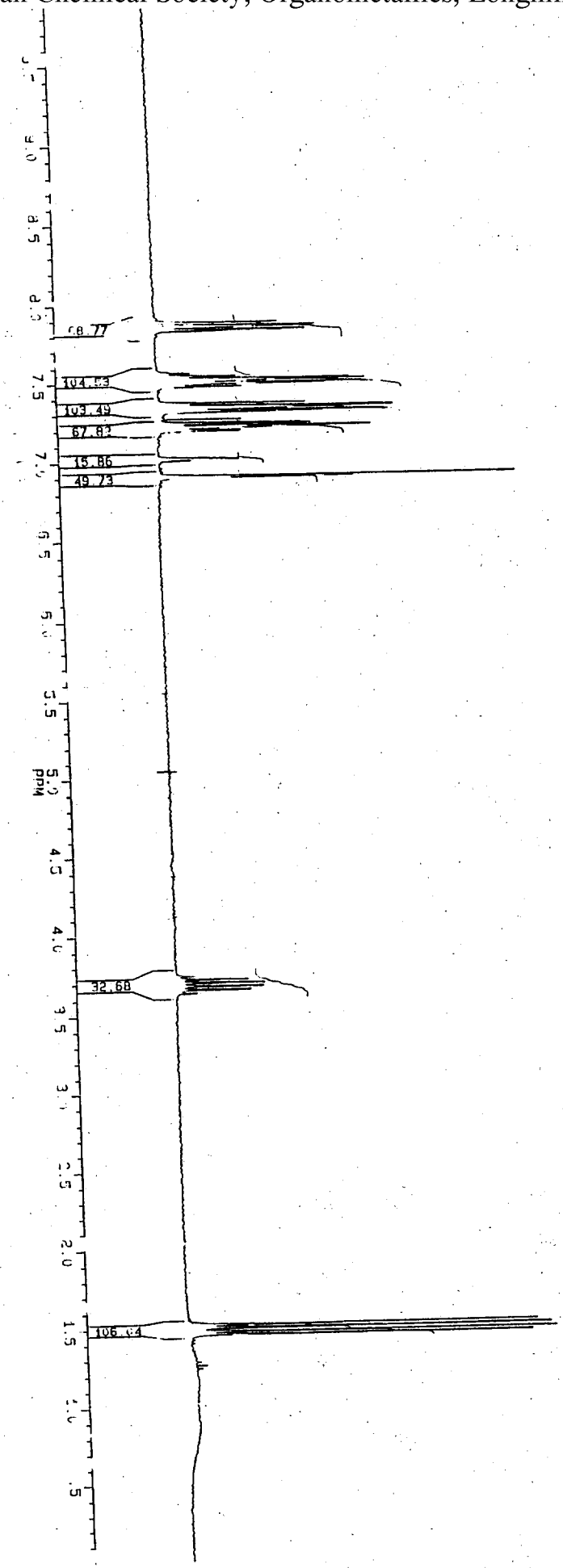
ORGANOMETALLICS
Organometallics, 1998, 17(20), 4374-4379, DOI:10.1021/om980461h



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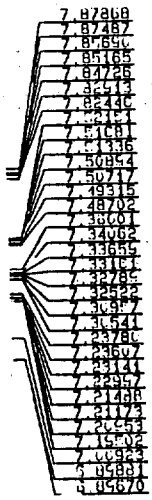
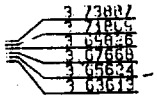
PPM





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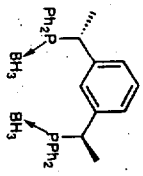
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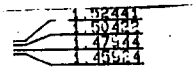

