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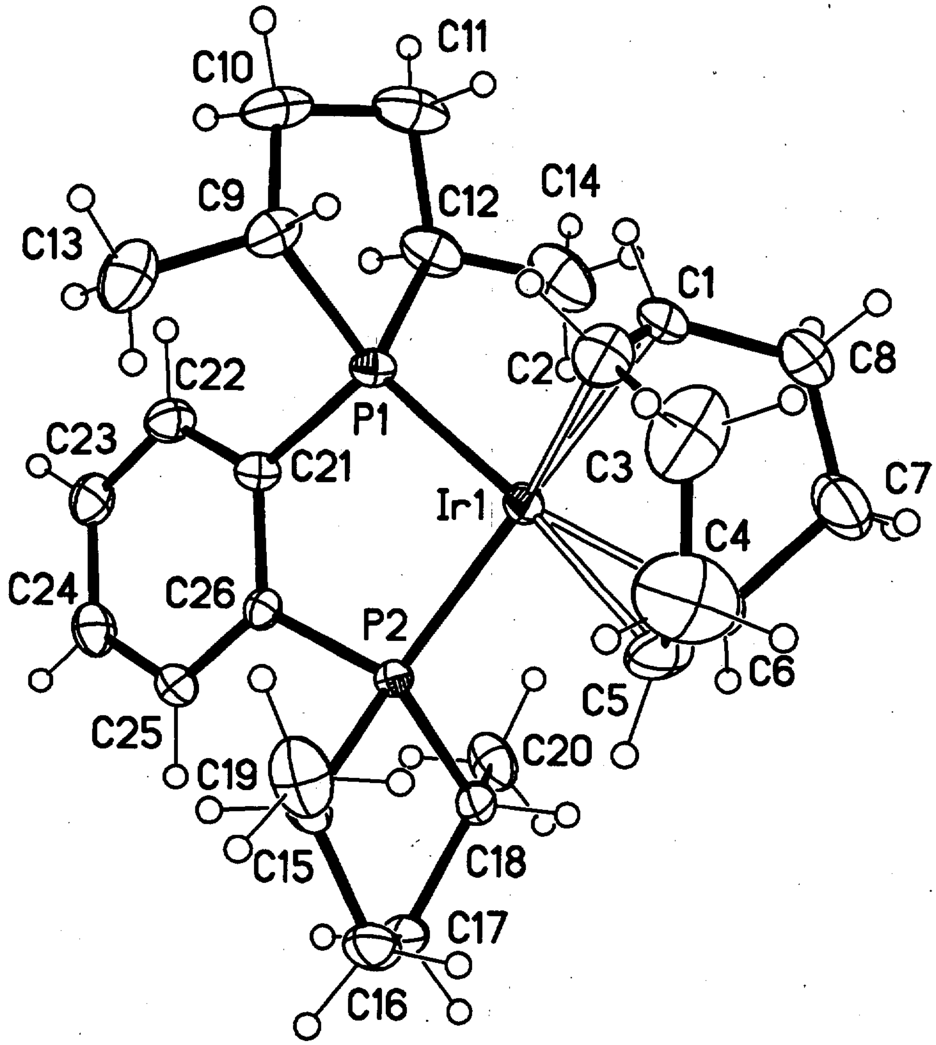

Figure 1. Complete structure and numbering scheme for Ir((*R,R*)-Me-DuPHOS)]BF_4 (**5**).

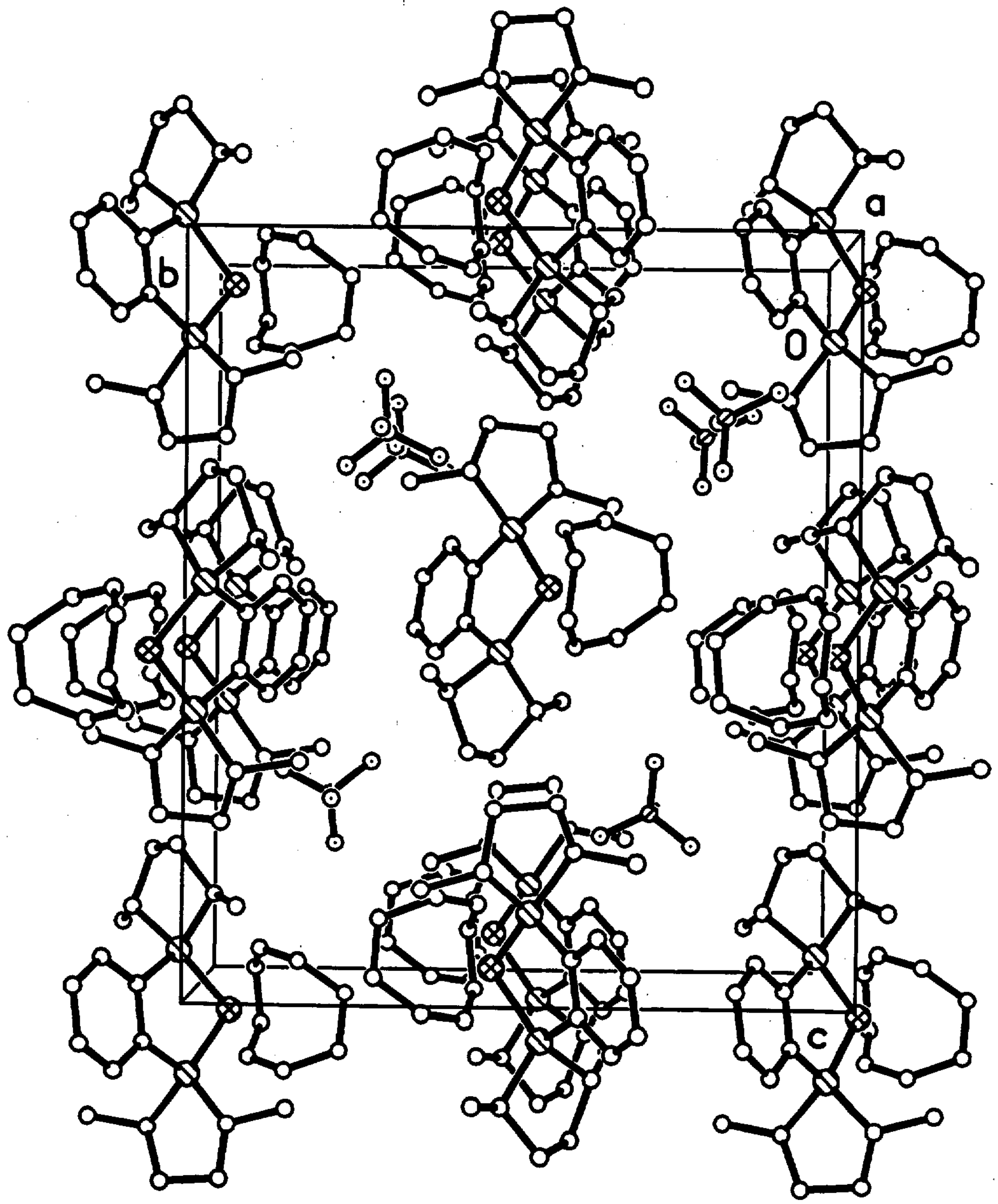

Figure 2. Unit cell diagram for [Ir((*R*,*R*)-Me-DuPHOS)(COD)]BF_4 (**5**).

Table 1. Bond Lengths (Å) and Bond Angles (°) for [Ir((*R*,*R*)-Me-DuPHOS)(COD)]BF_4.

Ir(1)-C(6)	2.188(4)	C(9)-C(13)	1.522(5)
Ir(1)-C(2)	2.197(3)	C(9)-C(10)	1.537(5)
Ir(1)-C(5)	2.214(4)	C(10)-C(11)	1.526(7)
Ir(1)-C(1)	2.233(3)	C(11)-C(12)	1.536(5)
Ir(1)-P(2)	2.2796(8)	C(12)-C(14)	1.522(6)
Ir(1)-P(1)	2.2839(8)	C(15)-C(19)	1.533(5)
P(1)-C(21)	1.821(3)	C(15)-C(16)	1.537(5)
P(1)-C(12)	1.861(3)	C(16)-C(17)	1.530(6)
P(1)-C(9)	1.871(3)	C(17)-C(18)	1.538(5)
P(2)-C(26)	1.831(3)	C(18)-C(20)	1.518(5)
P(2)-C(18)	1.835(3)	C(21)-C(22)	1.403(4)
P(2)-C(15)	1.854(3)	C(21)-C(26)	1.404(4)
C(1)-C(2)	1.373(6)	C(22)-C(23)	1.384(5)
C(1)-C(8)	1.507(6)	C(23)-C(24)	1.382(5)
C(2)-C(3)	1.507(6)	C(24)-C(25)	1.383(5)
C(3)-C(4	1.466(7)	C(25)-C(26)	1.399(4)
C(4)-C(5)	1.515(7)	B(1)-F(4)	1.379(5)
C(5)-C(6)	1.377(7)	B(1)-F(3)	1.384(5)
C(6)-C(7)	1.515(6)	B(1)-F(1)	1.386(5)
C(7)-C(8)	1.463(6)	B(1)-F(2)	1.389(5)
C(6)-Ir(1)-C(2)	89.08(15)	C(5)-C(6)-C(7)	123.2(5)
C(6)-Ir(1)-C(5)	36.5(2)	C(5)-C(6)-Ir(1)	72.8(2)
C(2)-Ir(1)-C(5)	80.02(14)	C(7-C(6)-Ir(1)	111.7(3)
C(6)-Ir(1)-C(1)	80.08(15)	C(8)-C(7)-C(6)	117.1(4)
C(2)-Ir(1)-C(1)	36.08(15)	C(7)-C(8)-C(1)	115.6(4)
C(5)-Ir(1)-C(1)	93.26(15)	C(13)-C(9)-C(10)	114.9(3)
C(6)-Ir(1)-P(2)	98.96(10)	C(13)-C(9)-P(1)	115.6(3)
C(2)-Ir(1)-P(2)	153.09(11)	C(10)-C(9)-P(1)	104.9(2)
C(5)-Ir(1)-P(2)	91.25(10)	C(11)-C(10)-C(9)	107.7(3)
C(1)-Ir(1)-P(2)	170.74(11)	C(10)-C(11)-C(12)	107.5(3)
C(6)-Ir(1)-P(1)	149.71(14)	C(14)-C(12)-C(11)	116.1(3)
C(2)-Ir(1)-P(1)	100.59(11)	C(14)-C(12)-P(1)	117.6(3)
C(5)-Ir(1)-P(1)	173.45(13)	C(11)-C(12)-P(1)	104.1(2)
C(1)-Ir(1)-P(1)	90.93(11)	C(19)-C(15)-C(16)	114.8(3)
P(2)-Ir(1)-P(1)	85.33(3)	C(19)-C(15)-P(2)	116.3(3)
C(21)-P(1)-C(12)	104.1(2)	C(16)-C(15)-P(2)	105.2(2)
C(21)-P(1)-C(9)	108.0(2)	C(17)-C(16)-C(15)	108.2(3)
C(12)-P(1)-C(9)	94.9(2)	C(16)-C(17)-C(18)	105.5(3)
C(21)-P(1)-Ir(1)	109.68(10)	C(20)-C(18)-C(17)	116.6(3)
C(12)-P(1)-Ir(1)	120.23(13)	C(20)-C(18)-P(2)	114.7(2)
C(9)-P(1)-Ir(1)	118.23(11)	C(17)-C(18)-P(2)	106.0(2)
C(26-P(2)-C(18)	107.23(15)	C(22)-C(21)-C(26)	119.1(3)
C(26-P(2)-C(15)	105.07(15)	C(22)-C(21)-P(1)	123.2(2)
C(18-P(2)-C(15)	94.5(2)	C(26)-C(21)-P(1)	117.7(2)
C(26-P(2)-Ir(1)	109.72(11)	C(23)-C(22)-C(21)	120.6(3)
C(18-P(2)-Ir(1)	117.70(10)	C(24)-C(23)-C(22)	120.0(3)
C(15)-P(2)-Ir(1)	120.86(11)	C(23)-C(24)-C(25)	120.4(3)
C(2)-C(1)-C(8)	126.0(4)	C(24)-C(25)-C(26)	120.4(3)
C(2)-C(1)-Ir(1)	70.5(2)	C(25)-C(26)-C(21)	119.4(3)
C(8)-C(1)-Ir(1)	109.2(3)	C(25)-C(26)-P(2)	123.2(2)

C(1)-C(2)-C(3)	123.0(4)	C(21)-C(26)-P(2)	117.3(2)
C(1)-C(2)-Ir(1)	73.4(2)	F(4)-B(1)-F(3)	111.2(4)
C(3)-C(2)-Ir(1)	112.0(3)	F(4)-B(1)-F(1)	109.5(3)
C(4)-C(3)-C(2)	115.7(4)	F(3)-B(1)-F(1)	108.9(3)
C(3)-C(4)-C(5)	115.6(4)	F(4)-B(1)-F(2)	109.2(4)
C(6)-C(5)-C(4)	127.1(4)	F(3)-B(1)-F(2)	108.2(3)
C(6)-C(5)-Ir(1)	70.7(2)	F(1)-B(1)-F(2)	109.8(3)
C(4)-C(5)-Ir(1)	108.6(3)		

Table 2. Atomic Coordinates and Equivalent Isotropic Displacement Parameters (Å^2) for [Ir((*R*,*R*)-Me-DuPHOS)(COD)]BF_4.

	x	y	z	U(eq)
Ir(1)	0.664585(12)	0.459161(7)	0.456250(6)	0.01679(3)
P(1)	0.49742(9)	0.51608(5)	0.37848(4)	0.0181(2)
P(2)	0.54649(7)	0.53318(5)	0.54437(4)	0.01541(13)
C(1)	0.7468(5)	0.3749(2)	0.3686(2)	0.0337(8)
C(2)	0.8474(4)	0.4367(2)	0.3813(2)	0.0353(9)
C(3)	0.9887(5)	0.4218(4)	0.4212(3)	0.0559(14)
C(4)	0.9827(5)	0.4318(4)	0.5004(3)	0.072(2)
C(5)	0.8340(5)	0.4188(3)	0.5347(2)	0.0403(9)
C(6)	0.7390(6)	0.3537(2)	0.5222(2)	0.0407(11)
C(7)	0.7771(8)	0.2788(3)	0.4756(2)	0.071(2)
C(8)	0.7540(6)	0.2868(3)	0.3972(2)	0.0497(12)
C(9)	0.5659(4)	0.5815(2)	0.3014(2)	0.0263(7)
C(10)	0.4732(4)	0.5552(3)	0.2355(2)	0.0366(10)
C(11)	0.4409(4)	0.4622(3)	0.2429(2)	0.0387(9)
C(12)	0.3823(4)	0.4475(2)	0.3202(2)	0.0300(8)
C(13)	0.5710(5)	0.6751(3)	0.3155(3)	0.0423(10)
C(14)	0.3650(5)	0.3568(2)	0.3433(3)	0.0447(11)
C(15)	0.6443(4)	0.6129(2)	0.5989(2)	0.0253(7)
C(16)	0.6389(4)	0.5808(2)	0.6777(2)	0.0328(9)
C(17)	0.4934(4)	0.5357(3)	0.6889(2)	0.0298(7)
C(18)	0.4788(4)	0.4757(2)	0.6239(2)	0.0226(6)
C(19)	0.7967(4)	0.6377(3)	0.5719(3)	0.0398(10)
C(20)	0.3311(5)	0.4345(2)	0.6134(2)	0.0325(8)
C(21)	0.3658(3)	0.5778(2)	0.4297(2)	0.0192(6)
C(22)	0.2416(4)	0.6140(2)	0.3982(2)	0.0247(7)
C(23)	0.1445(4)	0.6596(2)	0.4400(2)	0.0270(7)
C(24)	0.1716(4)	0.6716(2)	0.5133(2)	0.0258(6)
C(25)	0.2942(3)	0.6373(2)	0.5455(2)	0.0217(6)
C(26)	0.3905(3)	0.5883(2)	0.5046(2)	0.0168(6)
B(1)	0.4602(5)	0.7982(3)	0.7395(2)	0.0315(9)
F(1)	0.4030(3)	0.7350(2)	0.69668(15)	0.0457(6)
F(2)	0.6114(3)	0.7916(2)	0.74181(13)	0.0468(6)
F(3)	0.4249(3)	0.8744(2)	0.7086(2)	0.0585(8)
F(4)	0.4054(4)	0.7917(2)	0.8092(2)	0.0698(10)

U(eq) is defined as one third of the trace of the orthogonalized u_{ij} tensor.

Table 3. Anisotropic Displacement Parameters (Å^2) for [Ir((*R,R*)-Me-DuPHOS)(COD)]BF_4.