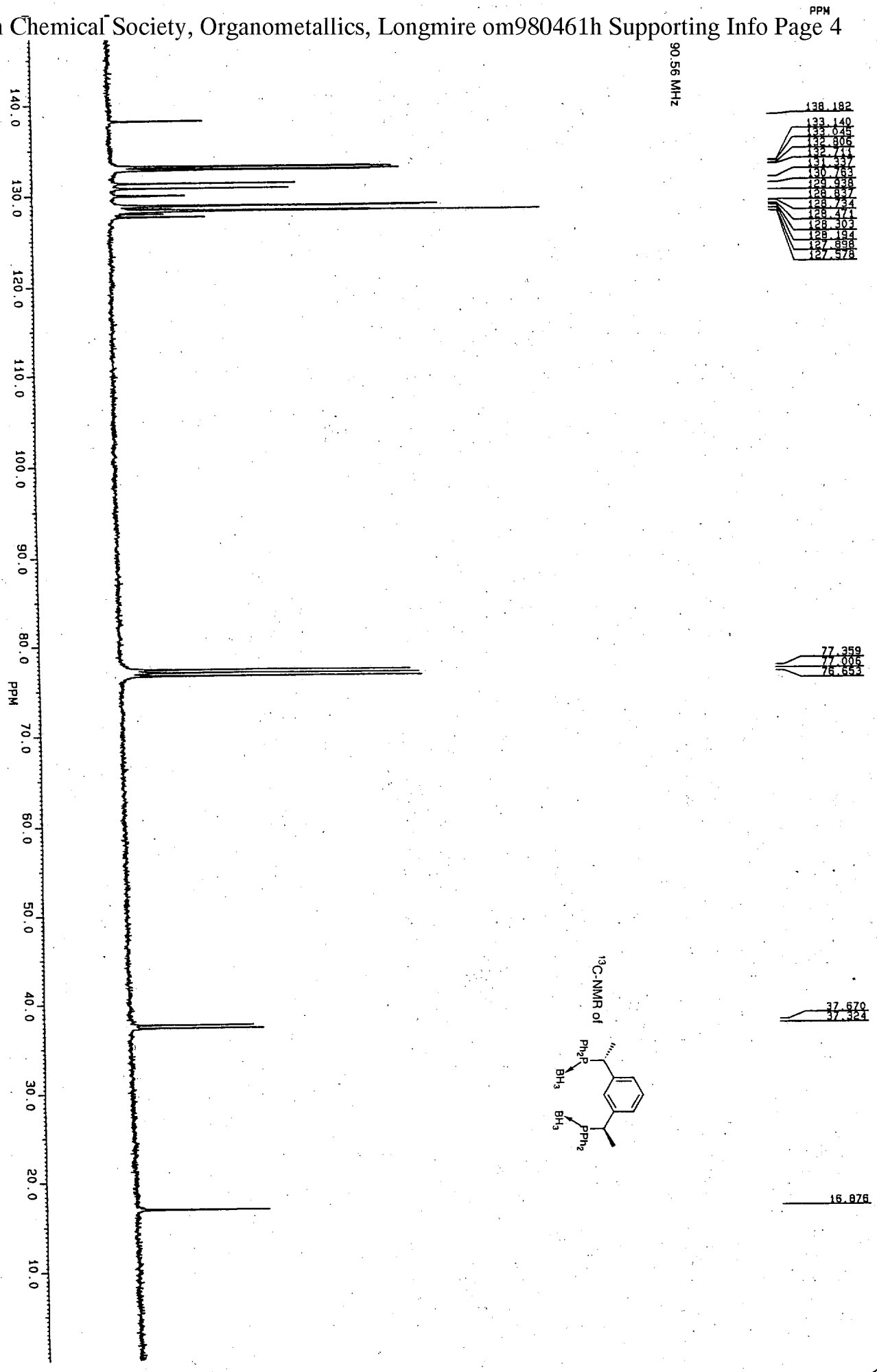

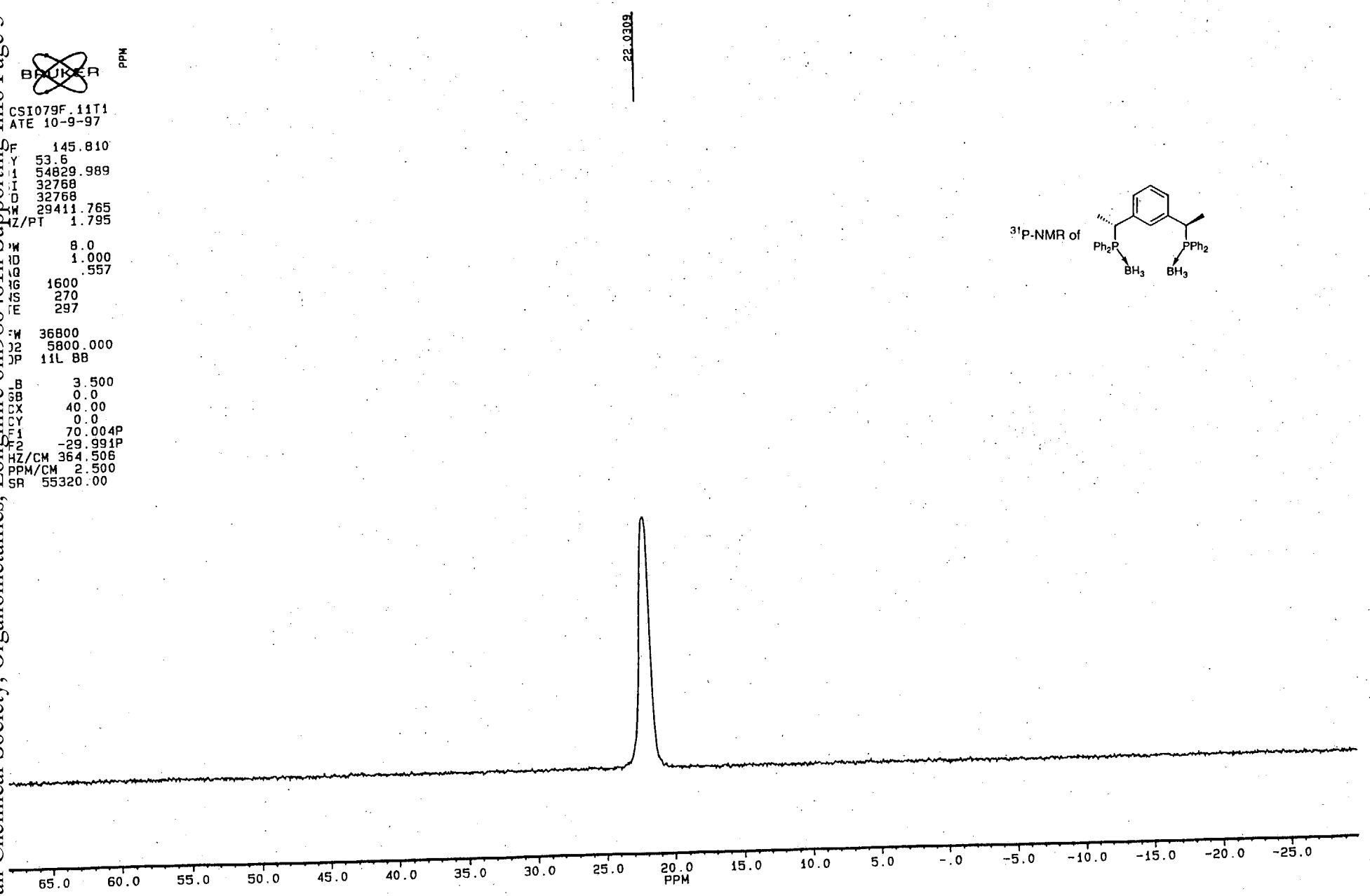

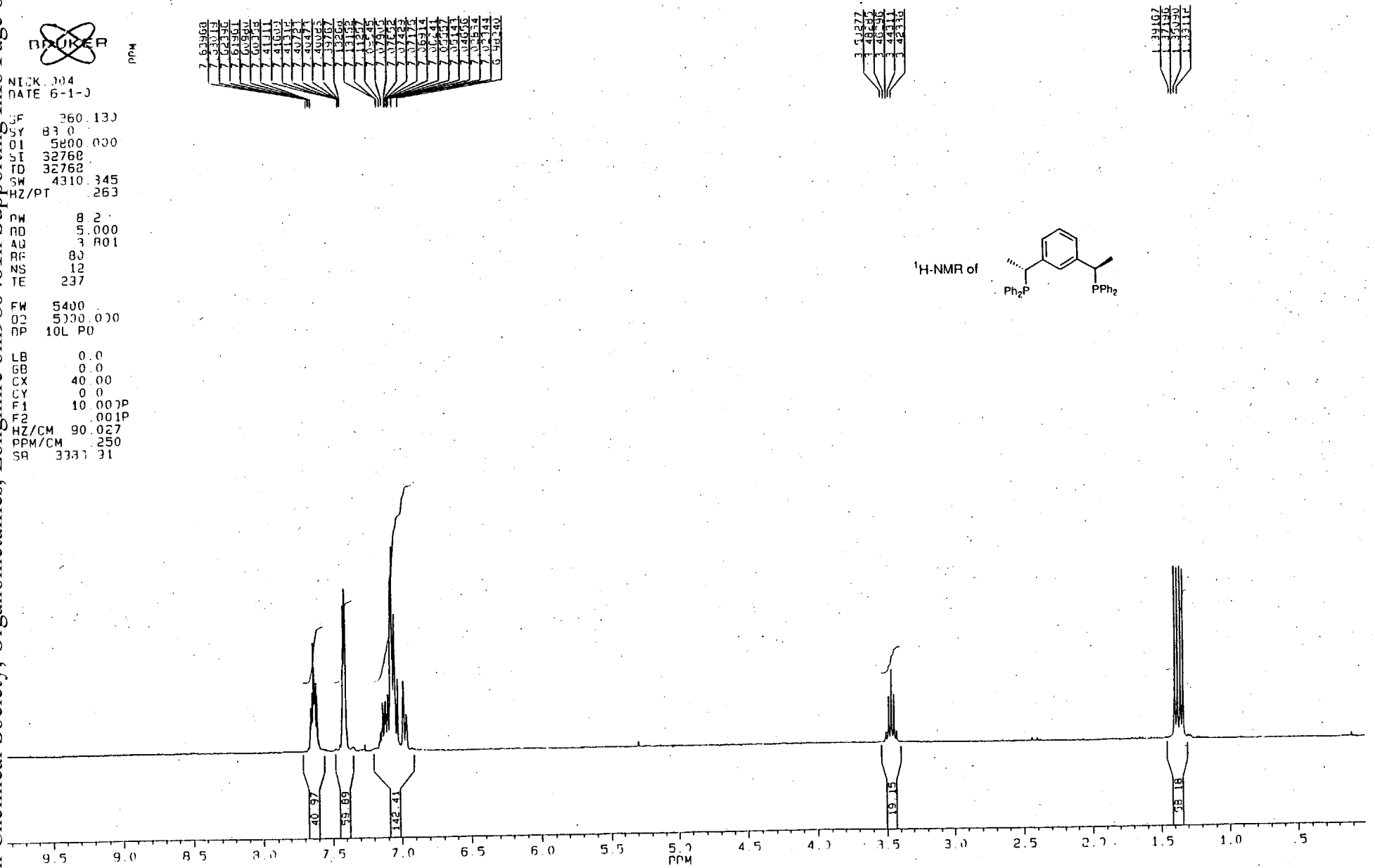

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JL-2-64 FILTERED

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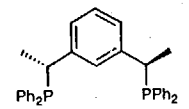