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Ir(1)	0.01737(5)	0.01676(5)	0.01622(5)	-0.00001(5)	0.00285(5)	0.00220(4)
P(1)	0.0173(3)	0.0223(4)	0.0147(4)	-0.0012(3)	0.0010(3)	-0.0004(3)
P(2)	0.0165(3)	0.0158(3)	0.0140(3)	0.0000(4)	-0.0003(3)	0.0015(2)
C(1)	0.052(2)	0.029(2)	0.020(2)	-0.003(2)	0.012(2)	0.013(2)
C(2)	0.029(2)	0.045(2)	0.032(2)	0.010(2)	0.021(2)	0.013(2)
C(3)	0.024(2)	0.072(3)	0.071(3)	0.025(3)	0.017(2)	0.007(2)
C(4)	0.026(2)	0.118(5)	0.073(4)	-0.022(4)	-0.013(2)	0.016(3)
C(5)	0.035(2)	0.062(3)	0.024(2)	-0.001(2)	-0.006(2)	0.022(2)
C(6)	0.070(3)	0.029(2)	0.023(2)	0.0041(15)	0.009(2)	0.023(2)
C(7)	0.147(6)	0.027(2)	0.038(3)	0.002(2)	0.030(3)	0.020(3)
C(8)	0.089(4)	0.027(2)	0.033(2)	-0.008(2)	0.002(2)	0.013(2)
C(9)	0.024(2)	0.034(2)	0.021(2)	0.0055(14)	0.0004(13)	0.0002(13)
C(10)	0.036(2)	0.059(3)	0.016(2)	0.002(2)	-0.0015(13)	0.003(2)
C(11)	0.029(2)	0.064(3)	0.023(2)	-0.014(2)	-0.0031(13)	0.002(2)
C(12)	0.0215(15)	0.040(2)	0.029(2)	-0.012(2)	-0.0004(12)	-0.0052(14)
C(13)	0.046(2)	0.035(2)	0.046(3)	0.015(2)	0.004(2)	-0.003(2)
C(14)	0.044(3)	0.035(2)	0.055(3)	-0.015(2)	0.012(2)	-0.016(2)
C(15)	0.024(2)	0.020(2)	0.031(2)	-0.0081(13)	-0.0049(13)	-0.0013(13)
C(16)	0.035(2)	0.038(2)	0.025(2)	-0.0103(15)	-0.0117(14)	0.011(2)
C(17)	0.041(2)	0.032(2)	0.0160(14)	-0.0016(15)	-0.0010(14)	0.013(2)
C(18)	0.031(2)	0.018(2)	0.0182(15)	0.0013(12)	0.0043(12)	0.0056(12)
C(19)	0.026(2)	0.032(2)	0.062(3)	-0.007(2)	-0.005(2)	-0.0041(14)
C(20)	0.038(2)	0.022(2)	0.038(2)	-0.0016(13)	0.014(2)	-0.005(2)
C(21)	0.019(2)	0.0229(15)	0.0156(14)	-0.0012(12)	0.0011(10)	-0.0004(11)
C(22)	0.024(2)	0.030(2)	0.020(2)	0.0000(14)	-0.0038(12)	0.0007(13)
C(23)	0.024(2)	0.027(2)	0.031(2)	0.0022(13)	-0.0049(13)	0.0077(12)
C(24)	0.0215(15)	0.023(2)	0.033(2)	-0.0014(13)	0.0041(15)	0.0059(14)
C(25)	0.0244(14)	0.0204(14)	0.0203(14)	-0.0025(14)	0.0013(13)	0.0035(10)
C(26)	0.0153(13)	0.0168(14)	0.0181(15)	0.0019(12)	-0.0003(11)	0.0017(10)
B(1)	0.035(2)	0.029(2)	0.030(2)	-0.008(2)	0.005(2)	-0.005(2)
F(1)	0.0478(14)	0.0365(13)	0.053(2)	-0.0239(12)	-0.0088(12)	0.0020(11)
F(2)	0.0366(12)	0.068(2)	0.0358(14)	0.0123(12)	-0.0042(10)	-0.0101(12)
F(3)	0.054(2)	0.0289(13)	0.093(2)	-0.0019(15)	-0.005(2)	0.0031(12)
F(4)	0.080(2)	0.080(2)	0.050(2)	-0.029(2)	0.036(2)	-0.044(2)

The aniotropic displacement factor exponent takes the form $-2\pi[(ha^*)^2U_{11} + \ldots + 2hka^*b^*U_{12}]$

Table 4. Hydrogen Coordinates and Isotropic Displacement Paramters [Å^2] for [Ir((*R,R*)-Me-DuPHOS)(COD)]BF_4.

	x	y	z	U(eq)
H(1)	0.6938(5)	0.3805(2)	0.3212(2)	0.040
H(2)	0.8550(4)	0.4786(2)	0.3411(2)	0.042
H(3A)	1.0222(5)	0.3644(4)	0.4103(3)	0.067
H(3B)	1.0630(5)	0.4608(4)	0.4018(3)	0.067
H(4A)	1.0168(5)	0.4887(4)	0.5127(3)	0.087
H(4B)	1.0520(5)	0.3918(4)	0.5227(3)	0.087
H(5)	0.8238(5)	0.4445(3)	0.5841(2)	0.048
H(6)	0.6739(6)	0.3405(2)	0.5644(2)	0.049
H(7A)	0.8812(8)	0.2652(3)	0.4839(2)	0.085
H(7B)	0.7189(8)	0.2307(3)	0.4931(2)	0.085
H(8A)	0.6618(6)	0.2581(3)	0.3844(2)	0.060
H(8B)	0.8343(6)	0.2573(3)	0.3718(2)	0.060
H(9)	0.6683(4)	0.5633(2)	0.2912(2)	0.032
H(10A)	0.3809(4)	0.5874(3)	0.2344(2)	0.044
H(10B)	0.5271(4)	0.5661(3)	0.1898(2)	0.044
H(11A)	0.5310(4)	0.4293(3)	0.2350(2)	0.046
H(11B)	0.3673(4)	0.4449(3)	0.2064(2)	0.046
H(12)	0.2820(4)	0.4722(2)	0.3212(2)	0.036
H(13A)	0.6295(5)	0.6860(3)	0.3591(3)	0.063
H(13B)	0.4716(5)	0.6961(3)	0.3229(3)	0.063
H(13C)	0.6152(5)	0.7033(3)	0.2737(3)	0.063
H(14A)	0.3396(5)	0.3544(2)	0.3951(3)	0.067
H(14B)	0.4570(5)	0.3270(2)	0.3351(3)	0.067
H(14C)	0.2873(5)	0.3307(2)	0.3146(3)	0.067
H(15)	0.5832(4)	0.6647(2)	0.5973(2)	0.030
H(16A)	0.7211(4)	0.5420(2)	0.6867(2)	0.039
H(16B)	0.6472(4)	0.6282(2)	0.7121(2)	0.039
H(17A)	0.4115(4)	0.5761(3)	0.6895(2)	0.036
H(17B)	0.4936(4)	0.5045(3)	0.7353(2)	0.036
H(18)	0.5501(4)	0.4295(2)	0.6328(2)	0.027
H(19A)	0.7914(4)	0.6536(3)	0.5205(3)	0.060
H(19B)	0.8634(4)	0.5903(3)	0.5774(3)	0.060
H(19C)	0.8328(4)	0.6850(3)	0.6005(3)	0.060
H(20A)	0.3333(5)	0.3999(2)	0.5694(2)	0.049
H(20B)	0.2558(5)	0.4775(2)	0.6083(2)	0.049
H(20C)	0.3090(5)	0.3994(2)	0.6556(2)	0.049
H(22)	0.2240(4)	0.6072(2)	0.3475(2)	0.030
H(23)	0.0593(4)	0.6826(2)	0.4184(2)	0.032
H(24)	0.1056(4)	0.7036(2)	0.5418(2)	0.031
H(25)	0.3132(3)	0.6470(2)	0.5956(2)	0.026

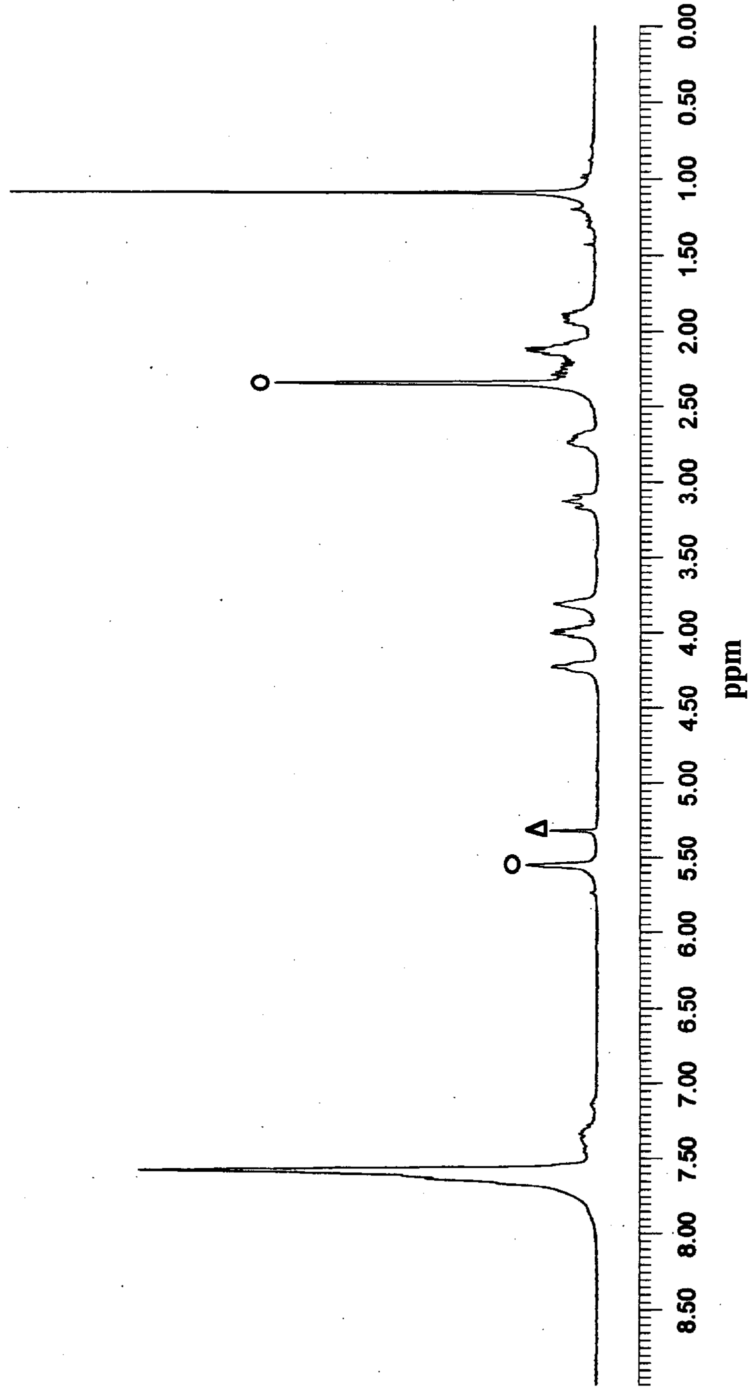

Figure 3. 300 MHz ^{1}H NMR of [Ir((*S*,*S*)-DIOP)(COD)]BF_4 in CD_2Cl_2 at 25°C (O = free COD and Δ = solvent).

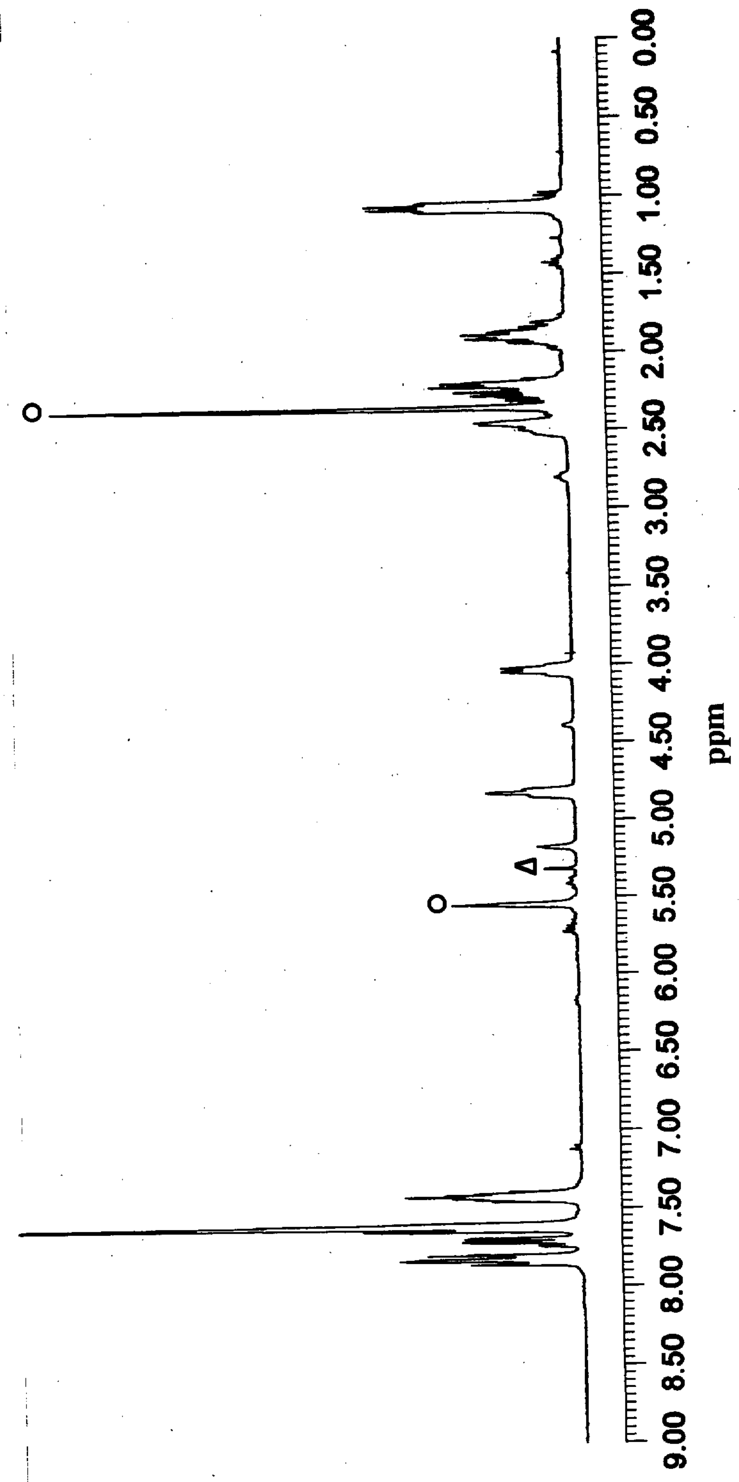

Figure 4. 300 MHz ^1H NMR of [Ir(*S*,*S*)-CHIRAPHOS)(COD)(]BF_4 in CD_2Cl_2 at 25°C (O = free COD and Δ = solvent).

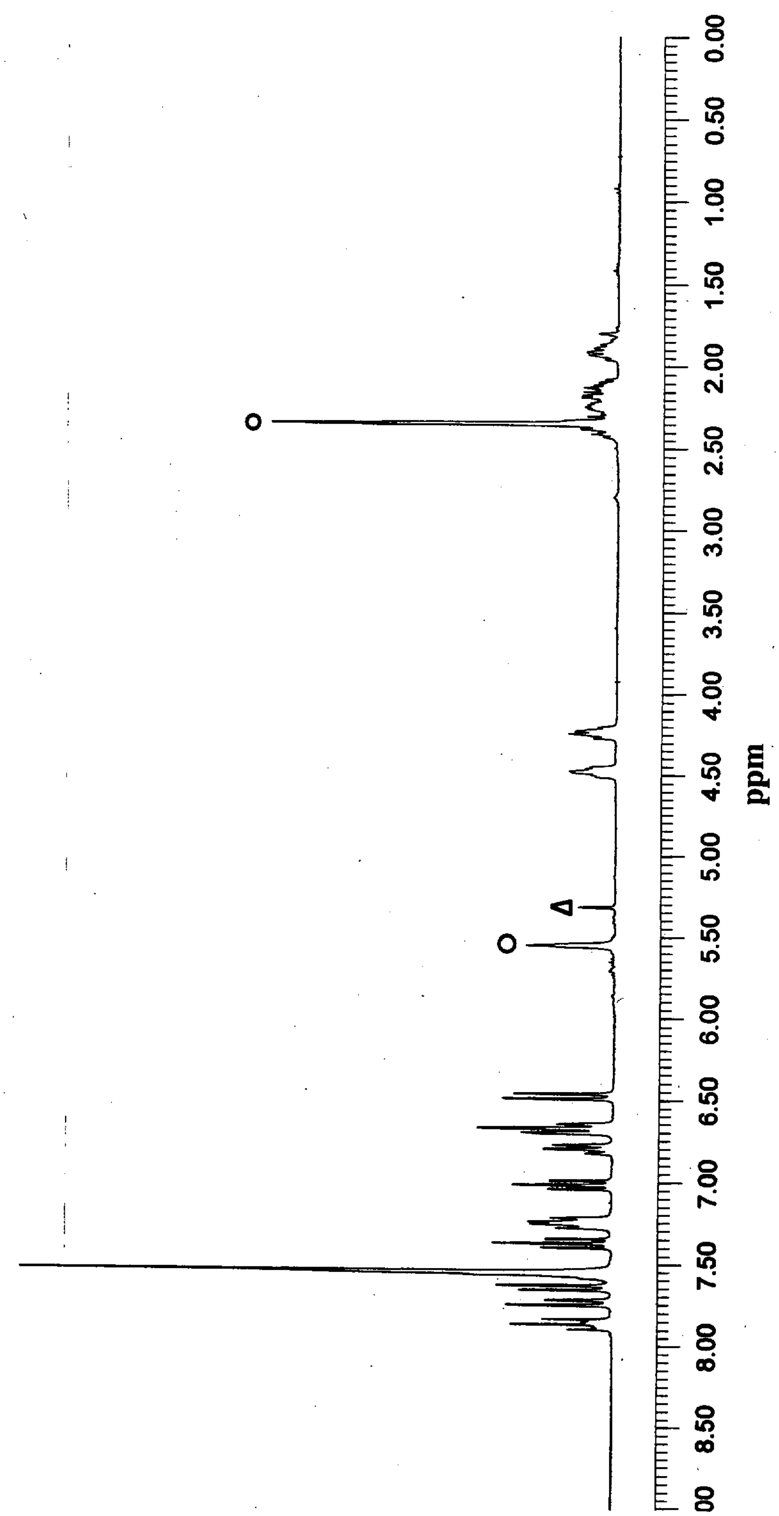

Figure 5. 300 MHz ^{1}H NMR of [Ir(((*R*)-BINAP)COD)]BF_4 in CD_2Cl_2 at 25°C (O = free COD and Δ = solvent).

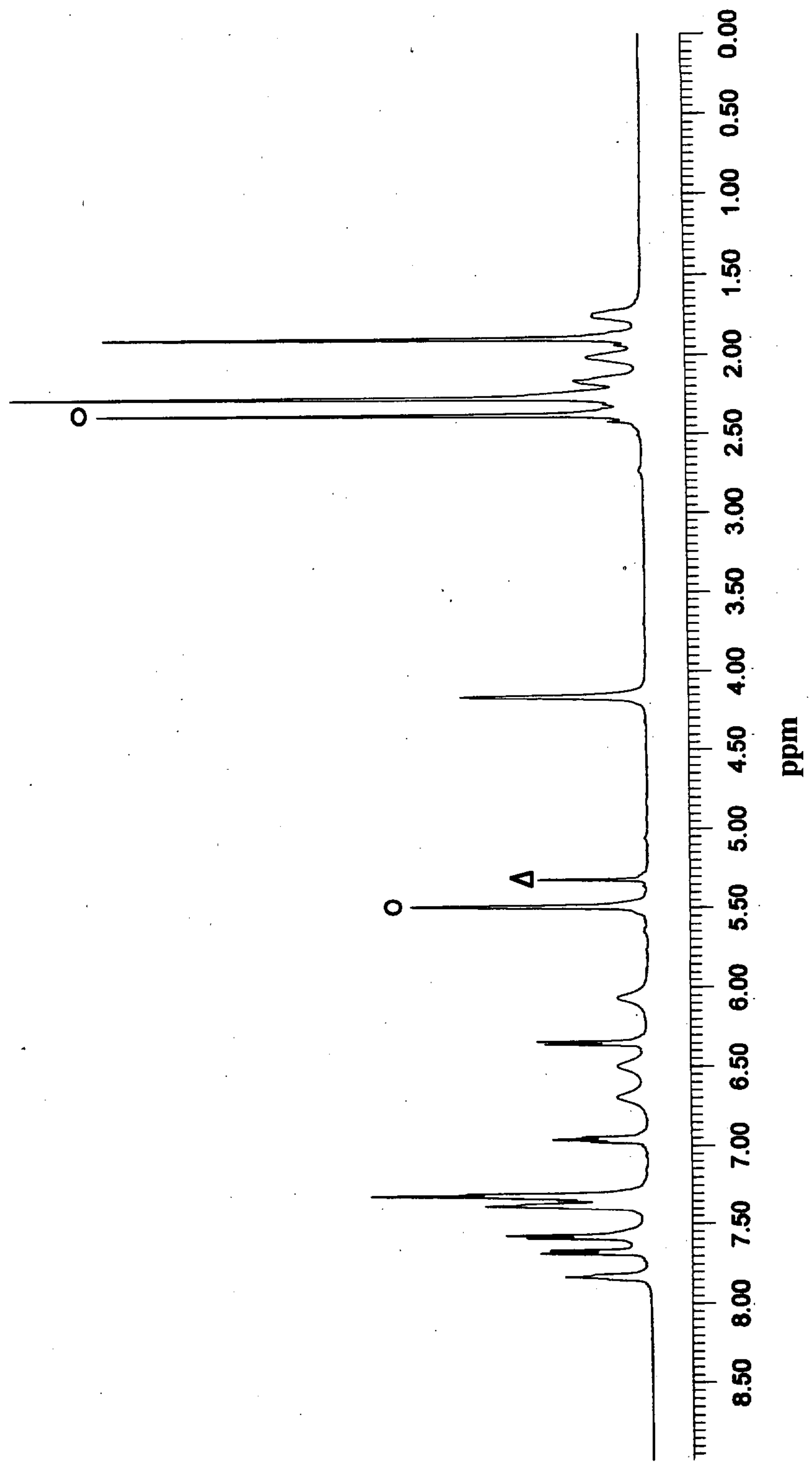

Figure 6. 300 MHz ^1H NMR of $[Ir((R)\text{-Tol-BINAP})(COD)]BF_4$ in CD_2Cl_2 at 25°C (O = free COD and **Δ** = solvent).