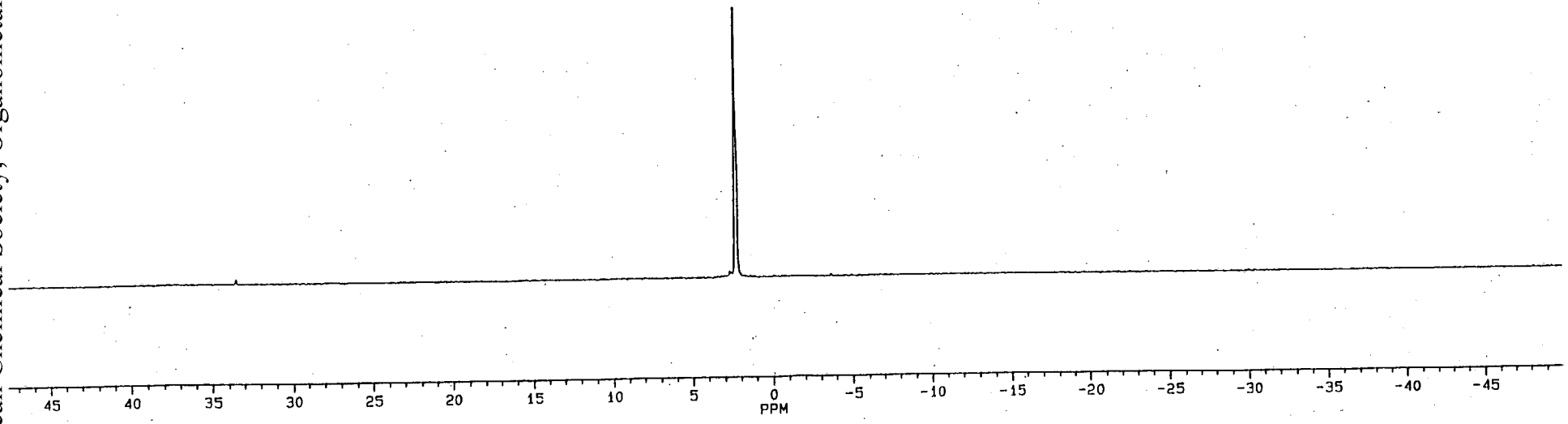

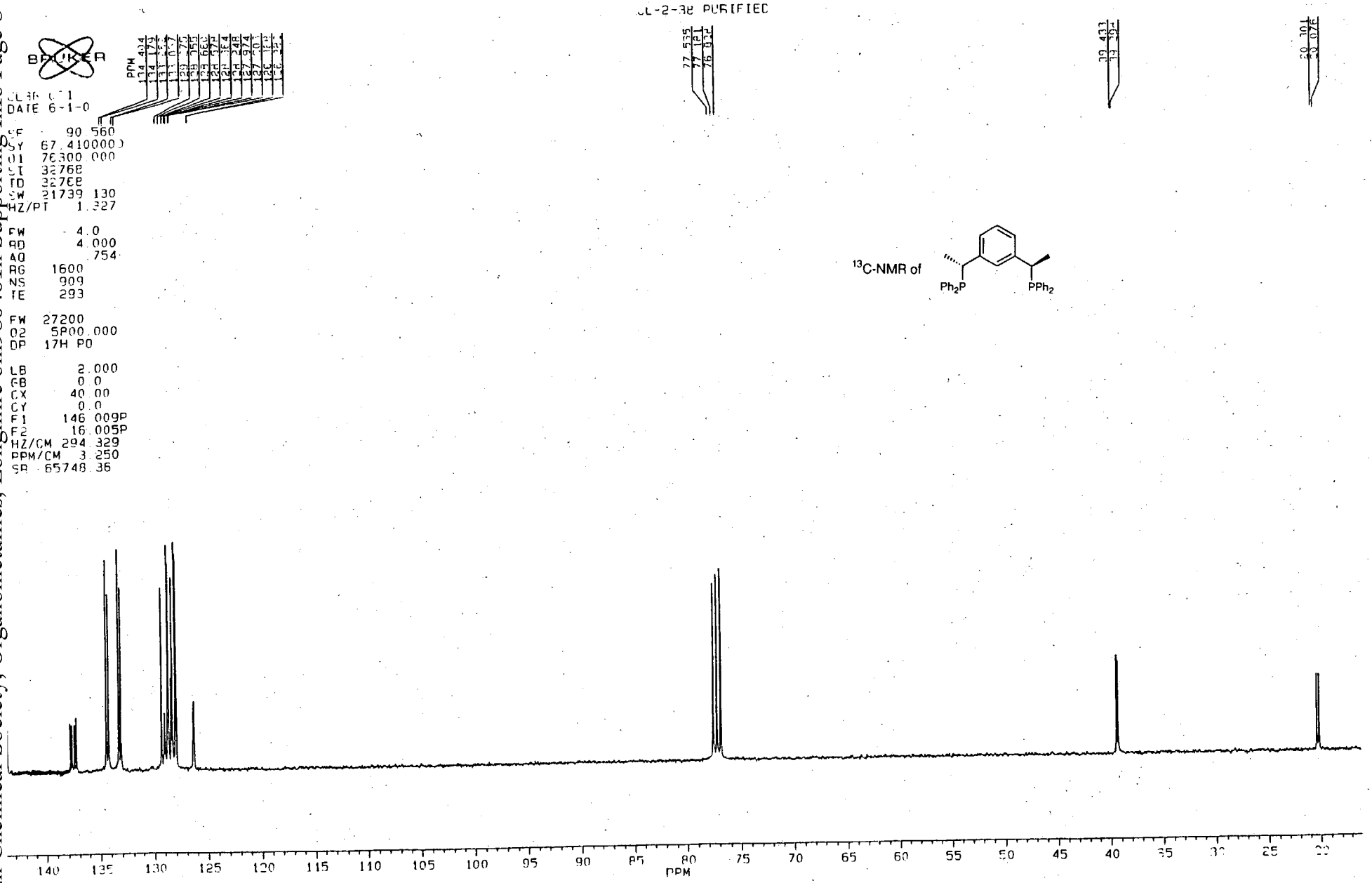

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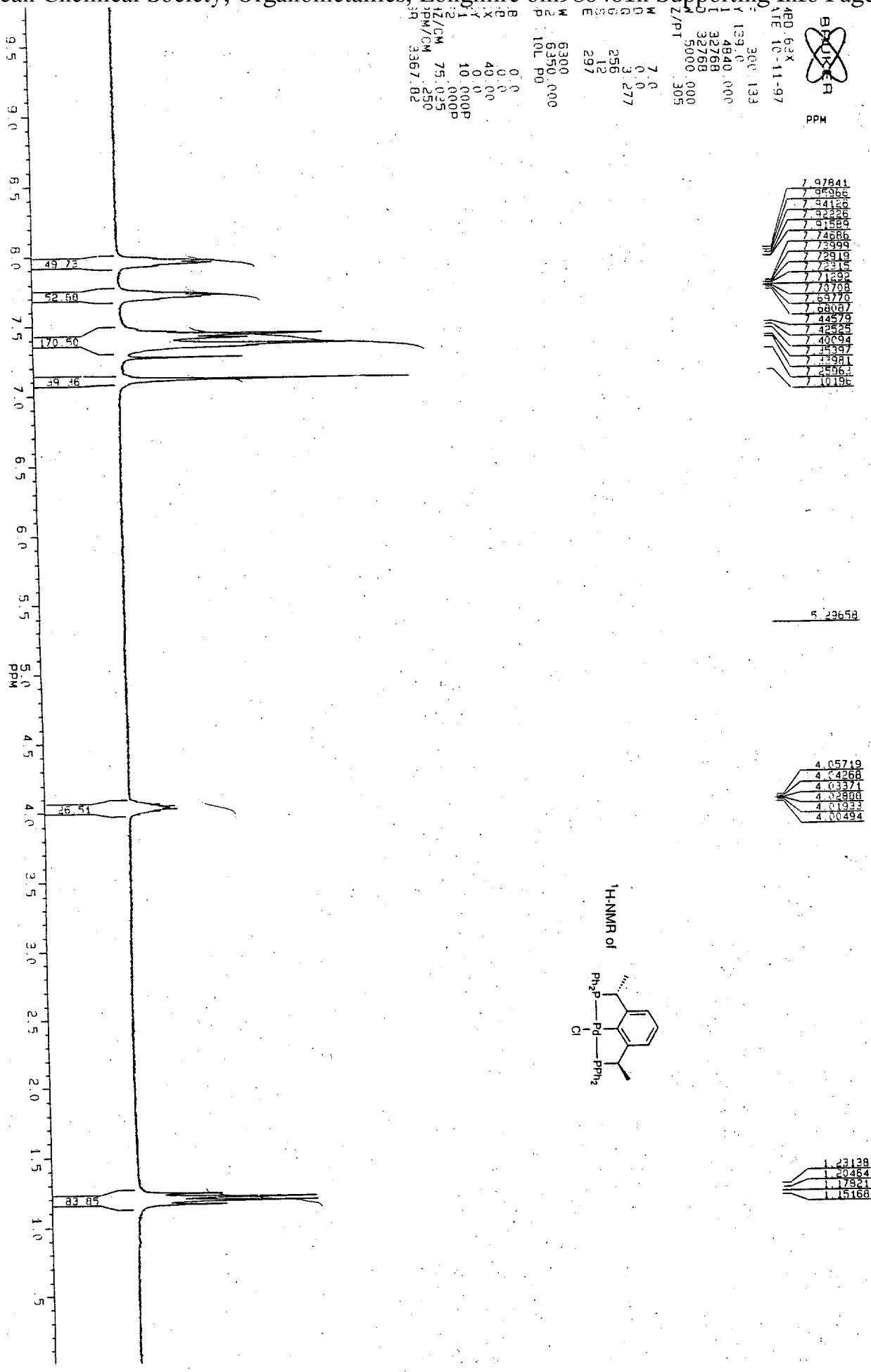
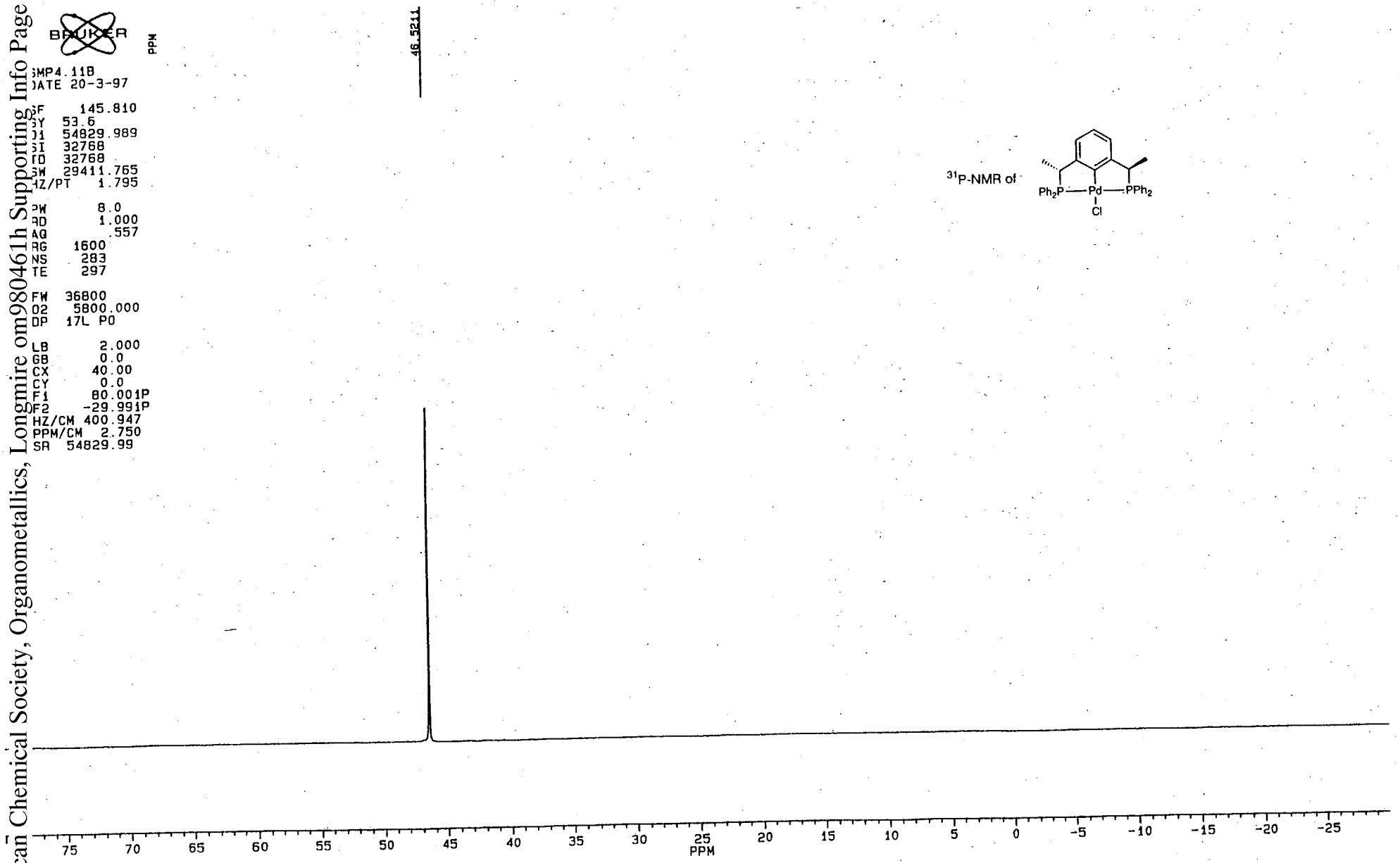


JL-2-65



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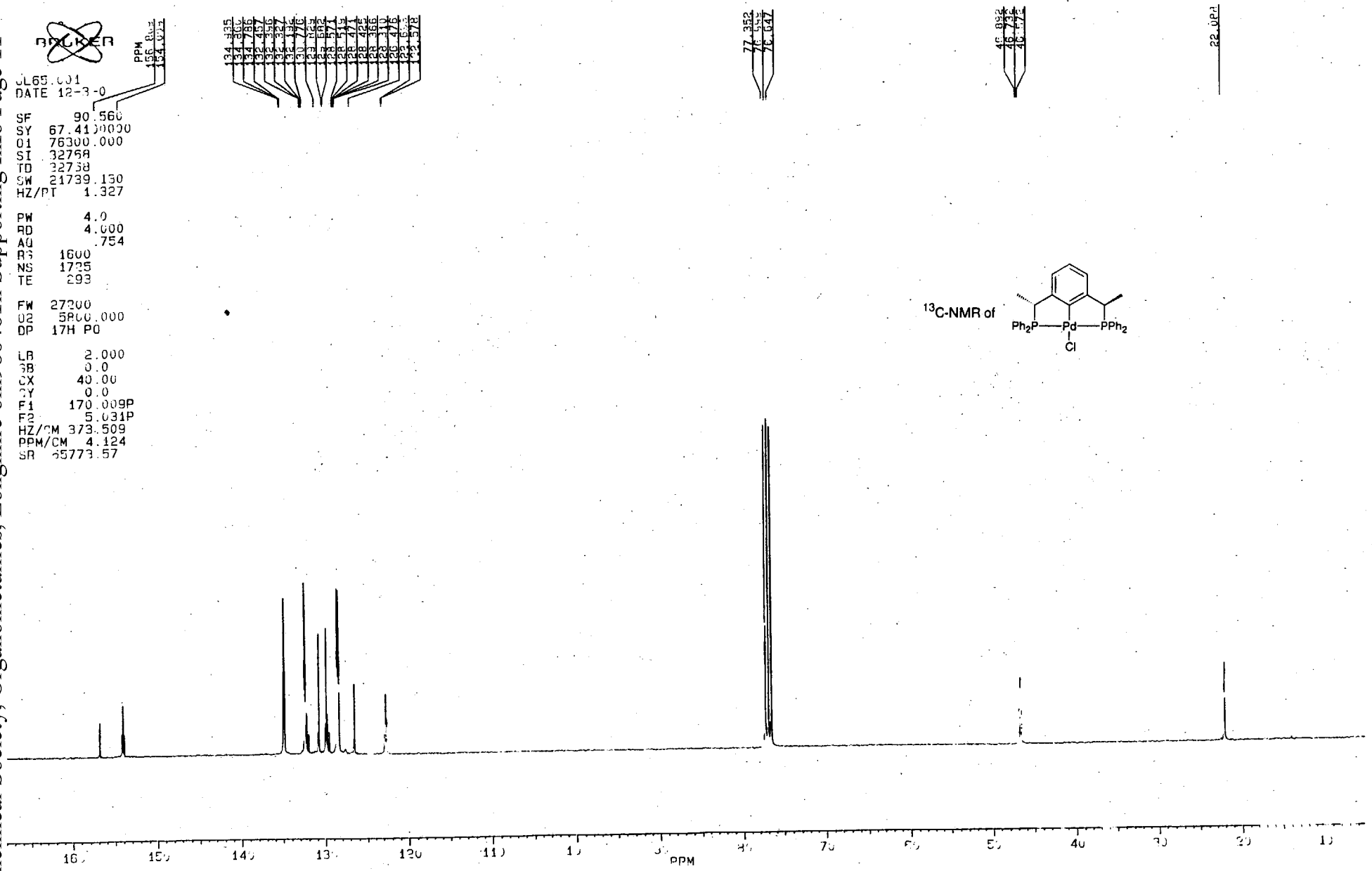

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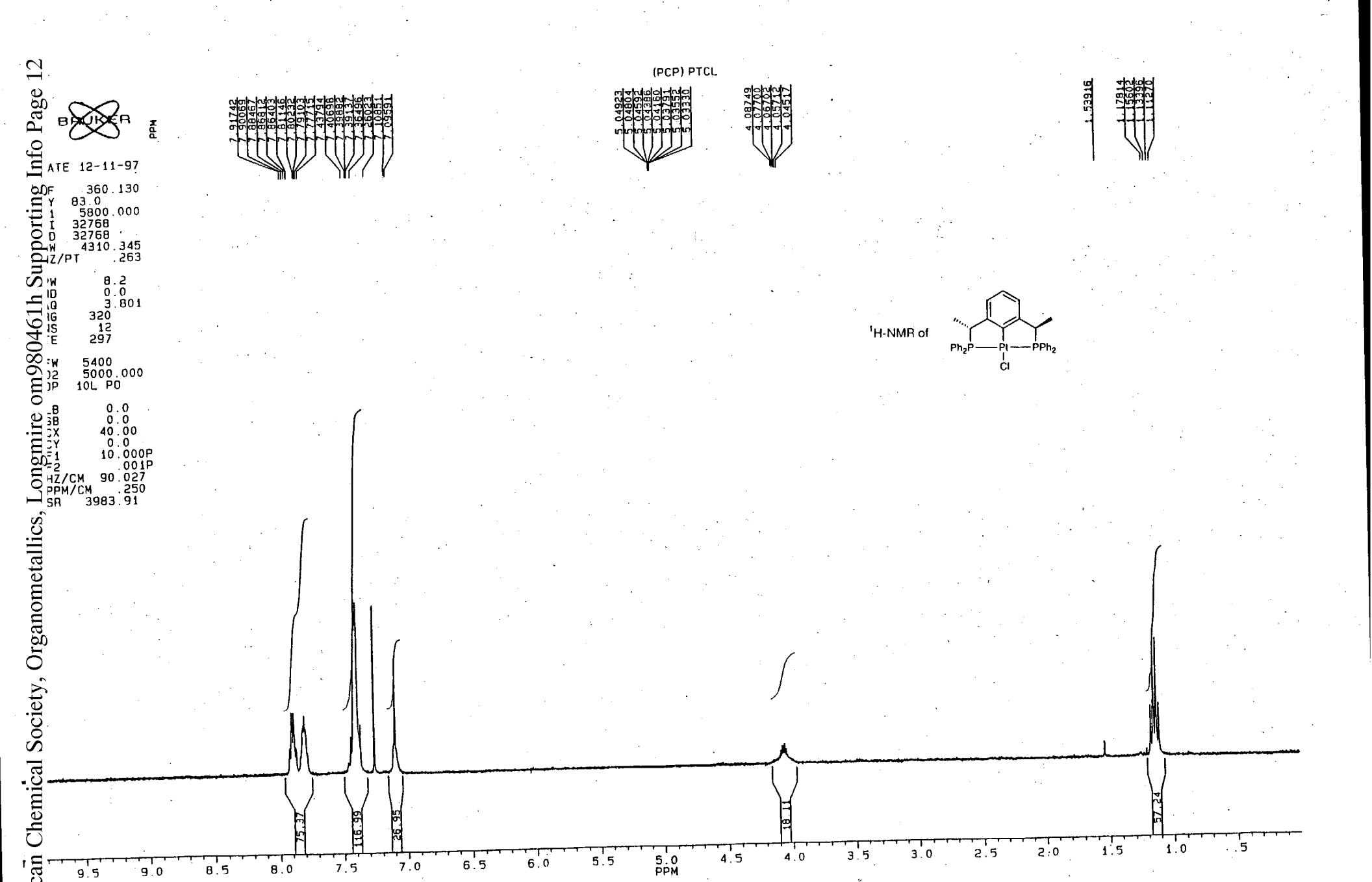