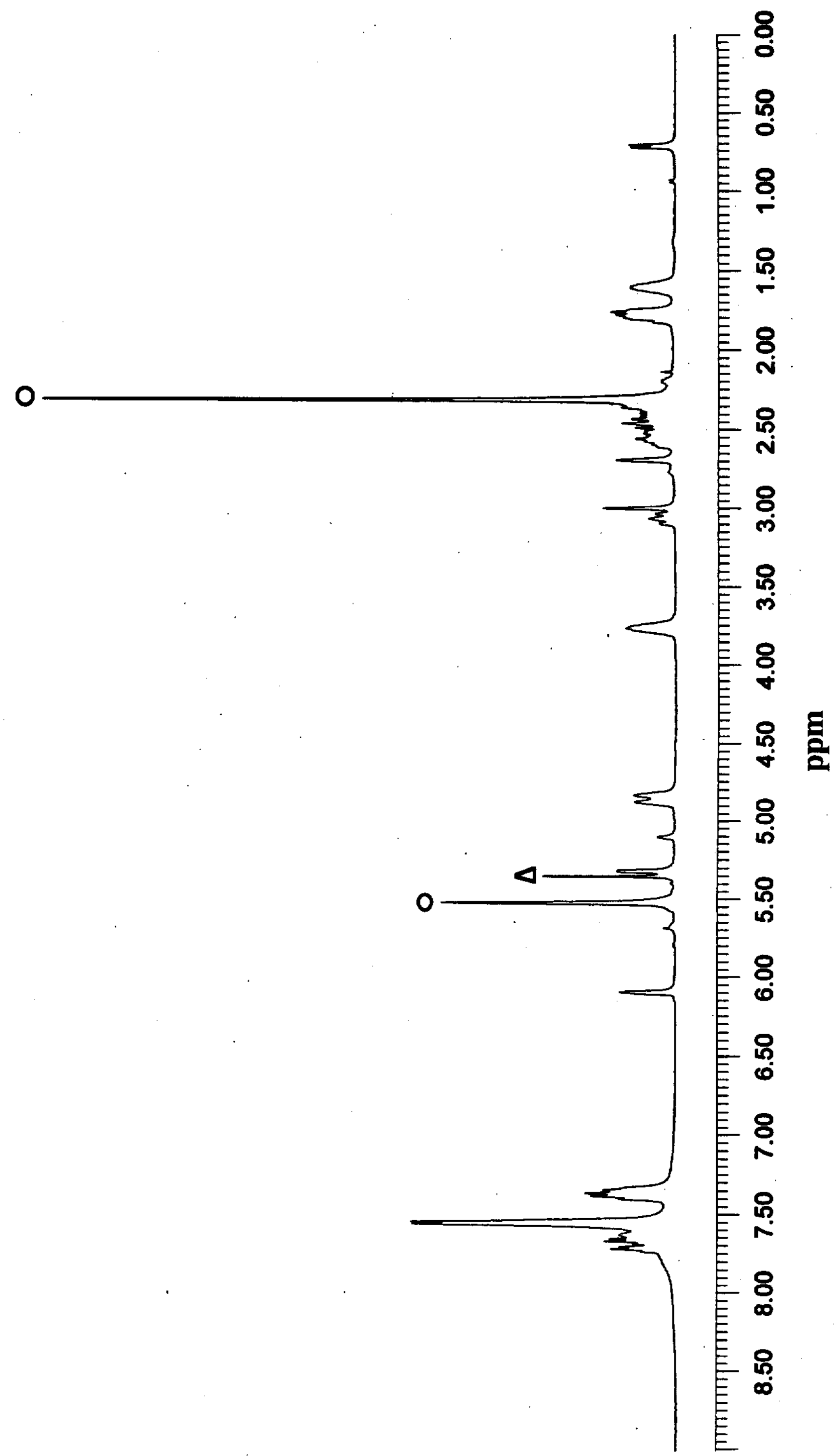

Figure 7. 300 MHz ^1H NMR of $[Ir((R,R)\text{-NORPHOS})(COD)]BF_4$ in CD_2Cl_2 at 25°C (O = free COD and **Δ** = solvent).

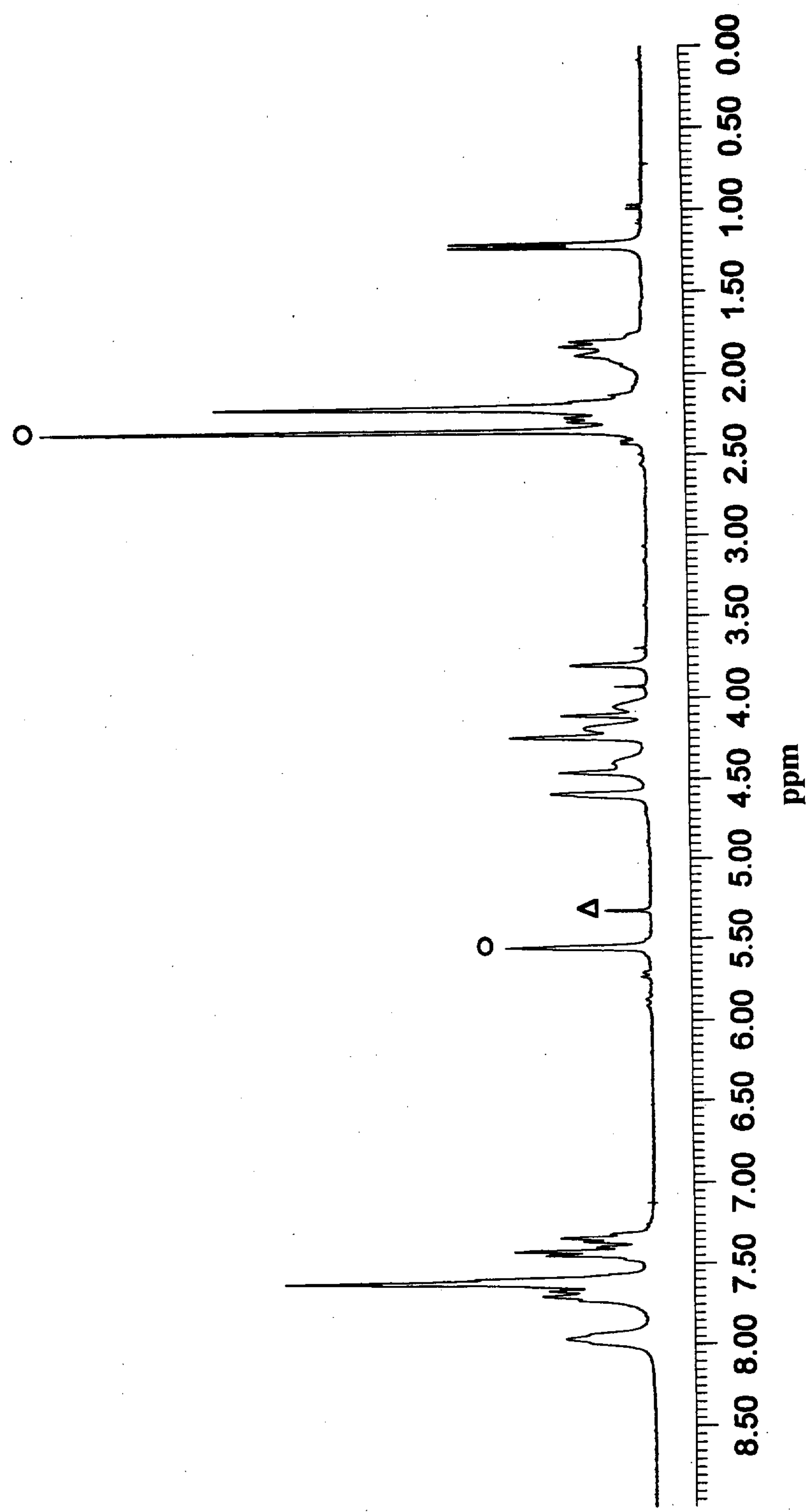

Figure 8. 300 MHz ^1H NMR of [Ir((*S*,*R*)-BPPFA)(COD)]BF_4 in CD_2Cl_2 at 25°C (O = free COD and Δ = solvent).

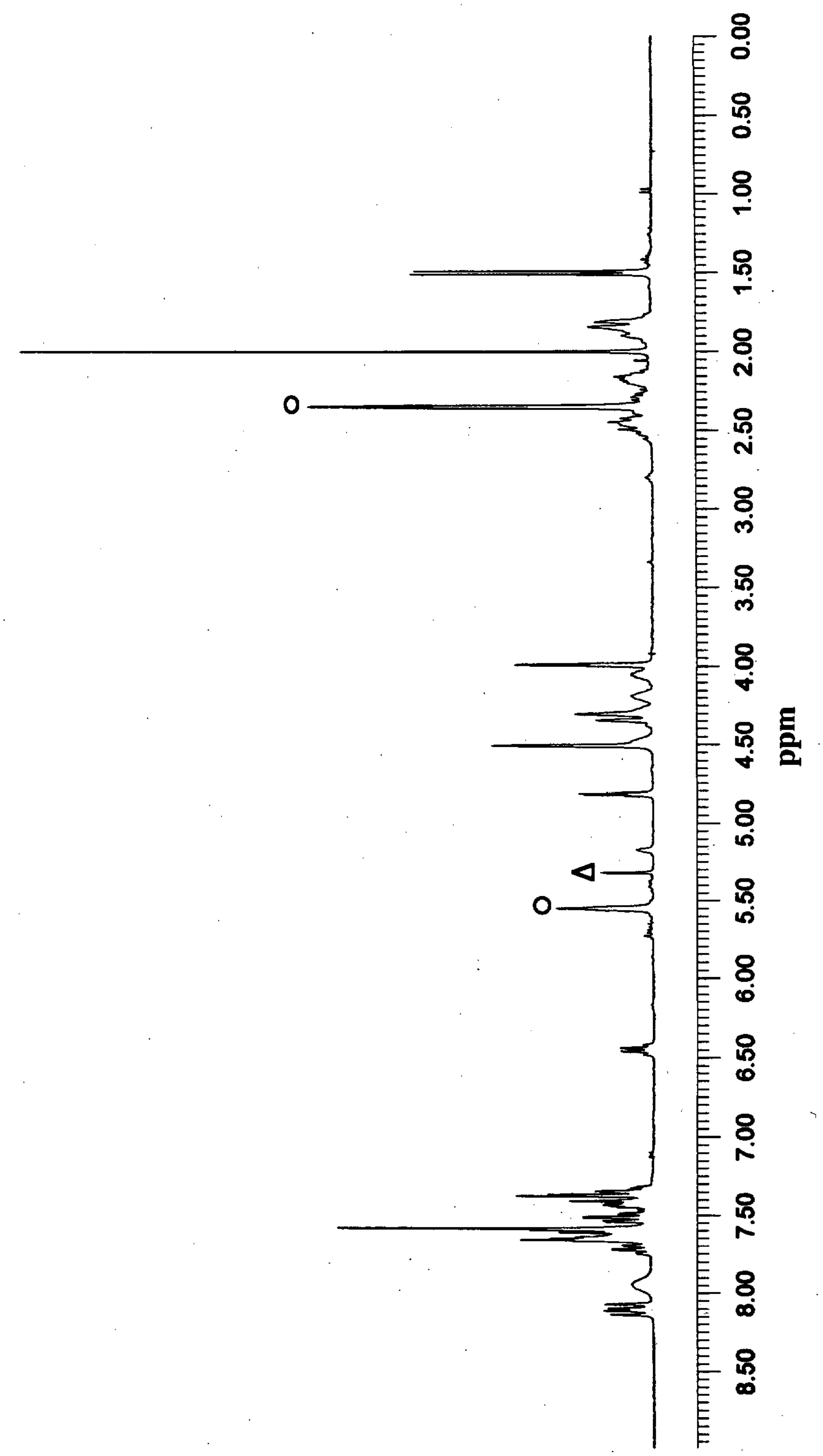

Figure 9. 300 MHz ^{1}H NMR of $[Ir((S,R)\text{-BPPFAc})(COD)]BF_4$ in CD_2Cl_2 at 25°C (O = free COD and Δ = solvent).

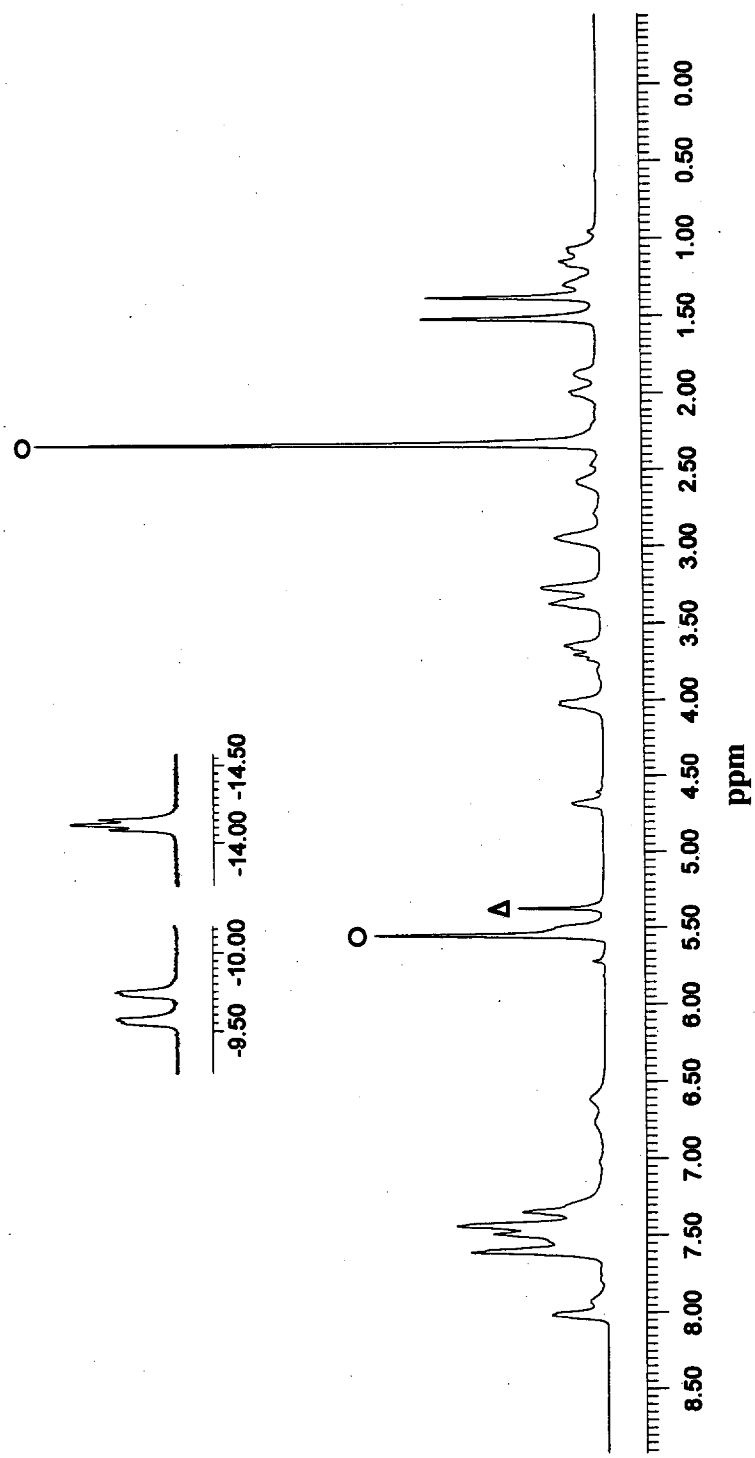

Figure 10. 500 MHz ^1H NMR of $[IrH_2((S,S)\text{-DIOP})(COD)]BF_4$ in CD_2Cl_2 at -80°C (O = free COD and Δ = solvent).

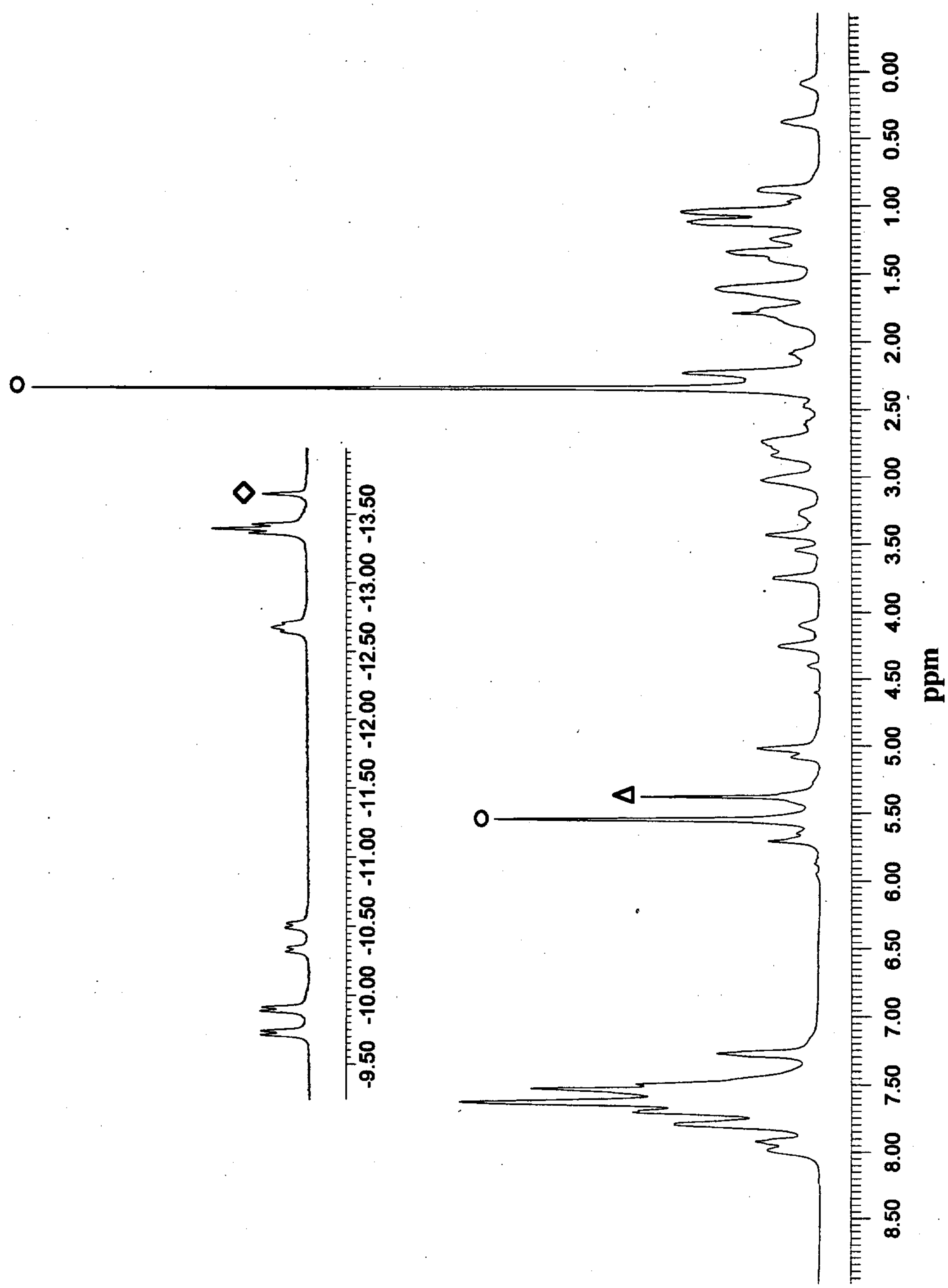

Figure 11. 500 MHz ^{1}H NMR of $[IrH_2(((S,S)\text{-CHIRAPHOS})COD)]BF_4$ in CD_2Cl_2 at -80°C (O = free COD, ◇ = trace $[IrH_2(COD)_2]BF_4$, and Δ = solvent).

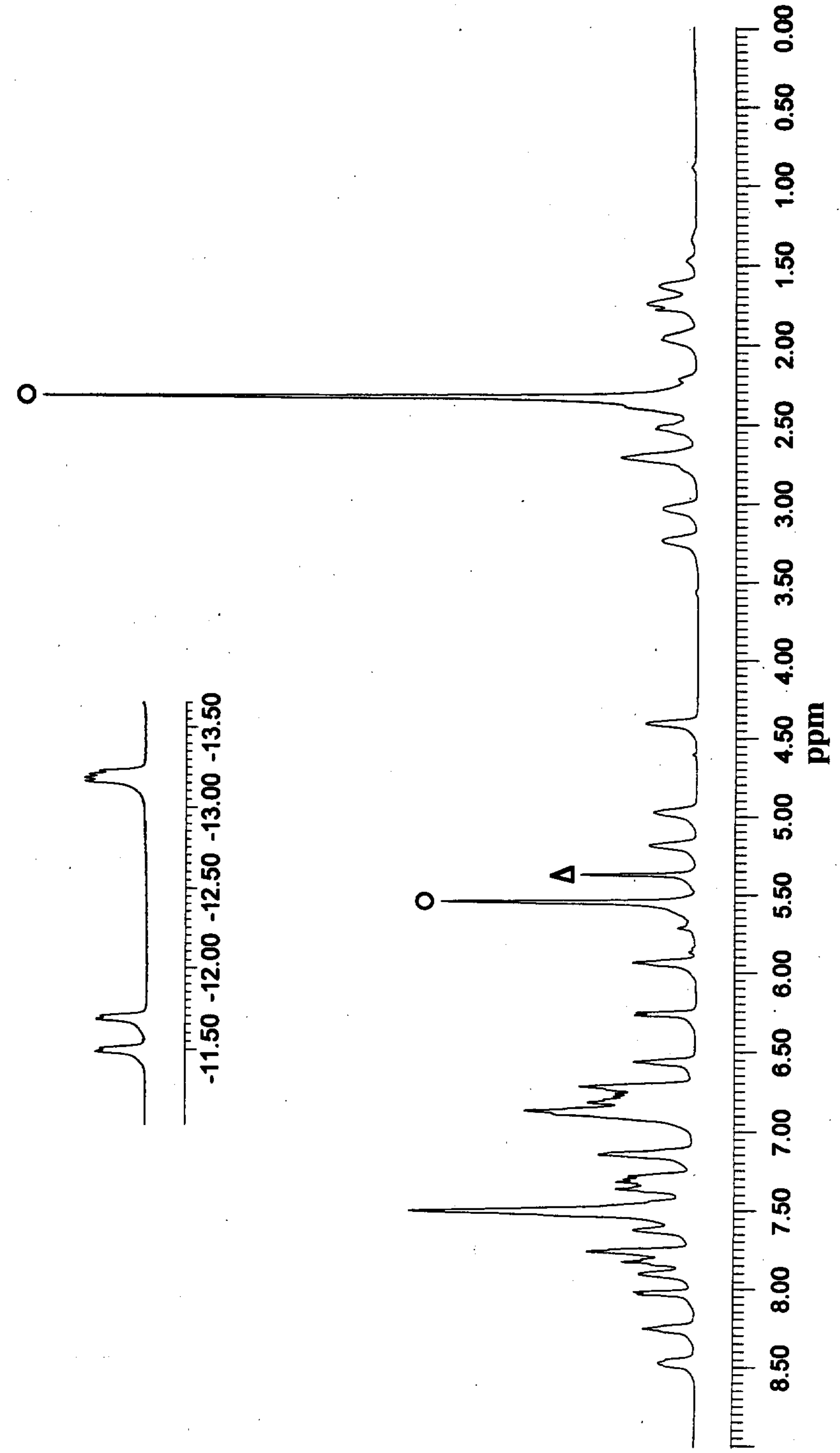

Figure 12. 500 MHz ^{1}H NMR of $[IrH_2((R)\text{-BINAP})(COD)]BF_4$ in CD_2Cl_2 at -80°C (ppm) (O = free COD and **Δ** = solvent).

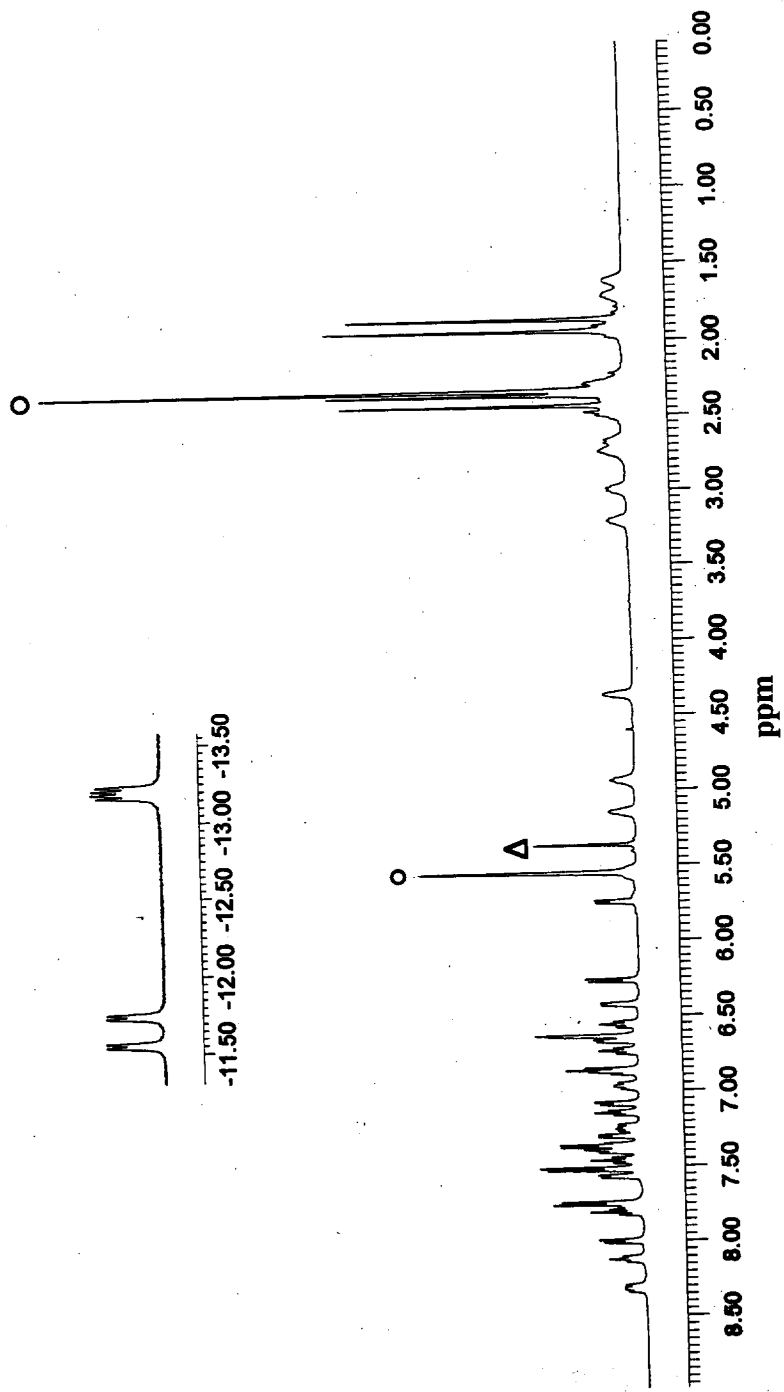

Figure 13. 500 MHz ^{1}H NMR of $[IrH_2((R)\text{-Tol-BINAP})(COD)]BF_4$ in CD_2Cl_2 at -80°C (O = free COD and Δ = solvent)..

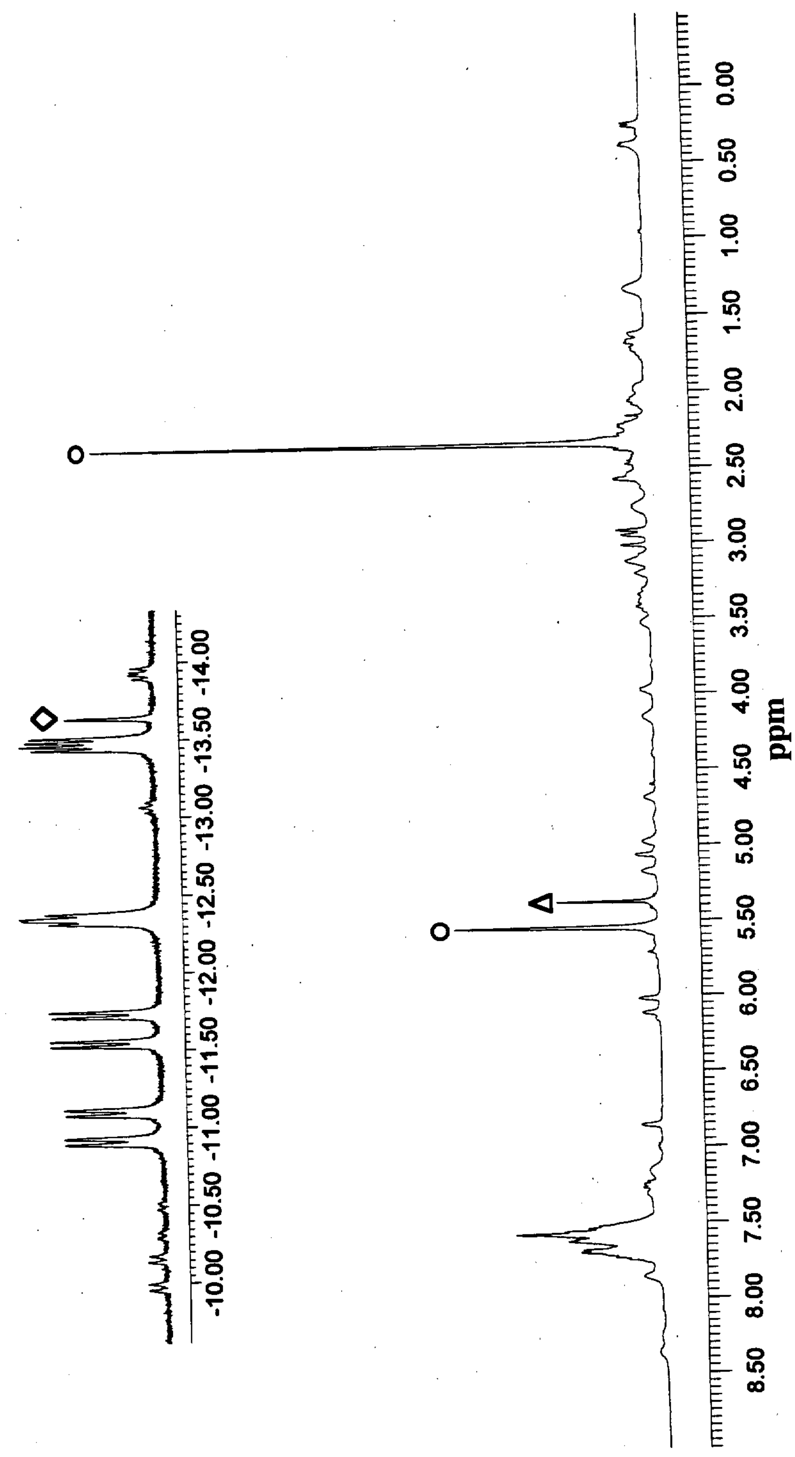

Figure 14. 500 MHz ^1H NMR of $[IrH_2((R,R)\text{-NORPHOS})(COD)]BF_4$ in CD_2Cl_2 at -80°C (O = free COD, ◇ = trace $[IrH_2(COD)_2]BF_4$, and Δ = solvent).

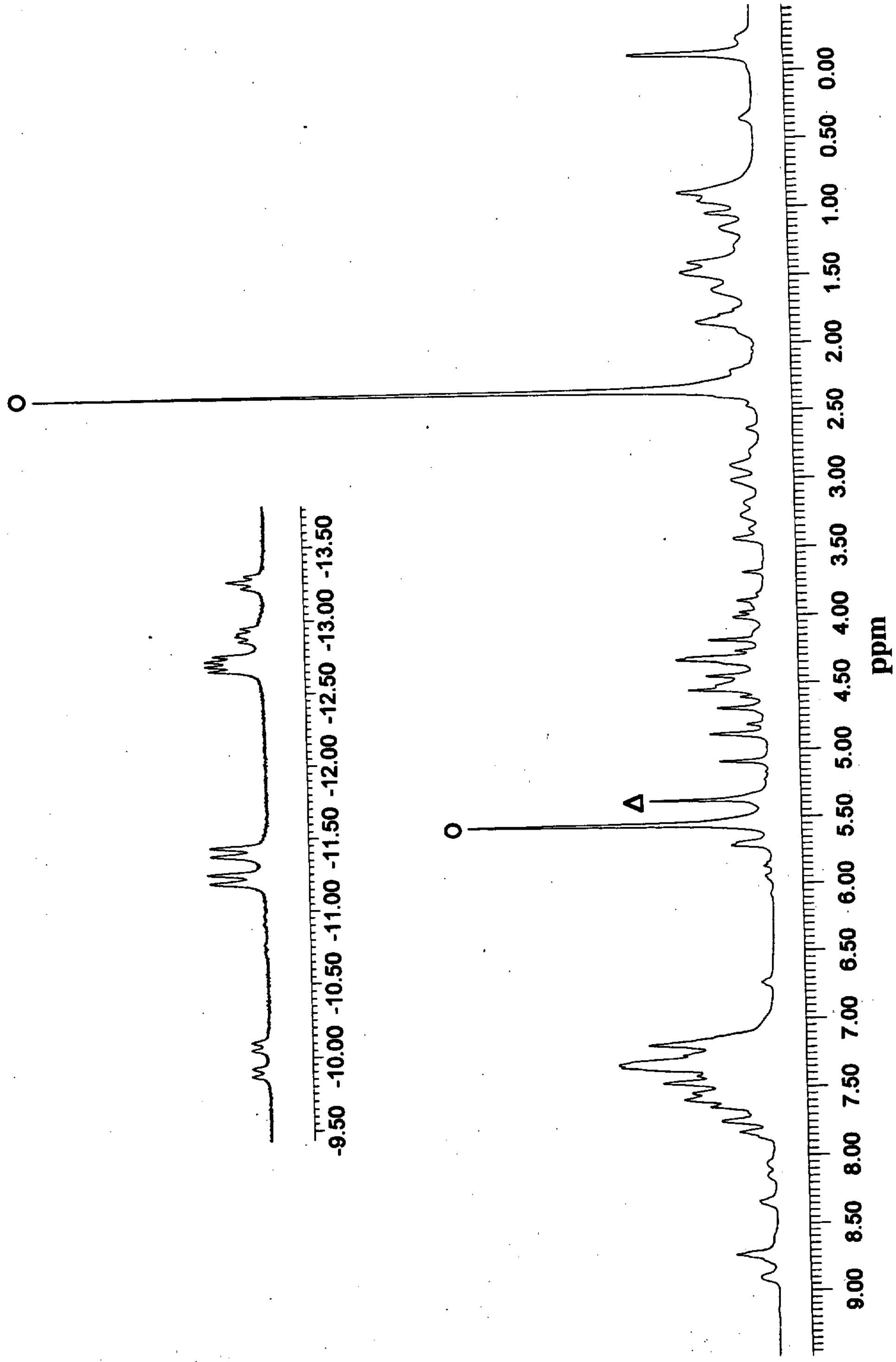

Figure 15. 500 MHz ^1H NMR of $[IrH_2((S,R)\text{-BPPFA})(COD)]BF_4$ in CD_2Cl_2 at -80°C (O = free COD and Δ = solvent).

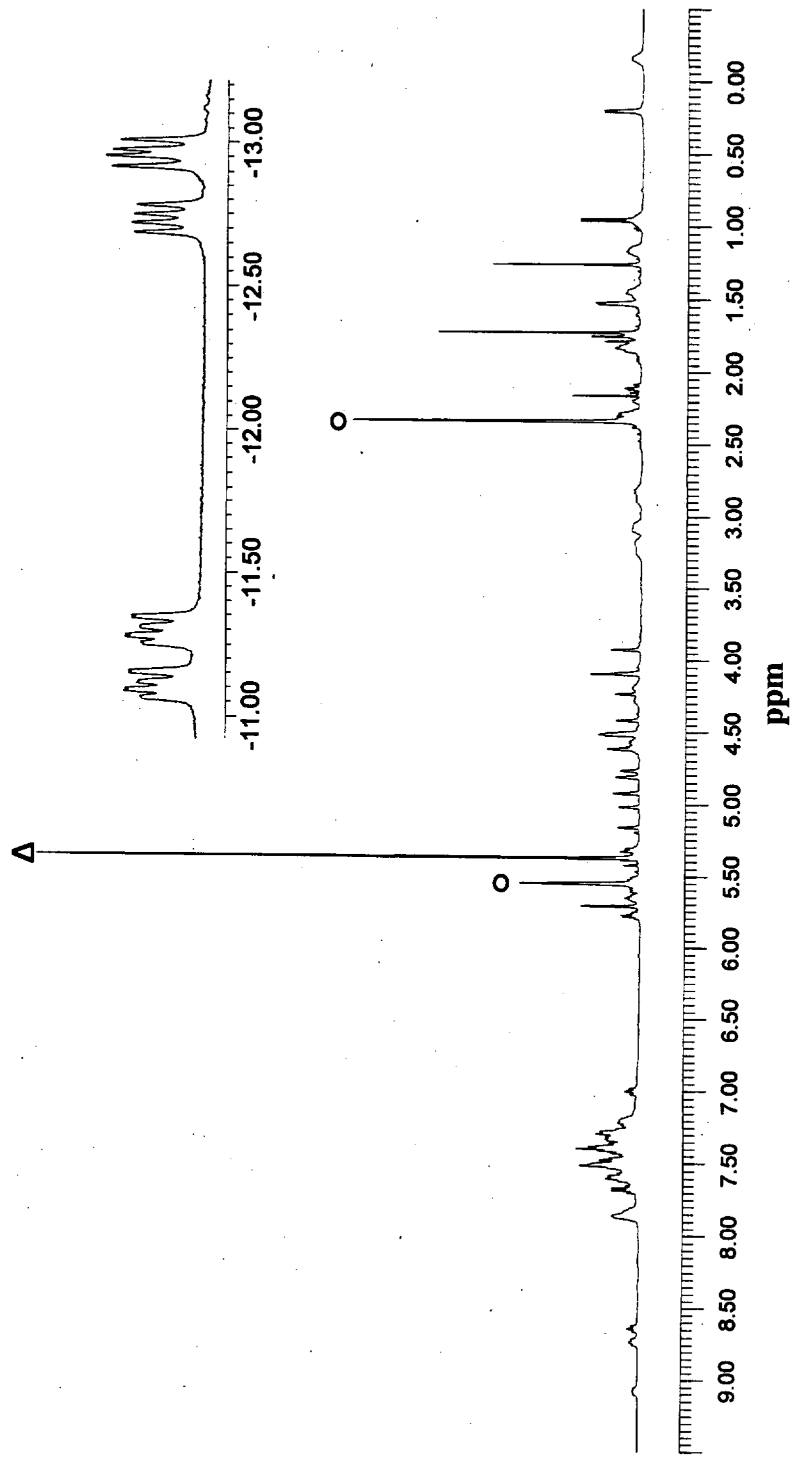

Figure 16. 500 MHz ^{1}H NMR of $[IrH_2((S,R)\text{-BPPFAc})(COD)]BF_4$ in CD_2Cl_2 at -80°C (○ = free COD, ◇ = trace $[IrH_2(COD)_2]BF_4$, and Δ = solvent).