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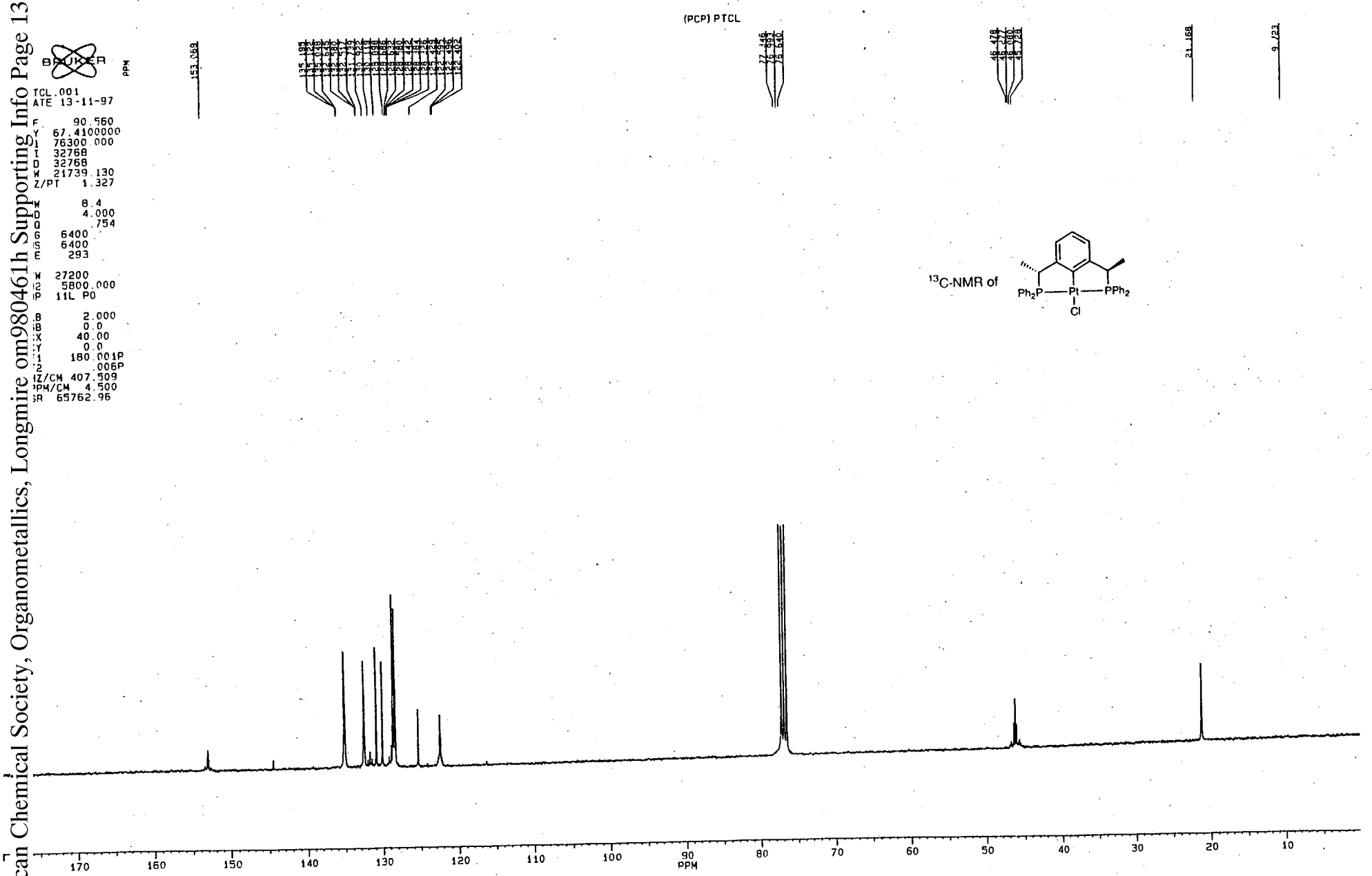

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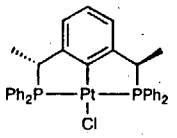

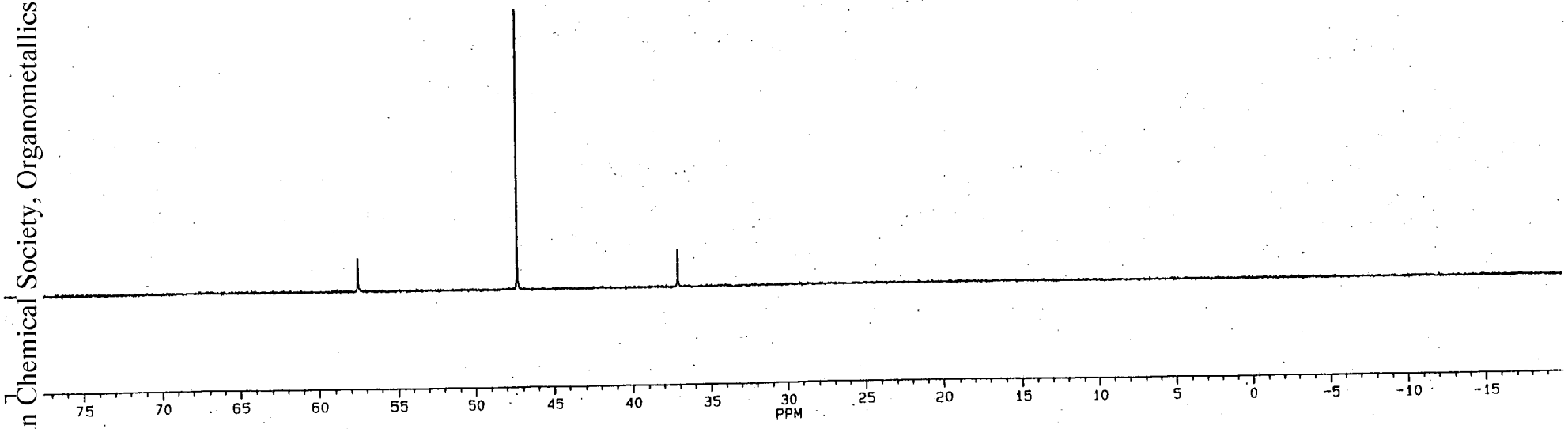

Table S1. Crystal data and structure refinement for (PSP*)PdCl·CH_2Cl_2.

Molecule	(PSP*)PdCl·CH_2Cl_2
Empirical formula	C_{35} H_{33} Cl_3 P_2 Pd
Formula weight	728.30
Crystal system	Monoclinic
Space group	$P2_1$
Unit cell dimensions	a = 9.8710(5) Å
	b = 15.1171(11) Å
	c = 11.5993(8) Å
	β = 98.795(5)°
Volume	1710.5(2) $Å^3$
Z	2
Density (calculated)	1.414 Mg/m^3
F(000)	740
Wavelength	0.71073 Å
Absorption coefficient	0.893 mm^{-1}
Crystal size	0.41 x 0.22 x 0.18 mm
Temperature	293(2) K
Diffractometer	Enraf-Nonius CAD4
Theta range for data collection	2.09 to 24.96°
Index ranges	$-11 \le h \le 0$, $-17 \le k \le 17$, $-13 \le l \le 13$
Scan method	θ/2θ
Scan rate	1.27 - 8.24 °/min (in ω)
Scan width	0.65° + 0.35° tanθ (in ω)
Total data collected	6371
Unique data	6005 [R(int) = 0.0139]
Unique observed data [$I>2\sigma(I)$]	5716
Decay correction	Linear decay (65.9%/69.1h)
Absorption correction	Semi-empirical from psi-scans
Max. and min. transmission	0.9980 and 0.9500
Refinement method	Full-matrix on F^2 (SHELXL-93)
Weighting scheme	sigma weight
Data / restraints / parameters	6005 / 7 / 379
Goodness-of-fit on F^2	1.262

Table S1. continued Page 2.

Final R indices [I>2σ(I)]	R_1 = 0.0325, wR_2 = 0.0820
R indices (all data)	R_1 = 0.0355, wR_2 = 0.0859
Absolute structure parameter	-0.05(3)
Largest diff. peak and hole	0.586 and -0.529 e·Å^{-3}

Table S2. Atomic coordinates and equivalent isotropic displacement parameters U_{eq} for (PSP*)PdCl·CH_2Cl_2.

	x	y	z	U_{eq}(Å^2)[a]
Pd	0.38582(2)	0.50038(2)	0.30816(2)	0.0401(1)
P(1)	0.48803(10)	0.59177(7)	0.45290(9)	0.0422(2)
C(1)	0.5355(5)	0.5601(3)	0.6049(4)	0.0528(11)
C(2)	0.5917(7)	0.6210(5)	0.6852(4)	0.080(2)
C(3)	0.6252(8)	0.5980(6)	0.8018(5)	0.103(2)
C(4)	0.6025(8)	0.5097(8)	0.8343(5)	0.113(3)
C(5)	0.5467(10)	0.4508(6)	0.7560(6)	0.110(3)
C(6)	0.5113(7)	0.4748(4)	0.6375(5)	0.078(2)
C(7)	0.6438(4)	0.6414(3)	0.4169(3)	0.0487(10)
C(8)	0.6740(6)	0.7306(4)	0.4312(6)	0.079(2)
C(9)	0.7977(8)	0.7617(6)	0.4090(7)	0.107(3)
C(10)	0.8915(7)	0.7079(7)	0.3707(6)	0.106(3)
C(11)	0.8629(6)	0.6199(7)	0.3553(6)	0.095(2)
C(12)	0.7374(5)	0.5848(4)	0.3781(5)	0.0718(14)
C(13)	0.3600(4)	0.6799(3)	0.4515(4)	0.0536(11)
C(14)	0.2537(6)	0.6547(5)	0.5289(5)	0.083(2)
C(15)	0.2967(4)	0.6885(3)	0.3266(4)	0.0482(10)
C(16)	0.2903(4)	0.6148(3)	0.2520(4)	0.0440(9)
C(17)	0.2218(4)	0.6233(3)	0.1376(4)	0.0495(10)
C(18)	0.1624(5)	0.7029(3)	0.0978(5)	0.0630(12)
C(19)	0.1711(5)	0.7749(4)	0.1710(5)	0.0690(14)
C(20)	0.2377(5)	0.7686(3)	0.2832(5)	0.0591(12)
C(21)	0.2201(5)	0.5448(3)	0.0539(4)	0.0534(10)
C(22)	0.3296(6)	0.5544(4)	-0.0244(5)	0.0721(14)
P(2)	0.24750(10)	0.44760(7)	0.14811(9)	0.0442(2)
C(23)	0.0817(4)	0.4144(3)	0.1823(4)	0.0535(11)
C(24)	0.0770(7)	0.3640(6)	0.2773(7)	0.114(3)
C(25)	-0.0436(8)	0.3368(8)	0.3075(9)	0.145(4)
C(26)	-0.1646(7)	0.3591(6)	0.2451(7)	0.107(3)
C(27)	-0.1624(6)	0.4113(6)	0.1544(8)	0.114(3)
C(28)	-0.0412(6)	0.4373(5)	0.1215(6)	0.088(2)

Table S2. continued Page 2.

C(29)	0.2993(5)	0.3573(3)	0.0600(4)	0.0539(10)
C(30)	0.4369(5)	0.3446(4)	0.0578(5)	0.0669(13)
C(31)	0.4786(8)	0.2800(4)	-0.0154(6)	0.086(2)
C(32)	0.3818(10)	0.2296(4)	-0.0837(5)	0.095(2)
C(33)	0.2490(9)	0.2414(5)	-0.0782(6)	0.095(2)
C(34)	0.2040(6)	0.3042(4)	-0.0078(5)	0.075(2)
Cl(1)	0.50324(14)	0.36649(8)	0.36590(11)	0.0648(3)
C(35)	-0.0677(11)	0.5423(7)	-0.3432(8)	0.222(9)
Cl(2A)	0.0423(7)	0.4553(4)	-0.2882(8)	0.225(4)[b]
Cl(3A)	-0.0179(7)	0.6281(4)	-0.2319(7)	0.220(4)[b]
Cl(2B)	0.0259(20)	0.5285(14)	-0.2103(10)	0.290(10)[c]
Cl(3B)	-0.0388(12)	0.4506(7)	-0.4389(9)	0.171(4)[c]

[a] $U_{eq} = (1/3)\Sigma_i\Sigma_j U_{ij} a_i^* a_j^* \mathbf{a}_i \cdot \mathbf{a}_j$.

[b] The occupancy coefficient was 0.668(7).