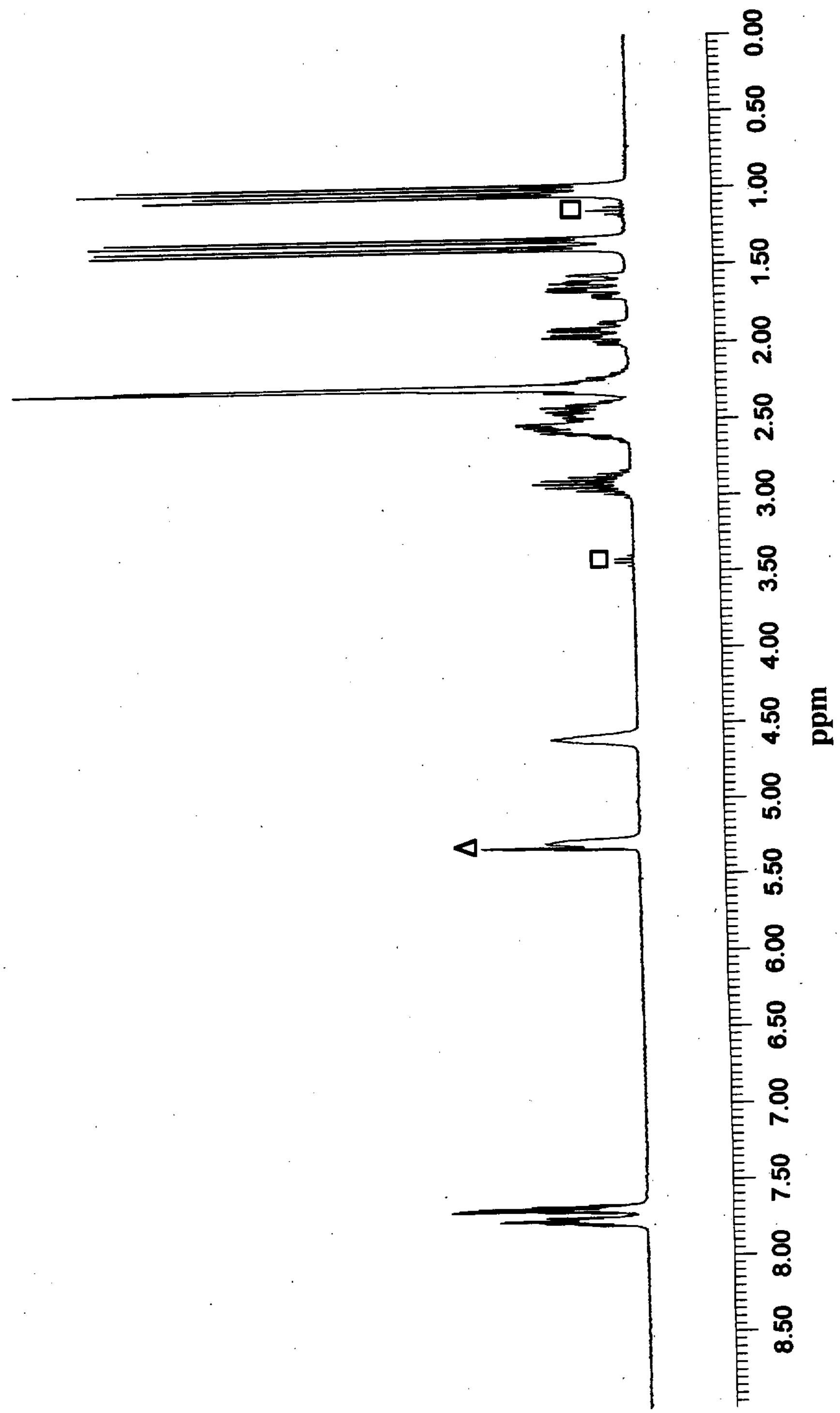

Figure 17. 300 MHz ^{1}H NMR of [Ir((*R*,*R*)-Me-DuPHOS)(COD)]BF_4 in CD_2Cl_2 at 25°C (□ = Et_2O and Δ = solvent).

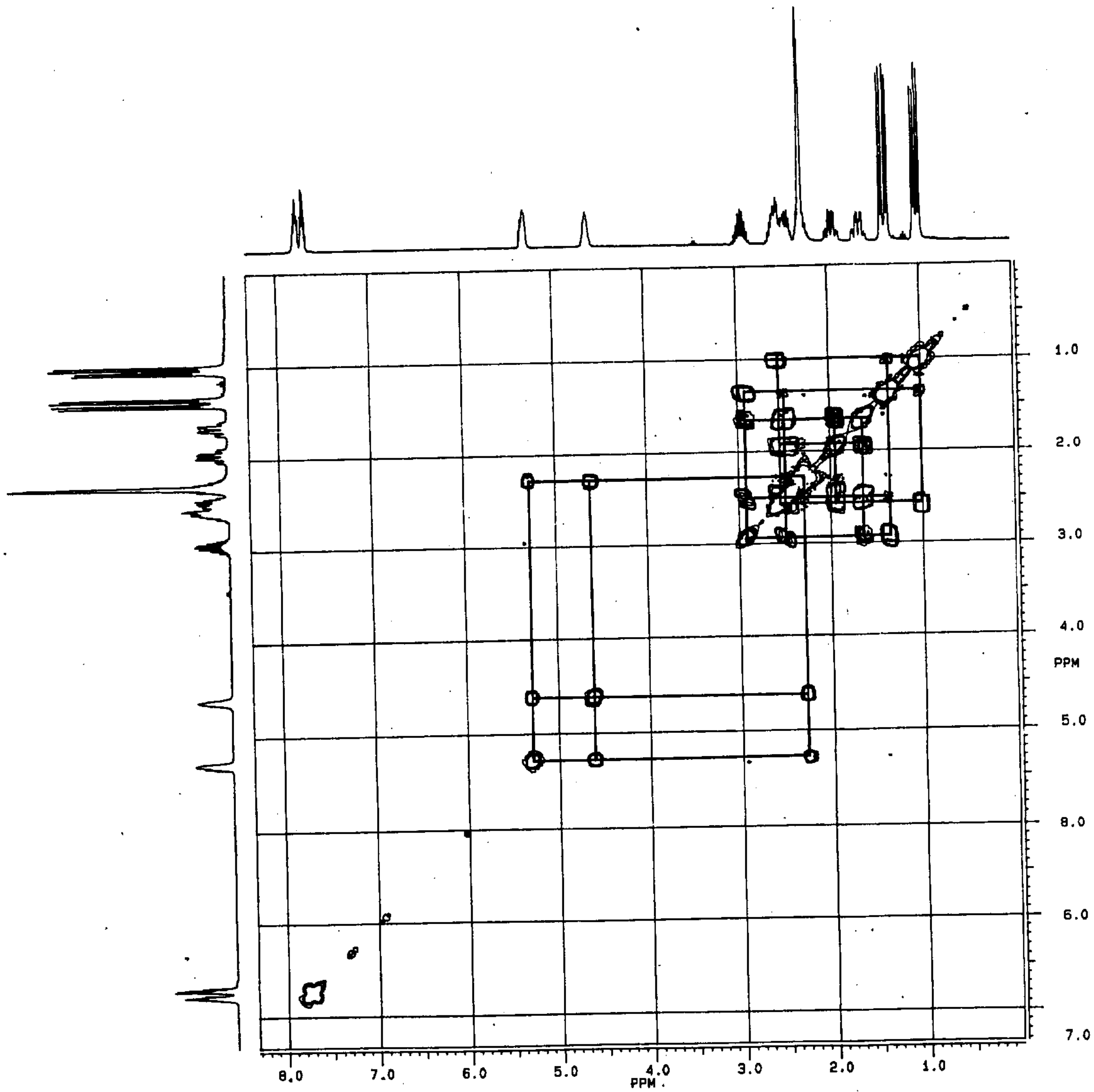

Figure 18. 300 MHz ^1H–^1H COSY 45 Spectrum of [Ir((*R*,*R*)-Me-DuPHOS)(COD)]BF_4 in CD_2Cl_2 at 25°C (□ = Et_2O and Δ = solvent).

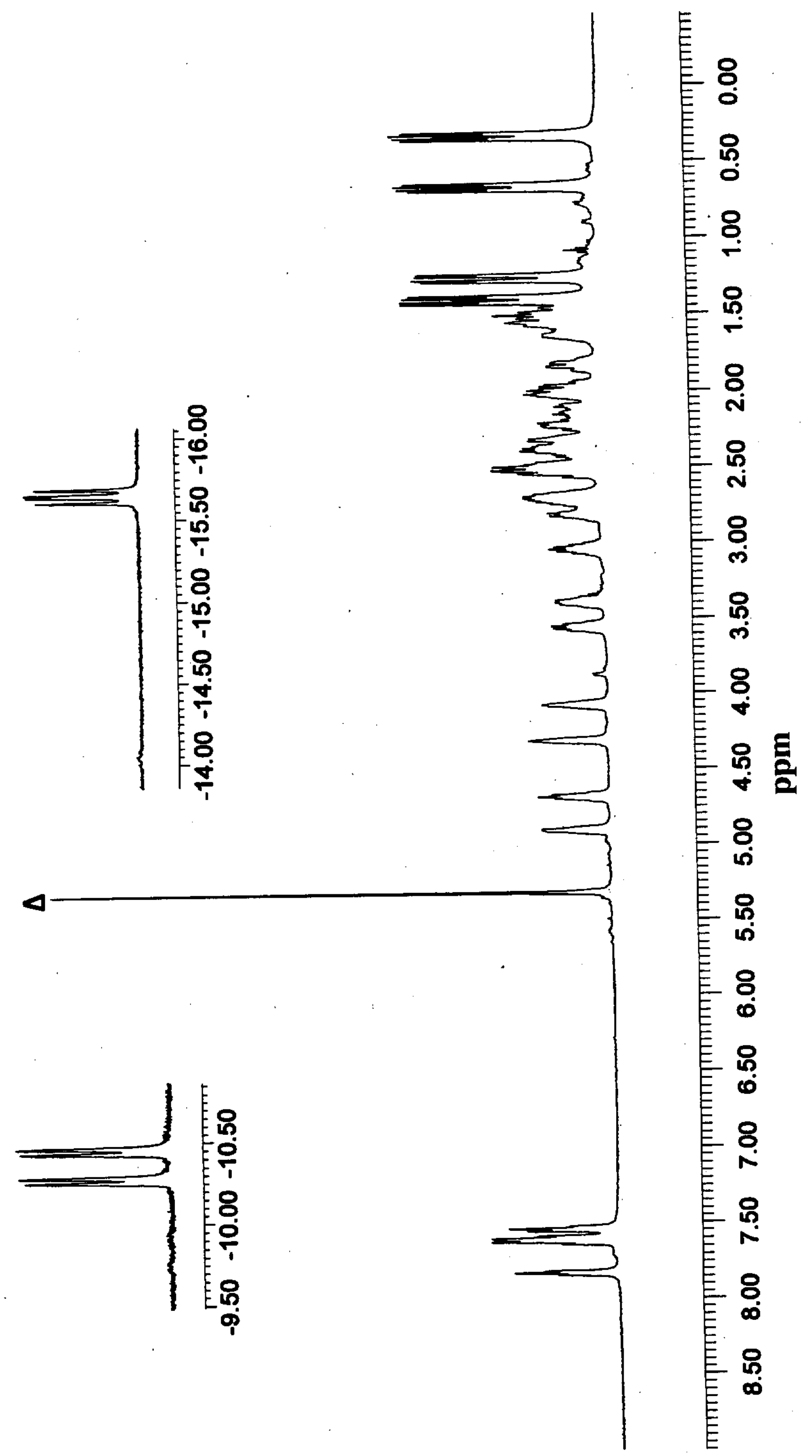

Figure 19. 500 MHz ^1H NMR of $[IrH_2(COD)((R,R)\text{-Me-DuPHOS})]BF_4$ in CD_2Cl_2 at -80°C (**Δ** = solvent).

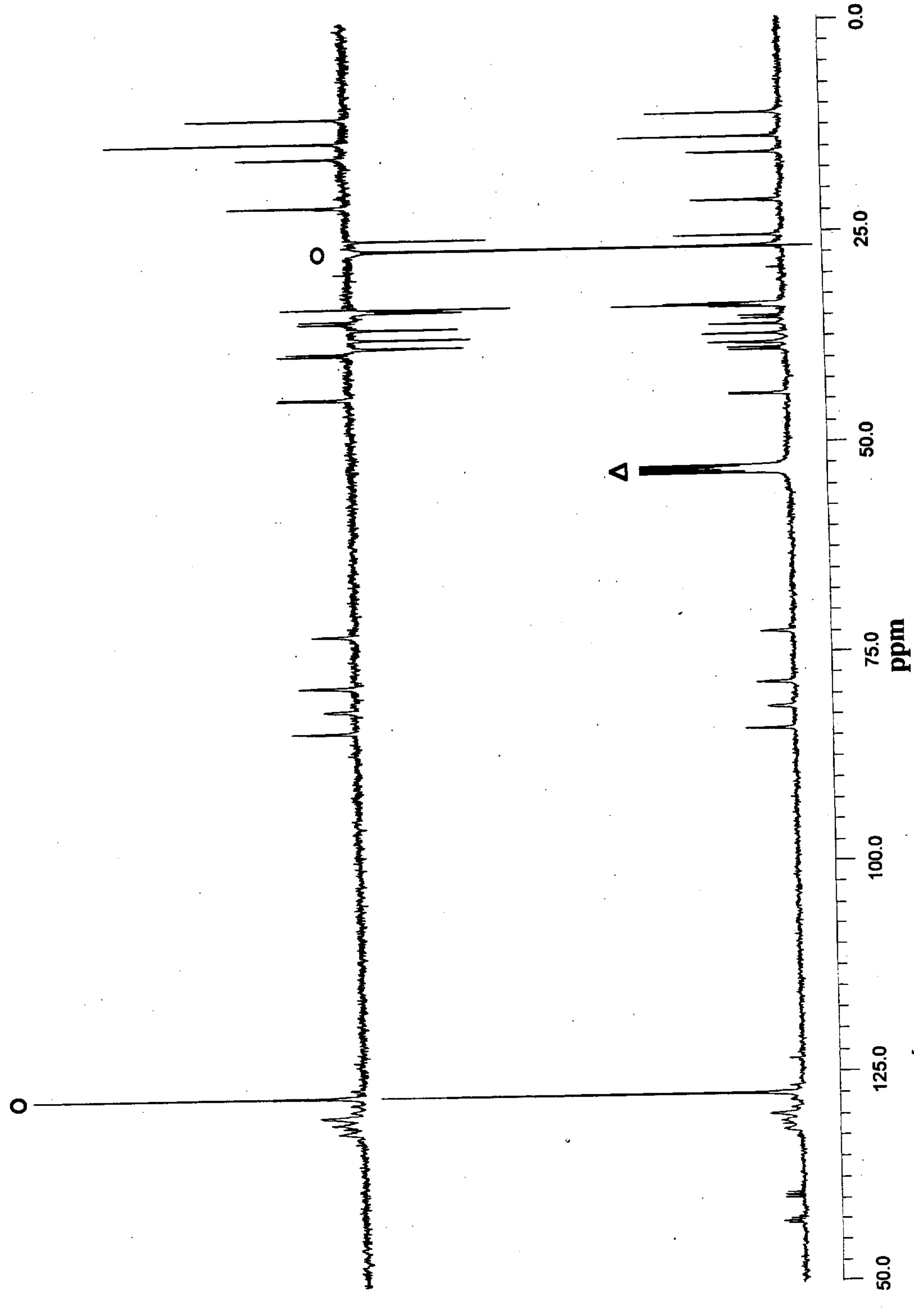

Figure 20. 126 MHz ^{13}C NMR and DEPT 135 of $[IrH_2(COD)((R,R)\text{-Me-DuPHOS})]BF_4$ in CD_2Cl_2 at -80°C (O = free COD and Δ = solvent).

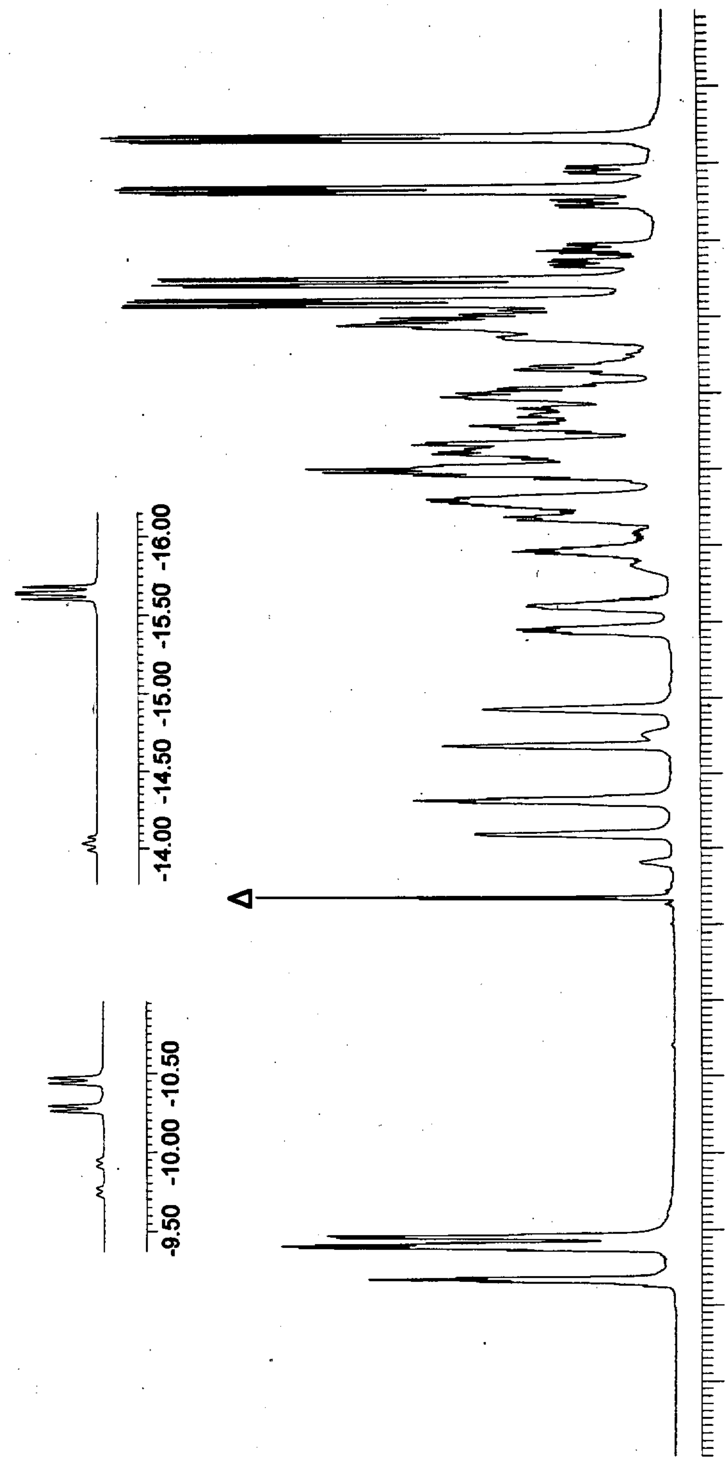

Figure 21. 500 MHz ^{1}H NMR of the equilibrium mixture (reached at -45°C) of $[IrH_2(COD)((R,R)\text{-Me-DuPHOS})]BF_4$ in CD_2Cl_2 taken at -80°C (**Δ** = solvent).

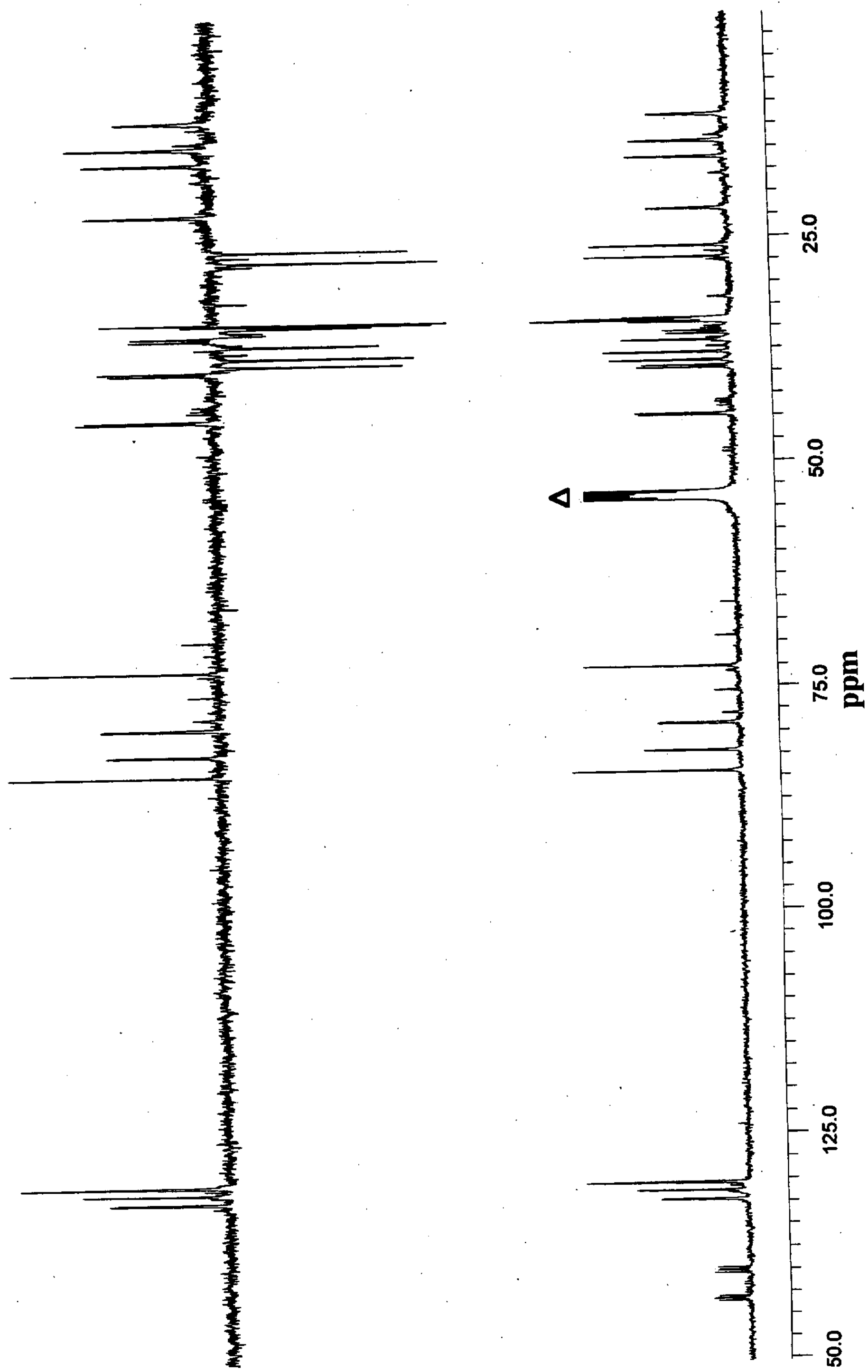

Figure 22. 126 MHz ^{13}C NMR and DEPT 135 of the equilibrium mixture (reached at -45°C) of $[IrH_2(COD)((R,R)\text{-Me-DuPHOS})]BF_4$ in CD_2Cl_2 taken at -80°C (**Δ** = solvent).

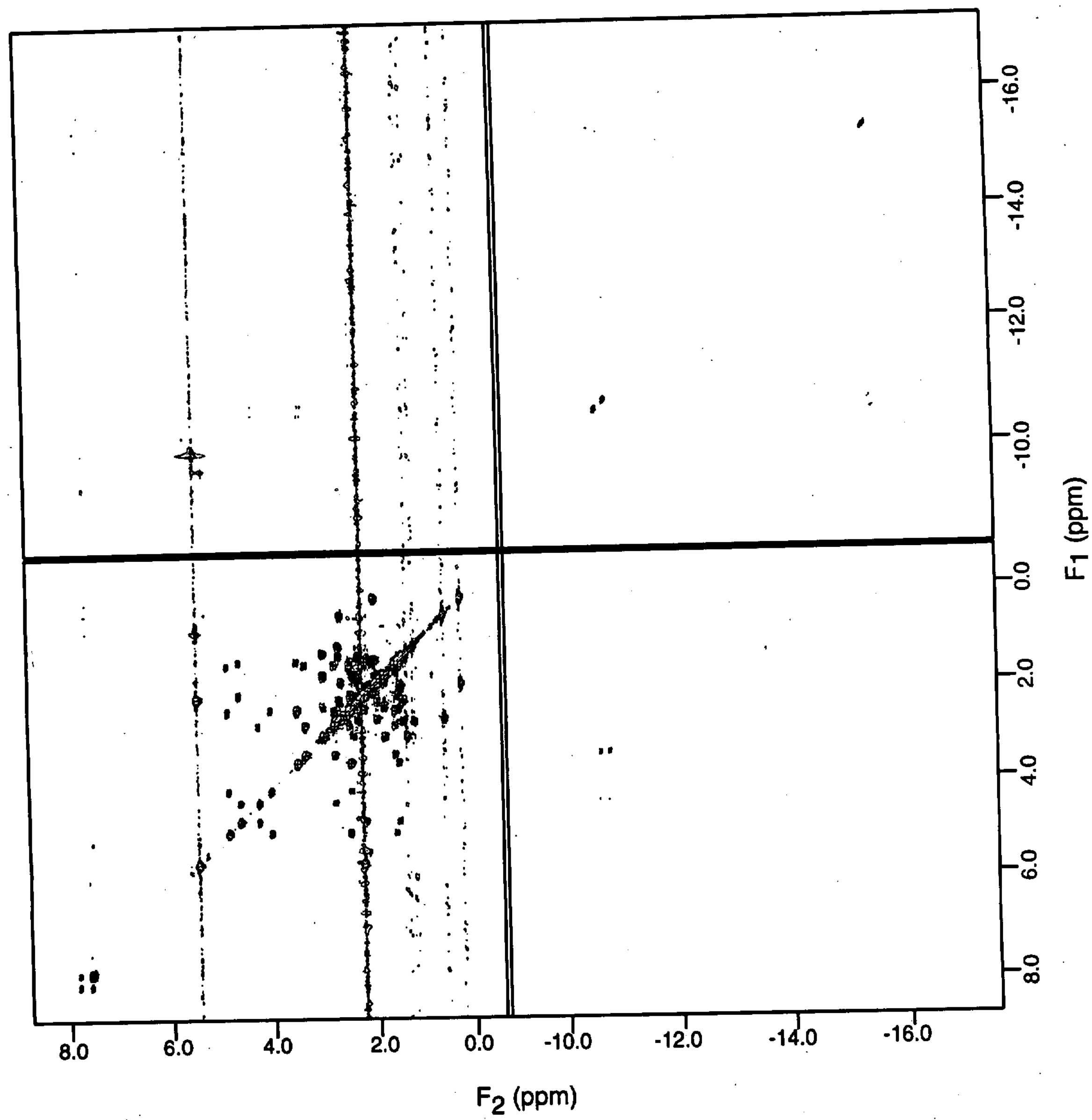

Figure 23. 500 MHz ^1H–^1H DQF COSY of $[IrH_2(COD)((R,R)\text{-Me-DuPHOS})]BF_4$, **10**^{maj}, at -80°C in CD_2Cl_2.

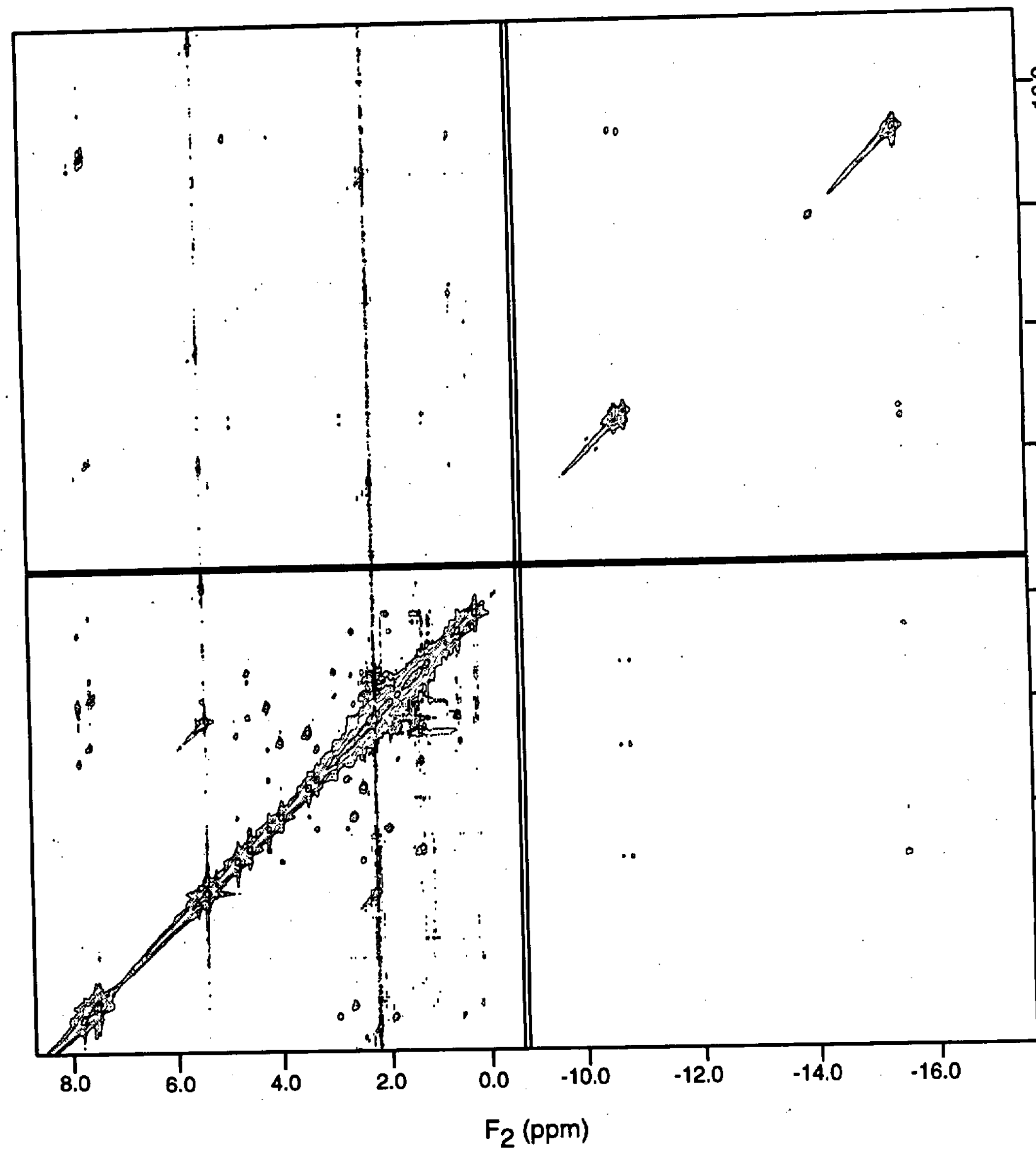

Figure 24. 500 MHz ^1H–^1H NOESY of $[IrH_2(COD)((R,R)\text{-Me-DuPHOS})]BF_4$, **10**^{maj}, at -80°C in CD_2Cl_2.

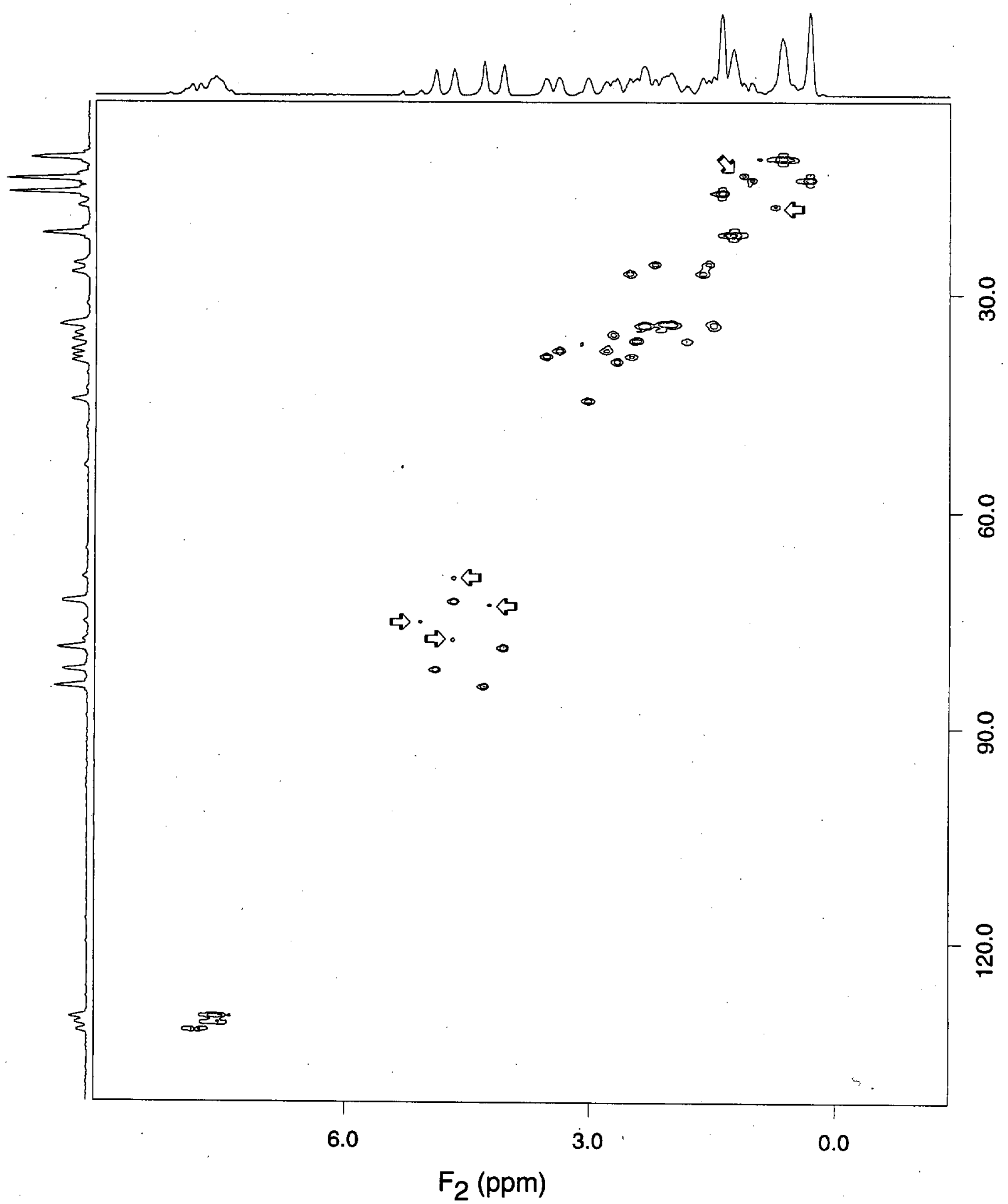

Figure 25. 500 MHz ^{1}H–^{13}C HMQC of the equilibrium mixture of $[IrH_2(COD)((R,R)\text{-Me-DuPHOS})]BF_4$, **10^{maj}/10^{min}**, at -80°C in CD_2Cl_2. The open arrows point to peaks of the minor diastereomer **10^{min}**.

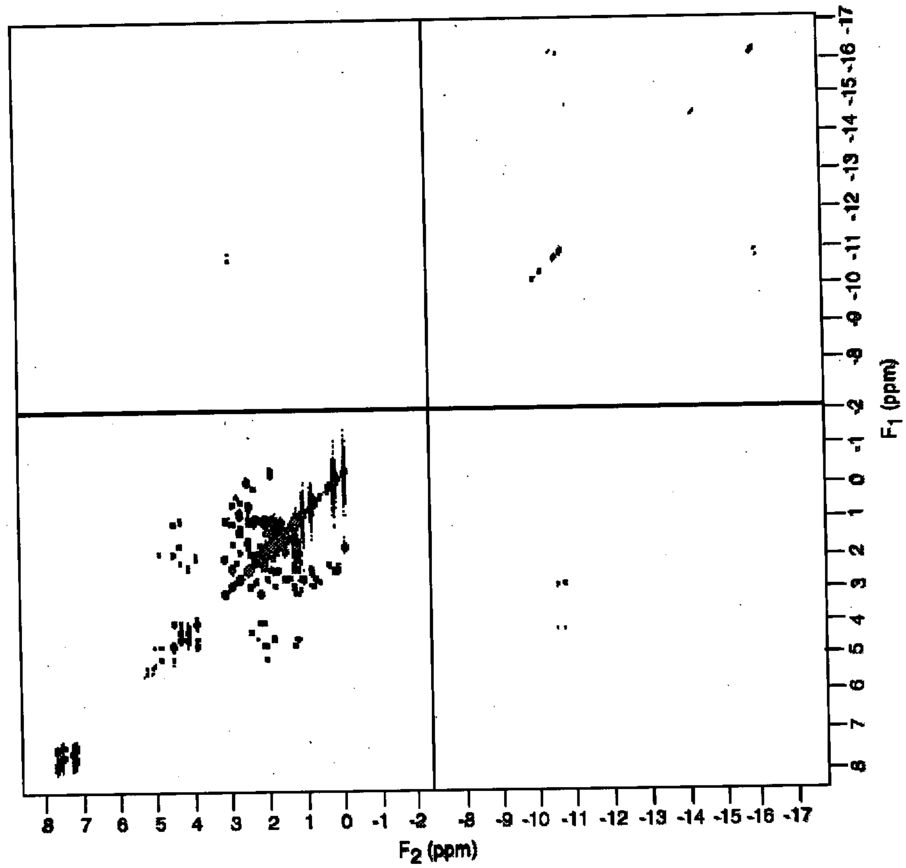

Figure 26. 500 MHz ^1H–^1H DQF COSY of $[IrH_2(COD)((R,R)\text{-Me-DuPHOS})]BF_4$, **$10^{maj}$**, at - 90°C in acetone-d_6.