[c] The occupancy coefficient was 0.332(7).

Table S3. Bond lengths (Å) for (PSP*)PdCl·CH_2Cl_2.

Pd-C(16)	2.030(4)	C(14)-H(14C)	0.96
Pd-P(2)	2.2742(11)	C(15)-C(20)	1.403(6)
Pd-P(1)	2.2864(11)	C(15)-C(16)	1.406(6)
Pd-Cl(1)	2.3773(12)	C(16)-C(17)	1.400(6)
P(1)-C(7)	1.816(4)	C(17)-C(18)	1.387(7)
P(1)-C(1)	1.818(4)	C(17)-C(21)	1.531(6)
P(1)-C(13)	1.835(4)	C(18)-C(19)	1.376(8)
C(1)-C(2)	1.365(8)	C(18)-H(18)	0.93
C(1)-C(6)	1.375(8)	C(19)-C(20)	1.368(7)
C(2)-C(3)	1.387(8)	C(19)-H(19)	0.93
C(2)-H(2)	0.93	C(20)-H(20)	0.93
C(3)-C(4)	1.415(13)	C(21)-C(22)	1.521(7)
C(3)-H(3)	0.93	C(21)-P(2)	1.827(5)
C(4)-C(5)	1.328(13)	C(21)-H(21)	0.98
C(4)-H(4)	0.93	C(22)-H(22A)	0.96
C(5)-C(6)	1.413(9)	C(22)-H(22B)	0.96
C(5)-H(5)	0.93	C(22)-H(22C)	0.96
C(6)-H(6)	0.93	P(2)-C(23)	1.813(4)
C(7)-C(12)	1.384(7)	P(2)-C(29)	1.825(5)
C(7)-C(8)	1.386(8)	C(23)-C(24)	1.347(8)
C(8)-C(9)	1.369(8)	C(23)-C(28)	1.352(8)
C(8)-H(8)	0.93	C(24)-C(25)	1.355(9)
C(9)-C(10)	1.357(12)	C(24)-H(24)	0.93
C(9)-H(9)	0.93	C(25)-C(26)	1.342(11)
C(10)-C(11)	1.366(12)	C(25)-H(25)	0.93
C(10)-H(10)	0.93	C(26)-C(27)	1.319(11)
C(11)-C(12)	1.410(9)	C(26)-H(26)	0.93
C(11)-H(11)	0.93	C(27)-C(28)	1.368(8)
C(12)-H(12)	0.93	C(27)-H(27)	0.93
C(13)-C(15)	1.494(7)	C(28)-H(28)	0.93
C(13)-C(14)	1.530(7)	C(29)-C(30)	1.375(7)
C(13)-H(13)	0.98	C(29)-C(34)	1.386(7)
C(14)-H(14A)	0.96	C(30)-C(31)	1.396(8)
C(14)-H(14B)	0.96	C(30)-H(30)	0.93

Table S3. continued Page 2.

C(31)-C(32)	1.375(10)	C(35)-Cl(3A)	1.843(8)
C(31)-H(31)	0.93	C(35)-H(35A)	0.97
C(32)-C(33)	1.334(11)	C(35)-H(35B)	0.97
C(32)-H(32)	0.93	C(35)-Cl(2B)	1.685(9)
C(33)-C(34)	1.371(9)	C(35)-Cl(3B)	1.825(9)
C(33)-H(33)	0.93	C(35)-H(35C)	0.97(2)
C(34)-H(34)	0.93	C(35)-H(35D)	0.97(2)
C(35)-Cl(2A)	1.761(8)		

Table S4. Bond angles (deg) for (PSP*)PdCl·CH_2Cl_2.

– C(16)-Pd-P(2)	81.11(12)	C(9)-C(8)-H(8)	120.3(5)
– C(16)-Pd-P(1)	81.49(12)	C(7)-C(8)-H(8)	120.3(3)
– P(2)-Pd-P(1)	162.53(4)	C(10)-C(9)-C(8)	121.9(7)
– C(16)-Pd-Cl(1)	177.22(12)	C(10)-C(9)-H(9)	119.0(4)
– P(2)-Pd-Cl(1)	97.89(5)	C(8)-C(9)-H(9)	119.0(5)
– P(1)-Pd-Cl(1)	99.57(4)	C(9)-C(10)-C(11)	119.3(6)
C(7)-P(1)-C(1)	103.3(2)	C(9)-C(10)-H(10)	120.4(4)
C(7)-P(1)-C(13)	107.7(2)	C(11)-C(10)-H(10)	120.4(4)
C(1)-P(1)-C(13)	106.0(2)	C(10)-C(11)-C(12)	120.8(7)
C(7)-P(1)-Pd	112.02(14)	C(10)-C(11)-H(11)	119.6(4)
C(1)-P(1)-Pd	124.9(2)	C(12)-C(11)-H(11)	119.6(5)
– C(13)-P(1)-Pd	101.9(2)	C(7)-C(12)-C(11)	118.5(6)
C(2)-C(1)-C(6)	121.0(5)	C(7)-C(12)-H(12)	120.7(3)
C(2)-C(1)-P(1)	120.1(4)	C(11)-C(12)-H(12)	120.7(5)
C(6)-C(1)-P(1)	118.9(4)	C(15)-C(13)-C(14)	111.6(4)
C(1)-C(2)-C(3)	120.5(7)	– C(15)-C(13)-P(1)	104.9(3)
C(1)-C(2)-H(2)	119.7(3)	C(14)-C(13)-P(1)	110.3(4)
C(3)-C(2)-H(2)	119.7(5)	C(15)-C(13)-H(13)	110.0(2)
C(2)-C(3)-C(4)	118.2(7)	C(14)-C(13)-H(13)	110.0(3)
C(2)-C(3)-H(3)	120.9(5)	P(1)-C(13)-H(13)	109.99(14)
C(4)-C(3)-H(3)	120.9(4)	C(13)-C(14)-H(14A)	109.5(3)
C(5)-C(4)-C(3)	121.1(6)	C(13)-C(14)-H(14B)	109.5(3)
C(5)-C(4)-H(4)	119.5(5)	H(14A)-C(14)-H(14B)	109.5
C(3)-C(4)-H(4)	119.5(4)	C(13)-C(14)-H(14C)	109.5(3)
C(4)-C(5)-C(6)	120.6(7)	H(14A)-C(14)-H(14C)	109.5
C(4)-C(5)-H(5)	119.7(5)	H(14B)-C(14)-H(14C)	109.5
C(6)-C(5)-H(5)	119.7(5)	C(20)-C(15)-C(16)	119.0(4)
C(1)-C(6)-C(5)	118.7(7)	C(20)-C(15)-C(13)	120.8(4)
C(1)-C(6)-H(6)	120.7(3)	– C(16)-C(15)-C(13)	120.1(4)
C(5)-C(6)-H(6)	120.7(5)	C(17)-C(16)-C(15)	118.8(4)
C(12)-C(7)-C(8)	119.9(5)	– C(17)-C(16)-Pd	121.0(3)
C(12)-C(7)-P(1)	116.8(4)	– C(15)-C(16)-Pd	120.2(3)
C(8)-C(7)-P(1)	123.2(4)	C(18)-C(17)-C(16)	120.9(4)
C(9)-C(8)-C(7)	119.5(6)	C(18)-C(17)-C(21)	119.9(4)

Table S4. continued Page 2.

C(16)-C(17)-C(21)	119.2(4)	C(25)-C(24)-H(24)	119.2(5)
C(19)-C(18)-C(17)	119.9(5)	C(26)-C(25)-C(24)	122.0(8)
C(19)-C(18)-H(18)	120.1(3)	C(26)-C(25)-H(25)	119.0(5)
C(17)-C(18)-H(18)	120.1(3)	C(24)-C(25)-H(25)	119.0(5)
C(20)-C(19)-C(18)	120.4(5)	C(27)-C(26)-C(25)	117.3(6)
C(20)-C(19)-H(19)	119.8(3)	C(27)-C(26)-H(26)	121.3(4)
C(18)-C(19)-H(19)	119.8(3)	C(25)-C(26)-H(26)	121.3(5)
C(19)-C(20)-C(15)	121.0(5)	C(26)-C(27)-C(28)	121.1(7)
C(19)-C(20)-H(20)	119.5(3)	C(26)-C(27)-H(27)	119.5(4)
C(15)-C(20)-H(20)	119.5(3)	C(28)-C(27)-H(27)	119.5(5)
C(22)-C(21)-C(17)	111.4(4)	C(23)-C(28)-C(27)	122.3(6)
C(22)-C(21)-P(2)	112.3(4)	C(23)-C(28)-H(28)	118.9(3)
C(17)-C(21)-P(2)	104.9(3)	C(27)-C(28)-H(28)	118.9(5)
C(22)-C(21)-H(21)	109.4(3)	C(30)-C(29)-C(34)	119.7(5)
C(17)-C(21)-H(21)	109.4(2)	C(30)-C(29)-P(2)	118.5(4)
P(2)-C(21)-H(21)	109.4(2)	C(34)-C(29)-P(2)	121.8(4)
C(21)-C(22)-H(22A)	109.5(3)	C(29)-C(30)-C(31)	119.5(6)
C(21)-C(22)-H(22B)	109.5(3)	C(29)-C(30)-H(30)	120.2(3)
H(22A)-C(22)-H(22B)	109.5	C(31)-C(30)-H(30)	120.2(4)
C(21)-C(22)-H(22C)	109.5(3)	C(32)-C(31)-C(30)	119.6(6)
H(22A)-C(22)-H(22C)	109.5	C(32)-C(31)-H(31)	120.2(4)
H(22B)-C(22)-H(22C)	109.5	C(30)-C(31)-H(31)	120.2(4)
C(23)-P(2)-C(29)	104.8(2)	C(33)-C(32)-C(31)	120.0(6)
C(23)-P(2)-C(21)	107.3(2)	C(33)-C(32)-H(32)	120.0(4)
C(29)-P(2)-C(21)	107.2(2)	C(31)-C(32)-H(32)	120.0(4)
C(23)-P(2)-Pd	111.6(2)	C(32)-C(33)-C(34)	122.1(7)
C(29)-P(2)-Pd	122.3(2)	C(32)-C(33)-H(33)	118.9(4)
C(21)-P(2)-Pd	102.8(2)	C(34)-C(33)-H(33)	118.9(4)
C(24)-C(23)-C(28)	115.6(5)	C(33)-C(34)-C(29)	119.0(6)
C(24)-C(23)-P(2)	118.7(4)	C(33)-C(34)-H(34)	120.5(4)
C(28)-C(23)-P(2)	125.7(4)	C(29)-C(34)-H(34)	120.5(3)
C(23)-C(24)-C(25)	121.6(7)	Cl(2A)-C(35)-Cl(3A)	100.8(5)
C(23)-C(24)-H(24)	119.2(3)	Cl(2A)-C(35)-H(35A)	111.6(5)

Table S4. continued Page 3.

Cl(3A)-C(35)-H(35A)	111.6(5)	Cl(2B)-C(35)-H(35C)	109.6(13)
Cl(2A)-C(35)-H(35B)	111.6(5)	Cl(3B)-C(35)-H(35C)	109.6(13)
Cl(3A)-C(35)-H(35B)	111.6(5)	Cl(2B)-C(35)-H(35D)	109.6(13)
H(35A)-C(35)-H(35B)	109.4	Cl(3B)-C(35)-H(35D)	109.6(13)
Cl(2B)-C(35)-Cl(3B)	110.3(7)	H(35C)-C(35)-H(35D)	108(2)

Table S5. Anisotropic displacement parameters ($Å^2$) for (PSP*)PdCl·CH_2Cl_2.