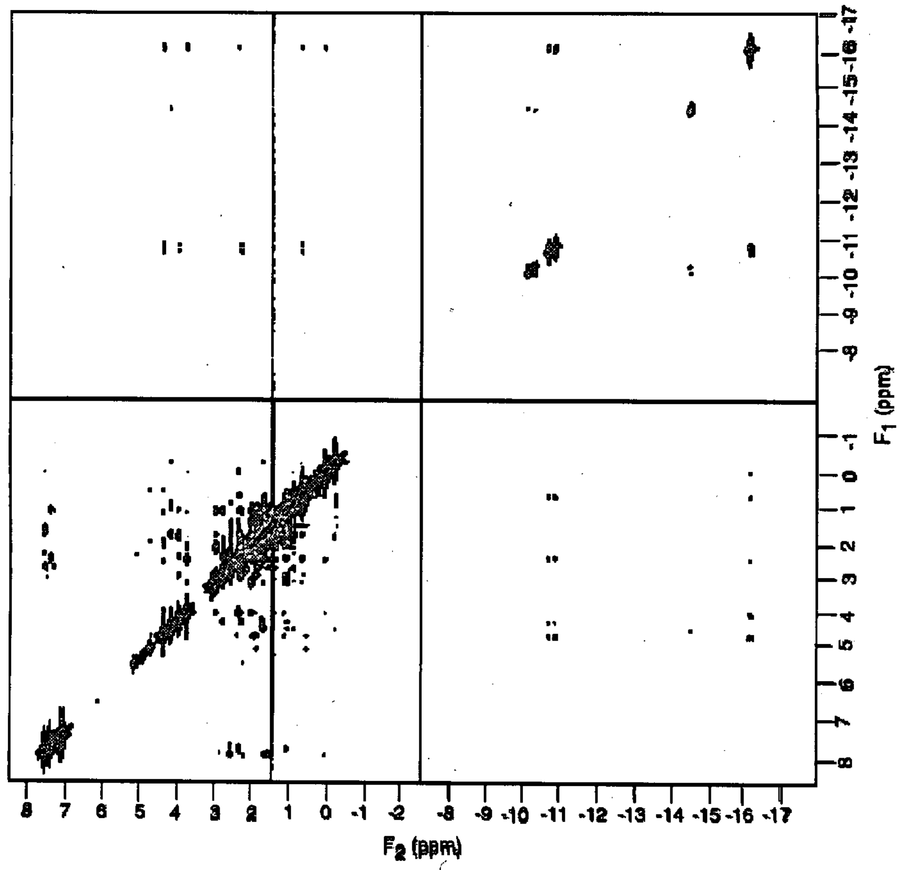

Figure 27. 500 MHz ^{1}H–^{1}H NOESY of $[IrH_2(COD)((R,R)\text{-Me-DuPHOS})]BF_4$, $\mathbf{10}^{maj}$, at - 90°C in acetone-d_6.

Table 5. ^{1}H Data for the Major Diastereomer of $[IrH_2((R,R)\text{-Me-DuPHOS})(COD)]BF_4$ ($\mathbf{10}^{maj}$) in acetone at -90°C.

H #	δ(^{1}H)	assignment
17	0.14	Me
6	-0.14	Me
18	1.00	Me
5	0.78	Me
22B	1.80	COD CH_2
22A	1.15	COD CH_2
26B	1.24	COD CH_2
26A	2.04	COD CH_2
4	1.86	$\underline{CH}CH_3$(6)
15A/B	1.68	Me-DuPHOS CH_2 *cis* to the adjacent Me
2A/B	1.80	Me-DuPHOS CH_2 *trans* to the adjacent Me
3A/B	1.60	Me-DuPHOS CH_2 *trans* to the adjacent Me
15A/B	1.47	Me-DuPHOS CH_2 *trans* to the adjacent Me
3A/B	1.20	Me-DuPHOS CH_2 *cis* to the adjacent Me
2A/B	1.15	Me-DuPHOS CH_2 *cis* to the adjacent Me
1	2.47	$\underline{CH}CH_3$(5)
14A/B	1.47	Me-DuPHOS CH_2 *cis* to the adjacent Me
14A/B	1.96	Me-DuPHOS CH_2 *trans* to the adjacent Me
25A	2.42	COD CH_2
25B	2.91	COD CH_2
21B	3.10	COD CH_2
21A	2.15	COD CH_2
16	2.50	$\underline{CH}CH_3$(17)
13	2.71	$\underline{CH}CH_3$(18)
23	4.32	COD vinyl
20	3.89	COD vinyl
19	4.51	COD vinyl
24	4.12	COD vinyl
8	7.56	phenyl
9	7.20	phenyl
10	7.26	phenyl
11	7.71	phenyl
27	-10.81	IrH trans
28	-16.16	IrH cis

Table 6. 2DCPA input data

34\ number of distinct NOESY groups of the major diastereomer.
1st number indicates whether methyl or not 1 = not methyl, 3 = methyl
2nd number is the number of protons in the group
3rd number is the atom number from the conformer file

1 1
1 \#1-*ortho*-aryl proton corresponds to H#11 in Figure 4 (Full paper)
1 1
2 \#2-*ortho*-aryl proton corresponds to H#8 in Figure 4 (Full paper)
1 1
3 \#3-*meta*-aryl proton corresponds to H#10 in Figure 4 (Full paper)
1 1
4 \#4-*meta*-aryl proton corresponds to H#9 in Figure 4 (Full paper)
1 1
5 \#5-vinyl proton corresponds to H#19 in Figure 4 (Full paper)
1 1
6 \#6-vinyl proton corresponds to H#23 in Figure 4 (Full paper)
1 1
7 \#7-vinyl proton corresponds to H#24 in Figure 4 (Full paper)
1 1
8 \#8-vinyl proton corresponds to H#20 in Figure 4 (Full paper)
1 1
9 \#9-CH2 proton on COD corresponds to H#21B in Figure 4 (Full paper)
1 1
10 \#10-CH2 proton on COD corresponds to H#25B in Figure 4 (Full paper)
1 1
11 \#11-CH proton on DuPhos corresponds to H#13 in Figure 4 (Full paper)
1 1
12 \#12-CH2 proton on COD corresponds to H#25A in Figure 4 (Full paper)
1 1
13 \#13-CH proton on DuPhos corresponds to H#1 in Figure 4 (Full paper)
1 1
14 \#14-CH proton on DuPhos corresponds to H#16 in Figure 4 (Full paper)
1 1
15 \#15-CH2 proton on COD corresponds to H#26A in Figure 4 (Full paper)
1 1
16 \#16-CH2 proton on COD corresponds to H#21A in Figure 4 (Full paper)

1 1
17 \#17-CH2 proton on COD corresponds to H#22B in Figure 4 (Full paper)
1 1
18 \#18-CH proton on DuPhos corresponds to H#4 in Figure 4 (Full paper)
1 1
19 \#19-CH2 proton on DuPhos corresponds to H#15A/B *cis* to the adjacent Me in Figure 4 (Full paper)
1 1
20 \#20-CH2 proton on DuPhos corresponds to H#14A/B *cis* to the adjacent Me in Figure 4 (Full paper)
1 1
21 \#21-CH2 proton on COD corresponds to H#26B in Figure 4 (Full paper)
1 1
22 \#22-CH2 proton on COD corresponds to H#22A in Figure 4 (Full paper)
1 1
23 \#23-CH2 proton on DuPhos corresponds to H#3A/B *cis* to the adjacent Me in Figure 4 (Full paper)
1 1
63 \#24-CH2 proton on DuPhos corresponds to H#2A/B *cis* to the adjacent Me in Figure 4 (Full paper)
3 3
25 43 44 42 \#25-Me protons (last number is the corresponding carbon) correspond to H#18 in Figure 4 (Full paper)
3 3
26 55 56 54 \#26-Me protons (last number is the corresponding carbon) correspond to H#5 in Figure 4 (Full paper)
3 3
27 48 49 47 \#27-Me protons (last number is the corresponding carbon) correspond to H#17 in Figure 4 (Full paper)
3 3
28 58 59 57 \#28-Me protons (last number is the corresponding carbon) correspond to H#6 in Figure 4 (Full paper)
1 1
29 \#29 the trans-hydride corresponds to H#27 in Figure 4 (Full paper)
1 1
30 \#30 the cis-hydride corresponds to H#11 in Figure 4 (Full paper)
1 1
46 \#31-CH2 proton corresponds to H#14A/B *trans* to the adjacent Me in Figure 4 (Full paper)
1 1
51 \#32-CH2 proton corresponds to H#15A/B *trans* to the adjacent Me in Figure 4 (Full paper)
1 1
24 \#33-CH2 proton corresponds to H#2A/B *trans* to the adjacent Me in Figure 4 (Full paper)
1 1
61 \#34-CH2 proton corresponds to H#3A/B *trans* to the adjacent Me in Figure 4 (Full paper)
1st number is isotropic rotational correlation time (in ns)
2nd number is methyl spin correlation. time (in ps)
3rd external relaxation rate (in sec, all extramolecular relaxation)

```
# 4th number is a bit flag that determines which relaxation parameter(s) is/are optimized
# by comparison with experimental data.  This flag is integer sum of three binary numbers
# 1=optimize tau(1), 2=optimize tau(2), 4=optimize rext;
# i.e. 3 means optimize both isotropic and methyl spin correlation times
# 5th number is optimization gradient cutoff
0.5596   167.701 0.3560   0          5E-4 \
6 \# number of mixing times (must include 0 mix time >= 2)
0        0.07      0.10      0.13      0.16      0.20 \# mixing time (in sec.)
#595 total points, 34 diagonal peaks, 49+4 good peaks,30 noisy peaks, 458 absent peaks,20 unresolved peaks
#Four groups of all data point are classified.
#Diagonal peaks  are from the same group.
#Good peaks are assigned if the observed intensities .GE. twice of the local noise level.
#Noisy peaks are assigned if the observed intensities are less than twice of the local noise level.
#Unresolved peaks are assigned if those are close to diagonal peaks.

# 1st two numbers are the group (group matrix elements)
# the input file only requires upper triangular part of the matrix
# next set of numbers is the volumes at each mixing time (arbitrary units)
# next number is weighting factor which can be of several types
# 999 for good peaks, 997 for noisy peaks and absent peaks, 0.0 for diagonal peaks and unresolved peaks.
```

1	1	2.294E+09	0.189E+10	0.184E+10	0.171E+10	0.156E+10	0.140E+10	0	0\diagonal peak
1	2	0.000E+00	7.282E+05	4.047E+05	5.611E+05	5.696E+05	9.572E+05	997	0\absent peak
1	3	0.000E+00	3.800E+07	4.570E+07	4.955E+07	5.175E+07	5.720E+07	999	0\good peak
1	4	0.000E+00	1.651E+05	8.331E+05	2.409E+04	8.612E+04	6.502E+05	997	0\absent peak
1	5	0.000E+00	4.424E+05	8.745E+05	1.194E+05	7.842E+05	5.439E+05	997	0\absent peak
1	6	0.000E+00	1.929E+05	1.735E+05	5.155E+05	8.398E+05	8.601E+05	997	0\absent peak
1	7	0.000E+00	4.552E+05	3.345E+05	1.512E+05	8.764E+05	2.925E+05	997	0\absent peak
1	8	0.000E+00	5.796E+05	2.367E+05	1.903E+05	8.510E+05	2.515E+05	997	0\absent peak
1	9	0.000E+00	8.211E+05	4.873E+05	6.368E+05	7.248E+05	5.478E+05	997	0\absent peak
1	10	0.000E+00	3.588E+04	7.429E+05	4.817E+05	3.472E+05	5.596E+05	997	0\absent peak
1	11	0.000E+00	1.690E+07	2.355E+07	2.940E+07	3.460E+07	3.905E+07	999	0\good peak
1	12	0.000E+00	7.814E+05	6.601E+05	9.624E+05	6.729E+05	9.798E+05	997	0\absent peak
1	13	0.000E+00	8.985E+05	4.570E+05	1.672E+04	5.775E+05	3.448E+05	997	0\absent peak
1	14	0.000E+00	7.299E+05	4.407E+05	7.721E+05	8.804E+05	3.904E+05	997	0\absent peak
1	15	0.000E+00	2.412E+05	6.391E+05	9.117E+04	2.758E+05	6.874E+04	997	0\absent peak
1	16	0.000E+00	3.074E+05	6.984E+05	3.667E+05	7.939E+05	4.731E+05	997	0\absent peak
1	17	0.000E+00	2.348E+05	5.906E+05	3.518E+05	6.719E+05	6.577E+05	997	0\absent peak
1	18	0.000E+00	9.921E+05	2.666E+04	2.862E+05	6.558E+04	2.313E+05	997	0\absent peak

1	19	0.000E+00	2.565E+07	3.575E+07	4.465E+07	5.000E+07	5.280E+07	999	0\good peak
1	20	0.000E+00	2.079E+05	5.047E+05	4.668E+05	8.647E+05	8.561E+05	997	0\absent peak
1	21	0.000E+00	3.110E+05	1.756E+05	8.424E+05	1.819E+05	8.951E+05	997	0\absent peak
1	22	0.000E+00	2.074E+05	5.284E+05	8.675E+05	7.825E+05	1.376E+05	997	0\absent peak
1	23	0.000E+00	7.250E+05	2.862E+05	4.788E+05	8.544E+05	5.790E+05	997	0\absent peak
1	24	0.000E+00	9.145E+05	2.105E+04	6.794E+05	5.651E+05	2.164E+05	997	0\absent peak
1	25	0.000E+00	-3.850E+04	3.360E+05	5.280E+05	9.690E+05	8.240E+05	997	0\noisy peak
1	26	0.000E+00	6.470E+05	1.442E+05	2.238E+05	9.534E+05	7.974E+05	997	0\absent peak
1	27	0.000E+00	1.478E+06	2.415E+06	2.615E+06	2.865E+06	3.175E+06	999	0\good peak
1	28	0.000E+00	7.340E+04	2.610E+05	6.430E+04	2.740E+04	2.860E+05	997	0\noisy peak
1	29	0.000E+00	2.494E+05	3.760E+05	7.547E+04	6.597E+04	6.191E+05	997	0\absent peak
1	30	0.000E+00	8.779E+05	4.407E+05	7.493E+05	6.716E+05	7.961E+05	997	0\absent peak
1	31	0.000E+00	7.081E+05	3.300E+05	1.917E+05	8.879E+04	5.465E+05	997	0\absent peak
1	32	0.000E+00	4.640E+05	3.270E+05	9.538E+05	1.241E+05	7.014E+05	997	0\absent peak
1	33	0.000E+00	6.827E+04	2.768E+04	4.649E+05	2.824E+05	1.346E+05	997	0\absent peak
1	34	0.000E+00	7.160E+05	1.077E+05	3.632E+05	6.509E+05	1.451E+05	997	0\absent peak
2	2	1.882E+09	0.158E+10	0.156E+10	0.146E+10	0.134E+10	0.122E+10	0	0\diagonal peak
2	3	0.000E+00	8.985E+05	4.570E+05	1.672E+04	5.775E+05	3.448E+05	997	0\absent peak
2	4	0.000E+00	6.940E+07	8.275E+07	8.035E+07	8.310E+07	8.045E+07	999	0\good peak
2	5	0.000E+00	8.104E+04	7.432E+04	3.421E+05	6.325E+04	4.995E+05	997	0\absent peak
2	6	0.000E+00	7.996E+04	5.351E+05	2.764E+05	7.396E+05	6.226E+05	997	0\absent peak
2	7	0.000E+00	3.087E+05	8.618E+05	9.524E+05	4.714E+05	9.075E+04	997	0\absent peak
2	8	0.000E+00	4.117E+05	1.809E+05	3.984E+05	6.026E+05	1.142E+05	997	0\absent peak
2	9	0.000E+00	2.332E+05	1.117E+05	5.488E+03	7.563E+04	8.082E+05	997	0\absent peak
2	10	0.000E+00	7.737E+05	6.609E+05	5.191E+05	2.919E+05	4.679E+05	997	0\absent peak
2	11	0.000E+00	8.029E+05	4.715E+05	3.647E+05	1.287E+05	9.255E+05	997	0\absent peak
2	12	0.000E+00	1.510E+05	1.140E+04	8.083E+04	2.097E+05	2.607E+05	997	0\absent peak
2	13	0.000E+00	2.580E+07	3.460E+07	4.415E+07	5.035E+07	5.740E+07	999	0\good peak
2	14	0.000E+00	3.816E+05	5.521E+05	9.558E+05	6.123E+05	4.611E+05	997	0\absent peak
2	15	0.000E+00	2.773E+05	1.006E+05	3.967E+05	3.589E+05	8.686E+05	997	0\absent peak
2	16	0.000E+00	6.059E+05	7.625E+05	8.014E+05	5.055E+05	4.397E+05	997	0\absent peak
2	17	0.000E+00	1.114E+05	7.635E+05	9.923E+05	1.209E+05	7.737E+05	997	0\absent peak
2	18	0.000E+00	5.280E+05	-3.930E+05	1.470E+05	-1.380E+05	2.610E+06	997	0\noisy peak
2	19	0.000E+00	4.334E+03	6.801E+05	8.815E+05	4.663E+05	3.927E+05	997	0\absent peak
2	20	0.000E+00	4.950E+04	4.971E+05	5.300E+05	8.811E+04	5.562E+05	997	0\absent peak
2	21	0.000E+00	5.126E+03	9.299E+05	2.413E+05	8.137E+05	1.825E+05	997	0\absent peak
2	22	0.000E+00	2.785E+05	3.473E+04	1.828E+05	6.089E+05	8.295E+05	997	0\absent peak
2	23	0.000E+00	1.160E+07	1.335E+07	1.890E+07	2.015E+07	2.230E+07	999	0\good peak
2	24	0.000E+00	2.661E+05	9.452E+05	6.572E+05	2.744E+04	2.372E+05	997	0\absent peak

2	25	0.000E+00	4.755E+04	2.574E+04	8.688E+05	6.318E+05	6.407E+05	997	0\absent peak
2	26	0.000E+00	-3.480E+04	5.900E+05	1.040E+06	1.070E+06	9.360E+05	997	0\noisy peak
2	27	0.000E+00	1.191E+05	3.305E+05	7.572E+05	2.703E+03	5.410E+05	997	0\absent peak
2	28	0.000E+00	1.579E+06	1.522E+06	7.165E+07	1.575E+07	1.565E+07	997	0\noisy peak
2	29	0.000E+00	7.727E+05	4.162E+05	8.586E+04	2.384E+05	1.152E+05	997	0\absent peak
2	30	0.000E+00	5.599E+04	6.538E+05	9.816E+05	5.156E+05	9.075E+05	997	0\absent peak
2	31	0.000E+00	6.299E+05	6.758E+05	2.347E+05	3.616E+05	3.331E+04	997	0\absent peak
2	32	0.000E+00	1.515E+05	6.235E+05	6.819E+05	8.759E+05	1.532E+05	997	0\absent peak
2	33	0.000E+00	0.387E+06	0.820E+06	0.221E+07	0.298E+07	0.300E+07	997	0\noisy peak
2	34	0.000E+00	0.323E+06	0.422E+06	0.689E+06	0.353E+06	0.140E+07	997	0\noisy peak
3	3	2.341E+09	0.209E+10	0.214E+10	0.206E+10	0.193E+10	0.183E+10	0	0\diagonal peak
3	4	0.000E+00	9.557E+06	9.448E+06	5.509E+06	8.578E+06	8.733E+06	0	0\unresolved peak
3	5	0.000E+00	1.082E+05	6.931E+05	5.229E+05	2.430E+05	6.937E+05	997	0\absent peak
3	6	0.000E+00	8.119E+05	7.438E+05	1.994E+05	3.655E+04	8.460E+04	997	0\absent peak
3	7	0.000E+00	8.088E+05	5.854E+05	2.709E+05	4.328E+05	4.364E+05	997	0\absent peak
3	8	0.000E+00	7.043E+05	6.499E+05	1.330E+05	5.301E+05	4.480E+05	997	0\absent peak
3	9	0.000E+00	1.173E+04	5.341E+05	2.551E+05	4.658E+05	6.888E+05	997	0\absent peak
3	10	0.000E+00	7.478E+05	8.370E+05	4.446E+04	5.357E+05	2.441E+05	997	0\absent peak
3	11	0.000E+00	0.200E+06	0.406E+06	0.850E+06	0.698E+06	0.144E+07	999	0\good peak
3	12	0.000E+00	8.414E+05	2.942E+05	7.975E+05	6.457E+05	8.995E+05	997	0\absent peak
3	13	0.000E+00	2.437E+05	2.174E+05	9.127E+05	9.985E+05	4.180E+05	997	0\absent peak
3	14	0.000E+00	8.199E+05	9.099E+04	8.956E+05	4.056E+05	7.804E+05	997	0\absent peak
3	15	0.000E+00	6.673E+05	5.015E+05	6.903E+05	2.773E+05	2.788E+05	997	0\absent peak
3	16	0.000E+00	4.094E+04	4.926E+05	5.165E+04	7.172E+05	2.016E+05	997	0\absent peak
3	17	0.000E+00	5.879E+05	6.965E+05	7.705E+05	3.250E+05	3.898E+05	997	0\absent peak
3	18	0.000E+00	4.119E+05	1.886E+05	2.665E+05	3.772E+05	5.089E+05	997	0\absent peak
3	19	0.000E+00	4.630E+05	-3.950E+04	-2.400E+03	8.220E+05	6.910E+05	997	0\noisy peak
3	20	0.000E+00	6.548E+05	5.581E+05	8.930E+05	5.225E+05	3.816E+05	997	0\absent peak
3	21	0.000E+00	5.927E+05	4.369E+05	4.911E+05	6.295E+05	3.818E+05	997	0\absent peak
3	22	0.000E+00	3.487E+05	8.342E+05	8.515E+05	9.966E+05	2.081E+05	997	0\absent peak
3	23	0.000E+00	7.050E+05	1.802E+05	4.025E+05	6.274E+04	3.437E+05	997	0\absent peak
3	24	0.000E+00	2.941E+05	5.759E+05	9.129E+05	6.140E+05	2.300E+05	997	0\absent peak
3	25	0.000E+00	8.094E+05	4.192E+05	3.605E+05	3.525E+05	9.079E+05	997	0\absent peak
3	26	0.000E+00	3.275E+05	7.693E+05	7.056E+05	3.207E+05	8.564E+04	997	0\absent peak
3	27	0.000E+00	3.880E+05	1.940E+05	5.240E+05	7.120E+05	5.370E+05	997	0\noisy peak
3	28	0.000E+00	8.481E+05	5.118E+04	5.482E+03	3.674E+04	4.905E+05	997	0\absent peak
3	29	0.000E+00	6.143E+04	5.059E+05	7.550E+05	8.396E+04	7.251E+05	997	0\absent peak
3	30	0.000E+00	6.839E+05	3.603E+05	4.326E+05	9.780E+05	4.682E+05	997	0\absent peak
3	31	0.000E+00	5.111E+05	5.390E+05	5.320E+05	4.424E+05	1.352E+05	997	0\absent peak

3	32	0.000E+00	3.643E+05	1.844E+05	4.236E+04	2.355E+05	6.503E+05	997	0\absent peak
3	33	0.000E+00	8.962E+05	8.271E+05	4.382E+05	4.270E+05	3.835E+05	997	0\absent peak
3	34	0.000E+00	4.773E+05	2.331E+05	2.590E+05	2.692E+05	7.667E+05	997	0\absent peak
4	4	2.344E+09	0.213E+10	0.213E+10	0.205E+10	0.196E+10	0.186E+10	0	0\diagonal peak
4	5	0.000E+00	5.233E+05	7.045E+05	7.633E+05	2.379E+05	4.889E+05	997	0\absent peak
4	6	0.000E+00	5.048E+05	7.052E+05	9.878E+05	1.708E+05	6.160E+05	997	0\absent peak
4	7	0.000E+00	3.521E+05	3.789E+04	8.838E+05	3.938E+03	3.648E+05	997	0\absent peak
4	8	0.000E+00	1.399E+05	2.822E+05	9.003E+05	4.760E+05	3.176E+05	997	0\absent peak
4	9	0.000E+00	4.863E+05	7.334E+05	7.503E+05	1.633E+05	1.624E+03	997	0\absent peak
4	10	0.000E+00	5.662E+05	2.510E+05	2.767E+05	1.600E+05	1.360E+05	997	0\absent peak
4	11	0.000E+00	5.673E+05	2.122E+04	6.667E+04	5.015E+05	8.357E+05	997	0\absent peak
4	12	0.000E+00	6.871E+05	2.327E+05	5.497E+05	1.548E+05	8.768E+05	997	0\absent peak
4	13	0.000E+00	0.228E+06	0.476E+05	0.801E+06	0.565E+06	0.119E+07	997	0\noisy peak
4	14	0.000E+00	3.800E+05	5.946E+05	5.964E+05	7.903E+05	1.956E+05	997	0\absent peak
4	15	0.000E+00	9.676E+05	7.603E+05	7.945E+05	5.640E+05	5.675E+04	997	0\absent peak
4	16	0.000E+00	5.895E+05	6.475E+05	5.353E+05	8.236E+05	6.444E+05	997	0\absent peak
4	17	0.000E+00	1.382E+05	4.302E+05	8.323E+05	7.232E+05	6.230E+05	997	0\absent peak
4	18	0.000E+00	3.179E+05	9.237E+05	7.308E+04	5.363E+05	7.415E+05	997	0\absent peak
4	19	0.000E+00	7.179E+05	5.748E+05	8.986E+05	3.596E+05	7.639E+05	997	0\absent peak
4	20	0.000E+00	1.396E+05	6.516E+05	2.852E+05	3.580E+05	8.724E+05	997	0\absent peak
4	21	0.000E+00	7.034E+05	3.812E+05	7.557E+05	5.934E+05	5.951E+05	997	0\absent peak
4	22	0.000E+00	5.833E+05	7.552E+05	6.961E+05	3.566E+05	3.331E+05	997	0\absent peak
4	23	0.000E+00	5.350E+04	5.680E+04	1.280E+04	1.010E+05	4.200E+05	997	0\noisy peak
4	24	0.000E+00	2.958E+05	6.542E+05	7.796E+05	6.685E+05	5.702E+05	997	0\absent peak
4	25	0.000E+00	3.203E+05	1.338E+05	1.730E+04	6.986E+05	5.869E+05	997	0\absent peak
4	26	0.000E+00	4.715E+05	8.116E+05	6.154E+05	9.956E+05	6.604E+05	997	0\absent peak
4	27	0.000E+00	2.860E+05	5.277E+05	3.965E+05	1.068E+05	4.765E+05	997	0\absent peak
4	28	0.000E+00	1.780E+05	4.010E+04	8.810E+05	3.110E+05	1.510E+05	997	0\noisy peak
4	29	0.000E+00	4.098E+04	6.453E+05	4.699E+05	2.405E+05	4.306E+05	997	0\absent peak
4	30	0.000E+00	7.196E+05	6.938E+05	3.611E+05	2.686E+05	5.660E+05	997	0\absent peak
4	31	0.000E+00	4.844E+05	8.095E+05	5.257E+05	4.573E+05	3.747E+05	997	0\absent peak
4	32	0.000E+00	6.982E+05	9.391E+05	2.261E+05	6.813E+05	4.570E+05	997	0\absent peak
4	33	0.000E+00	1.697E+05	9.050E+05	2.544E+05	8.429E+05	3.197E+05	997	0\absent peak
4	34	0.000E+00	1.040E+04	1.588E+05	9.980E+05	5.508E+05	6.491E+05	997	0\absent peak
5	5	2.759E+09	0.229E+10	0.225E+10	0.209E+10	0.191E+10	0.173E+10	0	0\diagonal peak
5	6	0.000E+00	8.873E+04	9.112E+05	9.387E+05	8.464E+05	8.215E+05	997	0\absent peak
5	7	0.000E+00	4.562E+05	3.410E+05	8.377E+05	8.463E+05	7.074E+05	997	0\absent peak
5	8	0.000E+00	1.920E+07	2.365E+07	2.530E+07	2.700E+07	2.895E+07	999	0\good peak
5	9	0.000E+00	4.610E+05	9.590E+05	6.520E+05	5.340E+05	1.120E+06	997	0\noisy peak

5	10	0.000E+00	3.840E+05	2.110E+05	6.600E+05	7.720E+05	6.450E+05	997	0\noisy peak
5	11	0.000E+00	4.377E+05	2.658E+05	1.833E+05	4.537E+05	5.216E+05	997	0\absent peak
5	12	0.000E+00	5.950E+04	9.348E+05	5.986E+05	7.008E+05	7.370E+05	997	0\absent peak
5	13	0.000E+00	2.637E+05	9.491E+05	4.714E+05	7.156E+05	4.996E+05	997	0\absent peak
5	14	0.000E+00	1.810E+05	3.539E+05	6.581E+05	4.567E+05	9.106E+05	997	0\absent peak
5	15	0.000E+00	2.055E+07	2.825E+07	3.295E+07	3.450E+07	4.000E+07	999	0\good peak
5	16	0.000E+00	4.552E+05	3.345E+05	1.512E+05	8.764E+05	2.925E+05	997	0\absent peak
5	17	0.000E+00	8.811E+05	1.493E+04	3.062E+05	2.261E+05	4.756E+05	997	0\absent peak
5	18	0.000E+00	3.770E+05	4.828E+05	1.650E+05	5.292E+05	2.805E+05	997	0\absent peak
5	19	0.000E+00	2.061E+05	9.830E+05	6.883E+05	4.700E+05	9.733E+05	997	0\absent peak
5	20	0.000E+00	3.297E+04	9.886E+05	6.052E+05	6.741E+05	7.444E+05	997	0\absent peak
5	21	0.000E+00	3.565E+06	5.000E+06	5.745E+06	7.390E+06	7.315E+06	999	0\good peak
5	22	0.000E+00	8.606E+05	6.209E+05	5.645E+05	7.895E+05	6.125E+04	997	0\absent peak
5	23	0.000E+00	4.209E+05	3.754E+05	9.905E+05	8.793E+05	9.494E+05	997	0\absent peak
5	24	0.000E+00	6.626E+05	3.426E+05	5.040E+05	7.089E+05	4.383E+04	997	0\absent peak
5	25	0.000E+00	2.218E+04	5.724E+05	6.459E+04	7.814E+05	7.655E+05	997	0\absent peak
5	26	0.000E+00	9.161E+05	7.331E+05	3.323E+05	8.045E+04	6.809E+05	997	0\absent peak
5	27	0.000E+00	9.272E+05	8.318E+05	3.568E+05	9.041E+05	9.001E+05	997	0\absent peak
5	28	0.000E+00	2.118E+05	5.661E+04	2.925E+05	7.995E+05	9.954E+05	997	0\absent peak
5	29	0.000E+00	1.534E+07	2.048E+07	2.530E+07	2.785E+07	3.120E+07	999	0\good peak
5	30	0.000E+00	1.101E+07	1.515E+07	1.940E+07	2.310E+07	2.510E+07	999	0\good peak
5	31	0.000E+00	1.307E+05	3.667E+05	8.289E+05	1.672E+05	3.666E+05	997	0\absent peak
5	32	0.000E+00	4.611E+05	2.044E+05	2.462E+05	4.302E+05	3.796E+05	997	0\absent peak
5	33	0.000E+00	2.984E+05	7.285E+05	5.219E+05	8.549E+05	4.206E+05	997	0\absent peak
5	34	0.000E+00	6.376E+04	7.018E+05	3.815E+05	7.490E+05	1.668E+05	997	0\absent peak
6	6	2.681E+09	0.220E+10	0.214E+10	0.199E+10	0.181E+10	0.162E+10	0	0\diagonal peak
6	7	0.000E+00	9.190E+07	1.020E+08	9.400E+07	8.810E+07	7.940E+07	999	0\good peak
6	8	0.000E+00	8.932E+05	6.344E+05	4.816E+05	8.800E+04	1.861E+05	997	0\absent peak
6	9	0.000E+00	7.367E+05	7.090E+05	2.651E+05	6.901E+05	4.442E+05	997	0\absent peak
6	10	0.000E+00	6.142E+04	7.330E+04	8.389E+04	3.230E+05	1.859E+05	997	0\absent peak
6	11	0.000E+00	7.188E+05	3.955E+05	7.630E+05	8.109E+05	6.737E+04	997	0\absent peak
6	12	0.000E+00	7.443E+05	8.059E+05	8.969E+05	1.011E+05	6.695E+05	997	0\absent peak
6	13	0.000E+00	1.324E+05	3.501E+05	6.963E+05	4.391E+05	5.293E+05	997	0\absent peak
6	14	0.000E+00	5.598E+05	2.278E+05	3.284E+05	1.133E+05	9.882E+05	997	0\absent peak
6	15	0.000E+00	4.216E+05	2.477E+05	7.830E+05	4.202E+05	1.570E+05	997	0\absent peak
6	16	0.000E+00	5.396E+05	4.433E+04	9.896E+05	4.264E+05	9.822E+05	997	0\absent peak
6	17	0.000E+00	1.995E+07	2.820E+07	3.595E+07	3.975E+07	4.255E+07	999	0\good peak
6	18	0.000E+00	6.926E+05	8.451E+05	2.895E+05	6.731E+05	2.155E+05	0	0\unresolved peak
6	19	0.000E+00	6.032E+05	9.329E+05	3.110E+05	7.101E+05	1.923E+05	997	0\absent peak

6	20	0.000E+00	5.661E+04	2.974E+05	2.414E+05	9.918E+04	5.681E+04	997	0\absent peak
6	21	0.000E+00	5.307E+05	8.776E+05	1.841E+05	7.553E+05	2.171E+05	997	0\absent peak
6	22	0.000E+00	3.355E+06	6.385E+06	8.295E+06	1.019E+07	1.214E+07	999	0\good peak
6	23	0.000E+00	5.383E+05	2.771E+05	8.609E+05	9.885E+05	7.810E+05	997	0\absent peak
6	24	0.000E+00	8.553E+05	7.349E+05	9.804E+05	2.698E+05	6.410E+05	997	0\absent peak
6	25	0.000E+00	4.080E+06	9.090E+06	8.380E+06	9.760E+06	1.105E+07	999	0\good peak
6	26	0.000E+00	6.440E+04	8.553E+05	6.628E+05	3.554E+05	9.138E+05	997	0\absent peak
6	27	0.000E+00	4.739E+05	4.597E+05	2.632E+05	2.100E+05	1.100E+04	997	0\absent peak
6	28	0.000E+00	2.260E+06	4.215E+06	5.865E+06	5.240E+06	5.255E+06	997	0\noisy peak
6	29	0.000E+00	2.205E+05	3.657E+05	8.047E+05	1.527E+05	3.011E+05	997	0\absent peak
6	30	0.000E+00	3.218E+05	1.011E+05	9.051E+03	2.082E+05	9.328E+05	997	0\absent peak
6	31	0.000E+00	4.546E+05	1.645E+05	1.010E+05	4.933E+05	2.193E+05	997	0\absent peak
6	32	0.000E+00	6.165E+05	8.968E+05	1.766E+05	3.946E+05	9.870E+05	997	0\absent peak
6	33	0.000E+00	5.926E+05	1.847E+04	6.335E+05	7.280E+05	6.191E+05	997	0\absent peak
6	34	0.000E+00	7.454E+05	4.297E+05	5.565E+05	5.410E+04	2.562E+05	997	0\absent peak
7	7	2.238E+09	0.177E+10	0.170E+10	0.155E+10	0.139E+10	0.122E+10	0	0\diagonal peak
7	8	0.000E+00	2.550E+03	3.091E+05	2.669E+04	5.131E+05	3.230E+05	997	0\absent peak
7	9	0.000E+00	1.411E+05	9.148E+05	5.098E+05	7.232E+04	4.133E+05	997	0\absent peak
7	10	0.000E+00	1.045E+07	1.260E+07	1.620E+07	1.760E+07	2.120E+07	999	0\good peak
7	11	0.000E+00	6.829E+05	8.556E+05	4.395E+04	3.010E+05	8.900E+05	997	0\absent peak
7	12	0.000E+00	1.330E+07	1.820E+07	2.175E+07	2.350E+07	2.545E+07	999	0\good peak
7	13	0.000E+00	8.679E+05	4.741E+02	2.656E+05	4.252E+05	2.662E+05	997	0\absent peak
7	14	0.000E+00	3.982E+04	9.220E+05	4.827E+05	4.359E+05	5.908E+04	997	0\absent peak
7	15	0.000E+00	7.910E+05	2.265E+05	7.484E+05	9.097E+05	1.072E+05	997	0\absent peak
7	16	0.000E+00	1.092E+05	3.344E+05	3.401E+05	8.844E+05	3.871E+05	997	0\absent peak
7	17	0.000E+00	3.026E+04	7.095E+05	8.579E+04	1.998E+05	8.229E+05	997	0\absent peak
7	18	0.000E+00	4.590E+07	6.075E+07	7.740E+07	8.235E+07	9.365E+07	999	0\good peak
7	19	0.000E+00	5.319E+05	7.006E+05	4.055E+05	2.437E+05	5.111E+05	997	0\absent peak
7	20	0.000E+00	8.737E+05	7.201E+05	5.335E+05	4.411E+05	9.857E+05	997	0\absent peak
7	21	0.000E+00	1.685E+05	4.541E+05	9.667E+05	3.977E+05	3.077E+05	997	0\absent peak
7	22	0.000E+00	-2.600E+06	1.010E+06	6.510E+06	1.610E+06	5.310E+06	997	0\noisy peak
7	23	0.000E+00	6.683E+05	1.848E+05	7.361E+05	9.717E+05	8.970E+05	997	0\absent peak
7	24	0.000E+00	8.173E+04	6.184E+05	7.559E+05	4.780E+05	7.712E+05	997	0\absent peak
7	25	0.000E+00	6.492E+04	7.934E+05	3.765E+05	2.810E+05	2.251E+05	997	0\absent peak
7	26	0.000E+00	2.118E+05	1.812E+04	4.249E+05	2.819E+05	5.428E+05	997	0\absent peak
7	27	0.000E+00	8.492E+05	2.626E+05	7.968E+05	2.704E+04	8.501E+05	997	0\absent peak
7	28	0.000E+00	0.773E+06	0.122E+07	0.995E+06	0.181E+07	0.200E+07	997	0\noisy peak
7	29	0.000E+00	4.965E+06	6.630E+06	7.440E+06	8.660E+06	9.300E+06	999	0\good peak
7	30	0.000E+00	3.218E+05	1.011E+05	9.051E+03	2.082E+05	9.328E+05	997	0\absent peak