	U11	U22	U33	U23	U13	U12
Pd	0.0341(1)	0.0377(1)	0.0487(1)	-0.0008(2)	0.0067(1)	-0.0010(2)
P(1)	0.0361(5)	0.0447(5)	0.0461(6)	-0.0007(4)	0.0072(4)	-0.0002(4)
C(1)	0.055(3)	0.060(3)	0.045(2)	0.005(2)	0.017(2)	0.011(2)
C(2)	0.097(4)	0.089(4)	0.052(3)	0.004(3)	0.006(3)	-0.002(3)
C(3)	0.119(6)	0.142(7)	0.043(3)	-0.009(4)	-0.004(3)	0.019(5)
C(4)	0.133(6)	0.161(8)	0.051(3)	0.023(5)	0.034(3)	0.063(7)
C(5)	0.172(8)	0.102(5)	0.069(4)	0.030(4)	0.058(5)	0.037(5)
C(6)	0.110(5)	0.064(4)	0.067(3)	0.012(2)	0.034(3)	0.012(3)
C(7)	0.039(2)	0.066(3)	0.041(2)	-0.001(2)	0.005(2)	-0.009(2)
C(8)	0.077(4)	0.076(4)	0.087(4)	-0.014(3)	0.029(3)	-0.027(3)
C(9)	0.105(6)	0.117(6)	0.105(5)	-0.015(4)	0.036(5)	-0.068(5)
C(10)	0.059(4)	0.185(9)	0.076(4)	0.009(5)	0.011(3)	-0.055(5)
C(11)	0.046(3)	0.156(8)	0.089(4)	0.020(5)	0.024(3)	0.015(4)
C(12)	0.047(3)	0.085(4)	0.087(4)	0.011(3)	0.022(3)	0.005(3)
C(13)	0.047(2)	0.050(2)	0.065(3)	-0.015(2)	0.011(2)	0.003(2)
C(14)	0.064(3)	0.121(5)	0.068(3)	-0.004(3)	0.023(3)	0.025(3)
C(15)	0.034(2)	0.045(2)	0.066(3)	-0.001(2)	0.011(2)	0.003(2)
C(16)	0.031(2)	0.039(2)	0.063(3)	0.000(2)	0.010(2)	0.000(2)
C(17)	0.040(2)	0.049(2)	0.059(3)	0.003(2)	0.007(2)	0.000(2)
C(18)	0.055(3)	0.062(3)	0.071(3)	0.013(2)	0.008(2)	0.010(2)
C(19)	0.057(3)	0.055(3)	0.094(4)	0.012(3)	0.011(3)	0.018(2)
C(20)	0.054(3)	0.044(2)	0.079(3)	-0.002(2)	0.011(2)	0.005(2)
C(21)	0.046(2)	0.057(2)	0.057(3)	-0.002(2)	0.009(2)	-0.007(2)
C(22)	0.091(4)	0.067(3)	0.066(3)	-0.002(3)	0.034(3)	-0.006(3)
P(2)	0.0347(5)	0.0477(6)	0.0505(6)	-0.0040(5)	0.0077(4)	-0.0040(4)
C(23)	0.036(2)	0.063(3)	0.063(3)	-0.011(2)	0.014(2)	-0.007(2)
C(24)	0.057(3)	0.155(7)	0.129(6)	0.072(6)	0.014(4)	-0.018(4)
C(25)	0.081(5)	0.204(11)	0.152(8)	0.095(8)	0.027(5)	-0.020(6)
C(26)	0.051(3)	0.158(8)	0.117(6)	-0.004(5)	0.030(4)	-0.028(4)
C(27)	0.041(3)	0.160(8)	0.144(7)	0.033(6)	0.023(4)	-0.004(4)
C(28)	0.051(3)	0.125(6)	0.089(4)	0.021(4)	0.011(3)	-0.007(3)

Table S5. continued Page 2.

C(29)	0.059(3)	0.052(2)	0.052(2)	-0.004(2)	0.014(2)	0.004(2)
C(30)	0.064(3)	0.067(3)	0.074(3)	-0.003(3)	0.024(3)	0.008(3)
C(31)	0.099(5)	0.083(4)	0.089(4)	0.009(4)	0.052(4)	0.030(4)
C(32)	0.159(8)	0.078(4)	0.051(3)	-0.009(3)	0.024(4)	0.038(5)
C(33)	0.123(6)	0.086(4)	0.071(4)	-0.026(3)	0.001(4)	0.016(4)
C(34)	0.077(4)	0.083(4)	0.060(3)	-0.020(3)	-0.005(3)	0.003(3)
Cl(1)	0.0741(8)	0.0484(6)	0.0729(7)	0.0102(5)	0.0140(6)	0.0167(6)
C(35)	0.129(8)	0.421(30)	0.105(7)	0.027(11)	-0.015(6)	0.011(12)
Cl(2A)	0.182(6)	0.141(4)	0.358(12)	-0.024(6)	0.065(6)	0.016(4)
Cl(3A)	0.189(6)	0.167(5)	0.275(8)	-0.036(5)	-0.057(5)	0.004(4)

The anisotropic displacement factor exponent takes the form:

$-2\pi^2 [h^2 a^{*2} U11 + ... + 2 h k a^* b^* U12]$

Table S6. Hydrogen coordinates and isotropic displacement parameters (Å^2) for (PSP*)PdCl·CH_2Cl_2.

	x	y	z	U_{iso}(Å^2)
H(2)	0.6076(7)	0.6783(5)	0.6614(4)	0.096
H(3)	0.6617(8)	0.6396(6)	0.8572(5)	0.124
H(4)	0.6270(8)	0.4925(8)	0.9117(5)	0.136
H(5)	0.5307(10)	0.3934(6)	0.7795(6)	0.132
H(6)	0.4725(7)	0.4336(4)	0.5826(5)	0.094
H(8)	0.6106(6)	0.7692(4)	0.4557(6)	0.094
H(9)	0.8181(8)	0.8214(6)	0.4205(7)	0.129
H(10)	0.9743(7)	0.7307(7)	0.3551(6)	0.128
H(11)	0.9271(6)	0.5826(7)	0.3295(6)	0.115
H(12)	0.7178(5)	0.5249(4)	0.3673(5)	0.086
H(13)	0.4051(4)	0.7355(3)	0.4789(4)	0.064
H(14A)	0.2976(6)	0.6496(5)	0.6084(5)	0.124
H(14B)	0.2126(6)	0.5991(5)	0.5034(5)	0.124
H(14C)	0.1841(6)	0.6995(5)	0.5234(5)	0.124
H(18)	0.1167(5)	0.7076(3)	0.0217(5)	0.076
H(19)	0.1314(5)	0.8283(4)	0.1441(5)	0.083
H(20)	0.2441(5)	0.8181(3)	0.3313(5)	0.071
H(21)	0.1298(5)	0.5408(3)	0.0055(4)	0.064
H(22A)	0.3261(6)	0.5043(4)	-0.0757(5)	0.108
H(22B)	0.4183(6)	0.5574(4)	0.0228(5)	0.108
H(22C)	0.3135(6)	0.6076(4)	-0.0697(5)	0.108
H(24)	0.1586(7)	0.3474(6)	0.3234(7)	0.136
H(25)	-0.0424(8)	0.3017(8)	0.3734(9)	0.174
H(26)	-0.2467(7)	0.3385(6)	0.2651(7)	0.128
H(27)	-0.2447(6)	0.4308(6)	0.1120(8)	0.137
H(28)	-0.0434(6)	0.4720(5)	0.0549(6)	0.106
H(30)	0.5016(5)	0.3787(4)	0.1047(5)	0.080
H(31)	0.5713(8)	0.2712(4)	-0.0180(6)	0.104
H(32)	0.4089(10)	0.1872(4)	-0.1336(5)	0.114
H(33)	0.1849(9)	0.2058(5)	-0.1236(6)	0.114
H(34)	0.1108(6)	0.3112(4)	-0.0056(5)	0.090

Table S6. continued Page 2.

H(35A)	-0.1633(11)	0.5259(7)	-0.3474(8)	0.266
H(35B)	-0.0507(11)	0.5612(7)	-0.4197(8)	0.266
H(35C)	-0.0423(20)	0.5975(14)	-0.3769(10)	0.266
H(35D)	-0.1642(20)	0.5454(14)	-0.3361(10)	0.266

Table S7. Selected torsion angles (deg) for (PSP*)PdCl·CH_2Cl_2.

-89.88 (0.20)	C16 - Pd - P1 - C7
-94.85 (0.20)	P2 - Pd - P1 - C7
87.51 (0.17)	Cl1 - Pd - P1 - C7
144.36 (0.21)	C16 - Pd - P1 - C1
139.39 (0.20)	P2 - Pd - P1 - C1
-38.25 (0.18)	Cl1 - Pd - P1 - C1
25.02 (0.20)	C16 - Pd - P1 - C13
20.05 (0.22)	P2 - Pd - P1 - C13
-157.59 (0.16)	Cl1 - Pd - P1 - C13
53.02 (0.48)	C7 - P1 - C1 - C2
-60.11 (0.49)	C13 - P1 - C1 - C2
-177.60 (0.38)	Pd - P1 - C1 - C2
-128.31 (0.44)	C7 - P1 - C1 - C6
118.56 (0.45)	C13 - P1 - C1 - C6
1.07 (0.50)	Pd - P1 - C1 - C6
-0.20 (0.93)	C6 - C1 - C2 - C3
178.44 (0.52)	P1 - C1 - C2 - C3
1.40 (1.07)	C1 - C2 - C3 - C4
-2.01 (1.17)	C2 - C3 - C4 - C5
1.40 (1.18)	C3 - C4 - C5 - C6
-0.46 (0.90)	C2 - C1 - C6 - C5
-179.11 (0.51)	P1 - C1 - C6 - C5
-0.15 (1.07)	C4 - C5 - C6 - C1
87.58 (0.40)	C1 - P1 - C7 - C12
-160.58 (0.39)	C13 - P1 - C7 - C12
-49.28 (0.40)	Pd - P1 - C7 - C12
-89.71 (0.47)	C1 - P1 - C7 - C8
22.12 (0.49)	C13 - P1 - C7 - C8
133.42 (0.42)	Pd - P1 - C7 - C8
-1.38 (0.89)	C12 - C7 - C8 - C9
175.84 (0.50)	P1 - C7 - C8 - C9
1.47 (1.11)	C7 - C8 - C9 - C10
-0.95 (1.18)	C8 - C9 - C10 - C11
0.36 (1.11)	C9 - C10 - C11 - C12
0.81 (0.82)	C8 - C7 - C12 - C11
-176.59 (0.45)	P1 - C7 - C12 - C11
-0.30 (0.97)	C10 - C11 - C12 - C7
84.17 (0.32)	C7 - P1 - C13 - C15
-165.81 (0.30)	C1 - P1 - C13 - C15
-33.85 (0.31)	Pd - P1 - C13 - C15
-155.56 (0.35)	C7 - P1 - C13 - C14
-45.55 (0.42)	C1 - P1 - C13 - C14
86.42 (0.35)	Pd - P1 - C13 - C14
86.63 (0.56)	C14 - C13 - C15 - C20
-153.94 (0.36)	P1 - C13 - C15 - C20
-90.60 (0.52)	C14 - C13 - C15 - C16
28.83 (0.48)	P1 - C13 - C15 - C16
-1.72 (0.61)	C20 - C15 - C16 - C17
175.56 (0.38)	C13 - C15 - C16 - C17
175.73 (0.32)	C20 - C15 - C16 - Pd
-6.99 (0.53)	C13 - C15 - C16 - Pd
-18.11 (0.30)	P2 - Pd - C16 - C17
163.39 (0.33)	P1 - Pd - C16 - C17
50.91 (2.61)	Cl1 - Pd - C16 - C17
164.49 (0.33)	P2 - Pd - C16 - C15
-14.00 (0.30)	P1 - Pd - C16 - C15
-126.48 (2.38)	Cl1 - Pd - C16 - C15
0.59 (0.62)	C15 - C16 - C17 - C18
-176.84 (0.34)	Pd - C16 - C17 - C18
177.11 (0.38)	C15 - C16 - C17 - C21
-0.32 (0.52)	Pd - C16 - C17 - C21
0.37 (0.72)	C16 - C17 - C18 - C19
-176.12 (0.45)	C21 - C17 - C18 - C19
-0.18 (0.81)	C17 - C18 - C19 - C20
-1.00 (0.80)	C18 - C19 - C20 - C15
1.95 (0.70)	C16 - C15 - C20 - C19
-175.31 (0.45)	C13 - C15 - C20 - C19
78.58 (0.56)	C18 - C17 - C21 - C22
-97.97 (0.49)	C16 - C17 - C21 - C22
-159.64 (0.37)	C18 - C17 - C21 - P2

Table S7. continued Page 2.

23.82	(0.46)	C16 - C17 - C21 - P2
-153.69	(0.36)	C22 - C21 - P2 - C23
85.16	(0.32)	C17 - C21 - P2 - C23
-41.60	(0.42)	C22 - C21 - P2 - C29
-162.76	(0.28)	C17 - C21 - P2 - C29
88.53	(0.36)	C22 - C21 - P2 - Pd
-32.63	(0.30)	C17 - C21 - P2 - Pd
-88.27	(0.22)	C16 - Pd - P2 - C23
-83.29	(0.22)	P1 - Pd - P2 - C23
94.36	(0.19)	Cl1 - Pd - P2 - C23
146.59	(0.22)	C16 - Pd - P2 - C29
151.56	(0.21)	P1 - Pd - P2 - C29
-30.79	(0.19)	Cl1 - Pd - P2 - C29
26.44	(0.19)	C16 - Pd - P2 - C21
31.41	(0.21)	P1 - Pd - P2 - C21
-150.94	(0.16)	Cl1 - Pd - P2 - C21
87.32	(0.61)	C29 - P2 - C23 - C24
-158.98	(0.60)	C21 - P2 - C23 - C24
-47.08	(0.63)	Pd - P2 - C23 - C24
-94.12	(0.57)	C29 - P2 - C23 - C28
19.58	(0.60)	C21 - P2 - C23 - C28
131.48	(0.52)	Pd - P2 - C23 - C28
1.45	(1.37)	C28 - C23 - C24 - C25
-179.85	(0.90)	P2 - C23 - C24 - C25
-0.52	(1.88)	C23 - C24 - C25 - C26
-2.14	(1.81)	C24 - C25 - C26 - C27
3.77	(1.55)	C25 - C26 - C27 - C28
0.21	(1.15)	C24 - C23 - C28 - C27
-178.39	(0.64)	P2 - C23 - C28 - C27
-2.93	(1.42)	C26 - C27 - C28 - C23
-155.07	(0.42)	C23 - P2 - C29 - C30
91.14	(0.44)	C21 - P2 - C29 - C30
-26.91	(0.49)	Pd - P2 - C29 - C30
27.67	(0.50)	C23 - P2 - C29 - C34
-86.12	(0.48)	C21 - P2 - C29 - C34
155.82	(0.39)	Pd - P2 - C29 - C34
1.88	(0.81)	C34 - C29 - C30 - C31
-175.45	(0.42)	P2 - C29 - C30 - C31
-0.49	(0.89)	C29 - C30 - C31 - C32
-1.16	(1.01)	C30 - C31 - C32 - C33
1.44	(1.12)	C31 - C32 - C33 - C34
-0.04	(1.07)	C32 - C33 - C34 - C29
-1.63	(0.88)	C30 - C29 - C34 - C33
175.60	(0.50)	P2 - C29 - C34 - C33

EXPERIMENTAL

DATA COLLECTION

A colorless block-like crystal of (PCP*)PtCl·THF having approximate dimensions of 0.40 x 0.28 x 0.25 mm was mounted on a glass fiber in a random orientation. Preliminary examination and data collection were performed with MoKα radiation (λ = 0.71073 Å) on an Enraf-Nonius CAD4 computer controlled kappa axis diffractometer equipped with a graphite crystal, incident beam monochromator.

Cell constants and an orientation matrix for data collection were obtained from least-squares refinement, using the setting angles of 25 reflections in the range $34° < 2\theta < 36°$, measured by the computer controlled diagonal slit method of centering. The monoclinic cell parameters and calculated volume are: a = 9.956(2), b = 14.7439(13), c = 11.892(2) Å, β = 97.810(9)°, V = 1729.4(5) $Å^3$. For Z = 2 and F.W. = 804.17 the calculated density is 1.544 g/cm^3. As a check on crystal quality, an omega/theta profile analysis of reflections was carried out, which showed that Δω was less than 0.55° and Δθ was less than 0.60°, indicating good crystal quality. From the following systematic absence

$$0k0: \; k = 2n + 1$$

and the results of final structure refinement; the space group was determined to be $P2_1$ (No. 4).

The data were collected at a temperature of 20°C using the ω/2θ scan technique. The scan rate varied from 1.37 to 8.24°/min (in ω). The variable scan rate allows rapid data collection for intense reflections where a fast scan rate is used and assures good counting statistics for weak reflections and reflections with even negative intensity counts, where a slow scan rate is used. Data were collected to a maximum 2θ of 50.0°. The scan range (in degrees) was determined as a function of θ to correct for the separation of the Kα doublet; the scan width was calculated as follows:

$$\omega \text{ scan width} = 0.65° + 0.35°\tan\theta$$

Moving-crystal static-background counts were made by scanning an additional 25% nabove and below this range. Thus the ratio of peak counting time to

background counting time was 2:1. The counter aperture was also adjusted as a function of θ. The horizontal aperture width ranged from 2.0 to 2.4 mm; the vertical aperture was set at 4.0 mm. The diameter of the incident beam collimator was 0.8 mm and the crystal to detector distance was 21 cm. For intense reflections an attenuator was automatically inserted in front of the detector; the attenuator factor was 19.455.

A total of 6374 reflections were collected. As a check on crystal and electronic stability 3 representative reflections were measured every 120 minutes of X-ray exposure. An intensity loss of 27.4% was found for the three standard reflections during 42.1 hours of X-ray exposure for the data collection, therefore a linear decay correction was made to the data.

DATA REDUCTION

SDP software was used to precess intensity data on a VAXstation 3200 computer.[1] Lorentz and polarization corrections were applied to the data. The linear absorption coefficient is 42.55 cm^{-1} for MoKα radiation. An empirical absorption correction based on a series of psi-scans was applied to the data. Relative transmission coefficients ranged from 0.9988 to 0.8932.

STRUCTURE SOLUTION AND REFINEMENT

Structure solution and refinement were performed on a PC by using the SHELXTL package.[2] Most of the nonhydrogen atoms were located by the direct method, the remaining nonhydrogen atoms were found in succeeding difference Fourier synthesis. Least-squares refinement was carried out on F^2 for all reflections. After all nonhydrogen atoms were refined anisotropically, difference Fourier synthesis located all hydrogen atoms. In the final refinement the hydrogen atoms were treated with riding models. All reflections, including those with negative intensities, were included in the refinement and the $I > 2\sigma(I)$ criterion was used only for calculating R_1. The refinement converged to a final value of $R_1 = 0.0218$ and $wR_2 = 0.0551$ for observed unique reflections ($I > 2\sigma(I)$) and $R_1 = 0.0234$ and $wR_2 = 0.0569$ for

all unique reflections including those with negative intensities. The weighted R-factors, wR, are based on F^2 and conventional R-factors, R, on F, with F set to zero for negative intensities. The maximum and minimum residual electron densities on the final difference Fourier map were 0.379 e/Å^3 and -0.428 e/Å^3, respectively. All e.s.d's were estimated by the use of the full covariance matrix. The cell e.s.d's were included in the estimation of e.s.d's of bond distances and angles.

Refinement on its enantiomorph yielded consistently higher values for the above four convergence factors: 0.0562, 0.1518, 0.058, and 0.1527, and a detrimental value of 1.04(2) for the Flack absolute structure parameter, which fully confirmed the correctness of the above established enantiomorph.[3]

REFERENCES

(1) B. A. Frenz, ''The Enraf-Nonius CAD4 SDP - A Real-time System for Concurent X-Ray Data Collection and Crystal Structure Determination,'' in Computing in Crystallography, H. Schenk, R. Olthof-Hazelkamp, H. vanKonigsveld, and G. C. Bassi, Eds, Delft University Press. Delft, Holland, 1978, pp 64-71.

(2) SHELXTL V.5, Siemens Industrial Automation, Inc. 1994.

(3) H. D. Flack, Acta Cryst. A39 (1983) 876.

Table S1. Crystal data and structure refinement for (PCP*)PtCl·THF.

Molecule	(PCP*)PtCl·THF
Empirical formula	C_{38} H_{39} Cl O P_2 Pt
Formula weight	804.17
Crystal system	Monoclinic
Space group	$P2_1$
Unit cell dimensions	a = 9.956(2) Å
	b = 14.7439(13) Å
	c = 11.892(2) Å
	β = 97.810(9)°
Volume	1729.4(5) $Å^3$
Z	2
Density (calculated)	1.544 Mg/m^3
F(000)	800
Wavelength	0.71073 Å
Absorption coefficient	4.255 mm^{-1}
Crystal size	0.40 x 0.28 x 0.25 mm
Temperature	293(2) K
Diffractometer	Enraf-Nonius CAD4
Theta range for data collection	2.06 to 24.97 deg.
Index ranges	$-11 \le h \le 11$, $-17 \le k \le 17$, $0 \le l \le 14$
Scan method	θ/2θ
Scan rate	1.37 - 8.24 °/min (in ω)
Scan width	0.65° + 0.35° tanθ (in ω)
Total data collected	6374
Unique data	6067 [R(int) = 0.0381]
Unique observed data [$I>2\sigma(I)$]	5863
Decay correction	Linear decay (-27.4%/42.1 h.)
Absorption correction	Semi-empirical from psi-scans
Max. and min. transmission	0.9988 and 0.8932
Refinement method	Full-matrix on F^2 (SHELXL-93)
Weighting scheme	sigma weight
Data / restraints / parameters	6067 / 1 / 388
Goodness-of-fit on F^2	1.095

Table S1. continued Page 2.

Final R indices [I>2σ(I)]	R_1 = 0.0218, wR_2 = 0.0551
R indices (all data)	R_1 = 0.0234, wR_2 = 0.0569
Absolute structure parameter	-0.011(5)
Largest diff. peak and hole	0.379 and -0.428 e·Å^{-3}

Table S2. Atomic coordinates and equivalent isotropic displacement parameters Ueq for (PCP*)PtCl·THF.

	x	y	z	Ueq(Å^2)
Pt	0.37868(1)	0.50074(2)	0.30190(1)	0.0304(1)
P(1)	0.48389(11)	0.59128(7)	0.44181(9)	0.0324(2)
C(1)	0.5170(5)	0.5554(4)	0.5901(4)	0.0398(11)
C(2)	0.5767(6)	0.6143(5)	0.6720(5)	0.0602(14)
C(3)	0.5968(7)	0.5875(6)	0.7839(5)	0.077(2)
C(4)	0.5619(7)	0.4985(9)	0.8131(4)	0.080(2)
C(5)	0.5030(8)	0.4430(5)	0.7324(6)	0.076(2)
C(6)	0.4781(7)	0.4705(4)	0.6194(5)	0.059(2)
C(7)	0.6470(4)	0.6334(3)	0.4101(4)	0.0358(9)
C(8)	0.6914(5)	0.7209(4)	0.4328(5)	0.0512(12)
C(9)	0.8174(7)	0.7468(5)	0.4086(6)	0.067(2)
C(10)	0.8993(6)	0.6875(5)	0.3618(5)	0.067(2)
C(11)	0.8570(6)	0.6012(5)	0.3385(6)	0.064(2)
C(12)	0.7288(5)	0.5725(4)	0.3611(5)	0.0507(12)
C(13)	0.3679(5)	0.6885(3)	0.4388(4)	0.0437(11)
C(14)	0.2606(6)	0.6727(5)	0.5179(5)	0.066(2)
C(15)	0.3017(4)	0.6964(3)	0.3175(4)	0.0382(10)
C(16)	0.2906(4)	0.6187(3)	0.2473(4)	0.0339(9)
C(17)	0.2196(4)	0.6273(3)	0.1365(4)	0.0391(10)
C(18)	0.1634(5)	0.7094(4)	0.0996(5)	0.0505(13)
C(19)	0.1759(6)	0.7846(4)	0.1676(5)	0.0546(13)
C(20)	0.2460(5)	0.7784(3)	0.2759(5)	0.0498(12)
C(21)	0.2155(5)	0.5464(3)	0.0568(4)	0.0391(10)
C(22)	0.3260(6)	0.5543(4)	-0.0211(5)	0.0585(14)
P(2)	0.24271(11)	0.44611(8)	0.14809(10)	0.0336(2)
C(23)	0.0776(5)	0.4113(3)	0.1807(4)	0.0392(10)
C(24)	0.0725(6)	0.3654(5)	0.2816(6)	0.067(2)
C(25)	-0.0516(9)	0.3345(6)	0.3068(7)	0.093(3)
C(26)	-0.1688(7)	0.3512(5)	0.2380(7)	0.077(2)
C(27)	-0.1630(6)	0.3967(5)	0.1399(6)	0.074(2)
C(28)	-0.0418(5)	0.4262(4)	0.1105(5)	0.0562(14)

C(29)	0.2973(5)	0.3547(3)	0.0621(4)	0.0416(11)
C(30)	0.4344(6)	0.3433(4)	0.0573(5)	0.0551(13)
C(31)	0.4782(7)	0.2788(4)	-0.0141(6)	0.071(2)
C(32)	0.3843(8)	0.2249(5)	-0.0788(5)	0.076(2)
C(33)	0.2510(9)	0.2334(5)	-0.0720(6)	0.081(2)
C(34)	0.2062(6)	0.2984(4)	-0.0014(5)	0.061(2)
Cl	0.48889(15)	0.36096(8)	0.35745(11)	0.0525(3)
O	0.0153(6)	0.4961(8)	-0.1806(4)	0.118(2)
C(35)	-0.0364(16)	0.5764(11)	-0.2224(10)	0.162(6)
C(36)	-0.0546(14)	0.5715(12)	-0.3473(9)	0.169(6)
C(37)	0.0055(16)	0.4823(11)	-0.3739(8)	0.147(5)
C(38)	0.0762(13)	0.4517(9)	-0.2669(8)	0.124(3)

$U_{eq} = (1/3)\Sigma_i\Sigma_j U_{ij} a_i^* a_j^* \mathbf{a}_i \cdot \mathbf{a}_j$.

Table S3. Bond lengths (Å) for (PCP*)PtCl·THF.

Pt-C(16)	2.015(4)	C(14)-H(14C)	0.96
Pt-P(2)	2.2702(12)	C(15)-C(20)	1.392(7)
Pt-P(1)	2.2746(11)	C(15)-C(16)	1.413(6)
Pt-Cl	2.3855(12)	C(16)-C(17)	1.414(6)
P(1)-C(7)	1.826(4)	C(17)-C(18)	1.380(7)
P(1)-C(1)	1.828(5)	C(17)-C(21)	1.520(7)
P(1)-C(13)	1.838(5)	C(18)-C(19)	1.368(8)
C(1)-C(6)	1.369(8)	C(18)-H(18)	0.93
C(1)-C(2)	1.378(8)	C(19)-C(20)	1.381(8)
C(2)-C(3)	1.377(8)	C(19)-H(19)	0.93
C(2)-H(2)	0.93	C(20)-H(20)	0.93
C(3)-C(4)	1.412(14)	C(21)-C(22)	1.535(7)
C(3)-H(3)	0.93	C(21)-P(2)	1.833(5)
C(4)-C(5)	1.336(12)	C(21)-H(21)	0.98
C(4)-H(4)	0.93	C(22)-H(22A)	0.96
C(5)-C(6)	1.393(9)	C(22)-H(22B)	0.96
C(5)-H(5)	0.93	C(22)-H(22C)	0.96
C(6)-H(6)	0.93	P(2)-C(23)	1.813(5)
C(7)-C(8)	1.377(7)	P(2)-C(29)	1.819(5)
C(7)-C(12)	1.392(7)	C(23)-C(28)	1.375(7)
C(8)-C(9)	1.379(8)	C(23)-C(24)	1.385(8)
C(8)-H(8)	0.93	C(24)-C(25)	1.387(9)
C(9)-C(10)	1.366(10)	C(24)-H(24)	0.93
C(9)-H(9)	0.93	C(25)-C(26)	1.354(12)
C(10)-C(11)	1.356(10)	C(25)-H(25)	0.93
C(10)-H(10)	0.93	C(26)-C(27)	1.353(10)
C(11)-C(12)	1.405(8)	C(26)-H(26)	0.93
C(11)-H(11)	0.93	C(27)-C(28)	1.372(8)
C(12)-H(12)	0.93	C(27)-H(27)	0.93
C(13)-C(15)	1.507(7)	C(28)-H(28)	0.93
C(13)-C(14)	1.535(7)	C(29)-C(34)	1.378(8)
C(13)-H(13)	0.98	C(29)-C(30)	1.384(7)
C(14)-H(14A)	0.96	C(30)-C(31)	1.384(8)
C(14)-H(14B)	0.96	C(30)-H(30)	0.93

Table S3. continued Page 2.

C(31)-C(32)	1.379(10)	C(35)-H(35A)	0.97
C(31)-H(31)	0.93	C(35)-H(35B)	0.97
C(32)-C(33)	1.346(10)	C(36)-C(37)	1.50(2)
C(32)-H(32)	0.93	C(36)-H(36A)	0.97
C(33)-C(34)	1.388(8)	C(36)-H(36B)	0.97
C(33)-H(33)	0.93	C(37)-C(38)	1.441(14)
C(34)-H(34)	0.93	C(37)-H(37A)	0.97
O-C(35)	1.36(2)	C(37)-H(37B)	0.97
O-C(38)	1.421(13)	C(38)-H(38A)	0.97
C(35)-C(36)	1.47(2)	C(38)-H(38B)	0.97

Table S4. Bond angles (deg) for (PCP*)PtCl·THF.

C(16)-Pt-P(2)	82.00(13)	C(7)-C(8)-H(8)	120.2(3)
C(16)-Pt-P(1)	82.31(12)	C(9)-C(8)-H(8)	120.2(4)
P(2)-Pt-P(1)	164.25(4)	C(10)-C(9)-C(8)	121.2(6)
C(16)-Pt-Cl	176.87(12)	C(10)-C(9)-H(9)	119.4(4)
P(2)-Pt-Cl	96.78(5)	C(8)-C(9)-H(9)	119.4(4)
P(1)-Pt-Cl	98.96(4)	C(11)-C(10)-C(9)	119.9(6)
C(7)-P(1)-C(1)	104.4(2)	C(11)-C(10)-H(10)	120.1(4)
C(7)-P(1)-C(13)	107.7(2)	C(9)-C(10)-H(10)	120.1(4)
C(1)-P(1)-C(13)	106.0(2)	C(10)-C(11)-C(12)	120.6(6)
C(7)-P(1)-Pt	112.5(2)	C(10)-C(11)-H(11)	119.7(4)
C(1)-P(1)-Pt	122.7(2)	C(12)-C(11)-H(11)	119.7(4)
C(13)-P(1)-Pt	102.6(2)	C(7)-C(12)-C(11)	119.0(5)
C(6)-C(1)-C(2)	120.4(5)	C(7)-C(12)-H(12)	120.5(3)
C(6)-C(1)-P(1)	119.4(5)	C(11)-C(12)-H(12)	120.5(4)
C(2)-C(1)-P(1)	120.2(4)	C(15)-C(13)-C(14)	110.4(4)
C(3)-C(2)-C(1)	119.6(6)	C(15)-C(13)-P(1)	105.7(3)
C(3)-C(2)-H(2)	120.2(5)	C(14)-C(13)-P(1)	111.0(4)
C(1)-C(2)-H(2)	120.2(3)	C(15)-C(13)-H(13)	109.9(3)
C(2)-C(3)-C(4)	119.8(7)	C(14)-C(13)-H(13)	109.9(3)
C(2)-C(3)-H(3)	120.1(5)	P(1)-C(13)-H(13)	109.9(2)
C(4)-C(3)-H(3)	120.1(4)	C(13)-C(14)-H(14A)	109.5(3)
C(5)-C(4)-C(3)	119.4(5)	C(13)-C(14)-H(14B)	109.5(3)
C(5)-C(4)-H(4)	120.3(5)	H(14A)-C(14)-H(14B)	109.5
C(3)-C(4)-H(4)	120.3(4)	C(13)-C(14)-H(14C)	109.5(3)
C(4)-C(5)-C(6)	121.2(7)	H(14A)-C(14)-H(14C)	109.5
C(4)-C(5)-H(5)	119.4(5)	H(14B)-C(14)-H(14C)	109.5
C(6)-C(5)-H(5)	119.4(4)	C(20)-C(15)-C(16)	119.9(4)
C(1)-C(6)-C(5)	119.5(7)	C(20)-C(15)-C(13)	120.6(4)
C(1)-C(6)-H(6)	120.2(4)	C(16)-C(15)-C(13)	119.5(4)
C(5)-C(6)-H(6)	120.2(4)	C(17)-C(16)-C(15)	117.8(4)
C(8)-C(7)-C(12)	119.7(5)	C(17)-C(16)-Pt	121.2(3)
C(8)-C(7)-P(1)	123.3(4)	C(15)-C(16)-Pt	120.9(3)
C(12)-C(7)-P(1)	117.0(4)	C(18)-C(17)-C(16)	120.3(5)
C(7)-C(8)-C(9)	119.7(5)	C(18)-C(17)-C(21)	121.0(4)

Table S4. continued Page 2.

C(16)-C(17)-C(21)	118.6(4)
C(19)-C(18)-C(17)	121.6(5)
C(19)-C(18)-H(18)	119.2(3)
C(17)-C(18)-H(18)	119.2(3)
C(18)-C(19)-C(20)	119.4(5)
C(18)-C(19)-H(19)	120.3(3)
C(20)-C(19)-H(19)	120.3(3)
C(19)-C(20)-C(15)	121.0(5)
C(19)-C(20)-H(20)	119.5(3)
C(15)-C(20)-H(20)	119.5(3)
C(17)-C(21)-C(22)	110.9(4)
C(17)-C(21)-P(2)	105.9(3)
C(22)-C(21)-P(2)	111.0(4)
C(17)-C(21)-H(21)	109.7(2)
C(22)-C(21)-H(21)	109.7(3)
P(2)-C(21)-H(21)	109.7(2)
C(21)-C(22)-H(22A)	109.5(3)
C(21)-C(22)-H(22B)	109.5(3)
H(22A)-C(22)-H(22B)	109.5
C(21)-C(22)-H(22C)	109.5(3)
H(22A)-C(22)-H(22C)	109.5
H(22B)-C(22)-H(22C)	109.5
C(23)-P(2)-C(29)	105.0(2)
C(23)-P(2)-C(21)	106.9(2)
C(29)-P(2)-C(21)	107.2(2)
C(23)-P(2)-Pt	112.8(2)
C(29)-P(2)-Pt	121.7(2)
C(21)-P(2)-Pt	102.4(2)
C(28)-C(23)-C(24)	118.3(5)
C(28)-C(23)-P(2)	124.0(4)
C(24)-C(23)-P(2)	117.7(4)
C(23)-C(24)-C(25)	119.1(6)
C(23)-C(24)-H(24)	120.4(3)
C(25)-C(24)-H(24)	120.4(5)
C(26)-C(25)-C(24)	121.9(7)
C(26)-C(25)-H(25)	119.0(4)
C(24)-C(25)-H(25)	119.0(5)
C(25)-C(26)-C(27)	118.5(6)
C(25)-C(26)-H(26)	120.7(4)
C(27)-C(26)-H(26)	120.7(4)
C(26)-C(27)-C(28)	121.3(6)
C(26)-C(27)-H(27)	119.3(4)
C(28)-C(27)-H(27)	119.3(4)
C(27)-C(28)-C(23)	120.8(6)
C(27)-C(28)-H(28)	119.6(4)
C(23)-C(28)-H(28)	119.6(3)
C(34)-C(29)-C(30)	119.0(5)
C(34)-C(29)-P(2)	122.0(4)
C(30)-C(29)-P(2)	119.0(4)
C(31)-C(30)-C(29)	120.2(6)
C(31)-C(30)-H(30)	119.9(4)
C(29)-C(30)-H(30)	119.9(3)
C(32)-C(31)-C(30)	119.5(6)
C(32)-C(31)-H(31)	120.2(4)
C(30)-C(31)-H(31)	120.2(4)
C(33)-C(32)-C(31)	120.7(6)
C(33)-C(32)-H(32)	119.6(4)
C(31)-C(32)-H(32)	119.6(4)
C(32)-C(33)-C(34)	120.1(7)
C(32)-C(33)-H(33)	119.9(4)
C(34)-C(33)-H(33)	119.9(4)
C(29)-C(34)-C(33)	120.4(6)
C(29)-C(34)-H(34)	119.8(3)
C(33)-C(34)-H(34)	119.8(4)
C(35)-O-C(38)	108.4(9)
O-C(35)-C(36)	108.4(12)