Synthesis of monodentate ferrocenylphosphines and their application to the palladium catalysed Suzuki reaction of aryl chlorides

Tom E. Pickett, Francesc X. Roca and Christopher J. Richards

Supplementary Material

Table of Contents

Page S2.	Table S1. Crystal data and structure refinement for 5 .
Page S3.	Table S2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 5 .
Page S4.	Table S3. Bond lengths [$\text{\AA}$] and angles [$^\circ$] for 5 .
Page S13.	Table S4. Anisotropic displacement parameters for 5 .
Page S15.	^1H NMR of 2-methyl-1-diphenylphosphinoferrocene 11 .
Page S16.	^{31}P NMR of 2-methyl-1-diphenylphosphinoferrocene 11 .
Page S17.	^1H NMR of 2-methyl-1-dicyclohexylphosphinoferrocene 12 .
Page S18.	^{31}P NMR of 2-methyl-1-dicyclohexylphosphinoferrocene 12 .
Page S19.	^1H NMR of 2-methyl-1-di-tert-butylphosphinoferrocene 13 .
Page S20.	^{31}P NMR of 2-methyl-1-di-tert-butylphosphinoferrocene 13 .

Table S1. Crystal data and structure refinement for **5**.

Identification code	XR-72	
Empirical formula	C ₃₃ H ₃₃ Fe ₃ P	
Formula weight	628.11	
Temperature	160(2) K	
Wavelength	0.71073 Å	
Crystal system	Trigonal	
Space group	R3	
Unit cell dimensions	a = 18.723(4) Å	$\alpha = 90^\circ$.
	b = 18.723(4) Å	$\beta = 90^\circ$.
	c = 12.991(6) Å	$\gamma = 120^\circ$.
Volume	3944(2) Å ³	
Z	6	
Density (calculated)	1.587 Mg/m ³	
Absorption coefficient	1.716 mm ⁻¹	
F(000)	1944	
Crystal size	0.40 x 0.40 x 0.20 mm ³	
Theta range for data collection	2.01 to 25.01°.	
Index ranges	-22 ≤ h ≤ 13, -13 ≤ k ≤ 22, -14 ≤ l ≤ 15	
Reflections collected	4953	
Independent reflections	2969 [R(int) = 0.0424]	
Completeness to theta = 25.01°	99.7 %	
Max. and min. transmission	0.7253 and 0.5469	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	2969 / 1 / 311	
Goodness-of-fit on F ²	1.031	
Final R indices [I > 2σ(I)]	R1 = 0.0231, wR2 = 0.0612	
R indices (all data)	R1 = 0.0234, wR2 = 0.0615	
Absolute structure parameter	0.015(12)	
Largest diff. peak and hole	0.304 and -0.505 e.Å ⁻³	

Table S2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) . U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	7230(1)	4340(2)	-136(2)	14(1)
C(2)	7280(2)	4532(1)	932(2)	16(1)
C(3)	7835(2)	5384(2)	1065(2)	20(1)
C(4)	8132(2)	5736(2)	75(2)	21(1)
C(5)	7756(1)	5096(1)	-676(2)	16(1)
C(6)	5674(2)	4772(2)	534(3)	28(1)
C(7)	6171(2)	5592(2)	869(2)	29(1)
C(8)	6562(2)	6092(2)	-5(2)	24(1)
C(9)	6298(2)	5580(2)	-890(2)	23(1)
C(10)	5749(2)	4763(2)	-555(2)	26(1)
C(11)	3748(2)	4309(2)	-843(2)	23(1)
C(12)	3354(2)	3843(2)	-1732(2)	25(1)
C(13)	3637(2)	4378(2)	-2594(2)	29(1)
C(14)	4219(2)	5178(2)	-2231(3)	30(1)
C(15)	4283(2)	5137(2)	-1149(2)	27(1)
C(16)	2132(2)	4578(2)	-608(2)	20(1)
C(17)	1835(2)	4260(2)	-1603(2)	21(1)
C(18)	2227(1)	4919(1)	-2328(2)	17(1)
C(19)	2764(1)	5659(1)	-1767(2)	15(1)
C(20)	2705(2)	5433(2)	-699(2)	18(1)
C(21)	2109(2)	4842(2)	-3471(2)	25(1)
C(22)	7895(2)	5220(2)	-1811(2)	24(1)
Fe(1)	6872(1)	5191(1)	130(1)	15(1)
Fe(2)	3092(1)	4776(1)	-1555(1)	16(1)
P(3)	6667	3333	-771(1)	12(1)
P(4)	3333	6667	-2377(1)	13(1)

Table S3. Bond lengths [Å] and angles [°].

C(1)-C(2)	1.425(3)
C(1)-C(5)	1.440(3)
C(1)-P(3)	1.831(2)
C(1)-Fe(1)	2.044(2)
C(2)-C(3)	1.413(3)
C(2)-Fe(1)	2.034(2)
C(2)-H(2)	0.90(3)
C(3)-C(4)	1.425(4)
C(3)-Fe(1)	2.051(2)
C(3)-H(3)	0.89(4)
C(4)-C(5)	1.429(4)
C(4)-Fe(1)	2.050(3)
C(4)-H(4)	0.96(3)
C(5)-C(22)	1.495(4)
C(5)-Fe(1)	2.040(2)
C(6)-C(7)	1.409(5)
C(6)-C(10)	1.422(5)
C(6)-Fe(1)	2.040(3)
C(6)-H(6)	1.02(4)
C(7)-C(8)	1.420(4)
C(7)-Fe(1)	2.048(3)
C(7)-H(7)	0.94(4)
C(8)-C(9)	1.419(4)
C(8)-Fe(1)	2.048(3)
C(8)-H(8)	0.91(3)
C(9)-C(10)	1.418(4)
C(9)-Fe(1)	2.055(3)
C(9)-H(9)	0.95(3)
C(10)-Fe(1)	2.042(3)
C(10)-H(10)	0.94(3)
C(11)-C(12)	1.412(4)
C(11)-C(15)	1.418(4)
C(11)-Fe(2)	2.049(3)
C(11)-H(11)	0.92(4)
C(12)-C(13)	1.418(4)

C(12)-Fe(2)	2.049(3)
C(12)-H(12)	0.99(3)
C(13)-C(14)	1.422(4)
C(13)-Fe(2)	2.044(3)
C(13)-H(13)	0.92(4)
C(14)-C(15)	1.416(5)
C(14)-Fe(2)	2.050(3)
C(14)-H(14)	0.90(4)
C(15)-Fe(2)	2.050(3)
C(15)-H(15)	0.91(4)
C(16)-C(17)	1.416(4)
C(16)-C(20)	1.417(4)
C(16)-Fe(2)	2.052(2)
C(16)-H(16)	0.92(4)
C(17)-C(18)	1.429(4)
C(17)-Fe(2)	2.050(3)
C(17)-H(17)	0.96(3)
C(18)-C(19)	1.438(3)
C(18)-C(21)	1.498(3)
C(18)-Fe(2)	2.034(2)
C(19)-C(20)	1.438(3)
C(19)-P(4)	1.820(2)
C(19)-Fe(2)	2.052(2)
C(20)-Fe(2)	2.041(2)
C(20)-H(20)	0.96(3)
C(21)-H(21A)	1.00(4)
C(21)-H(21B)	0.98(4)
C(21)-H(21C)	0.88(4)
C(22)-H(22A)	0.96(4)
C(22)-H(22B)	0.90(4)
C(22)-H(22C)	0.88(4)
P(3)-C(1)#1	1.831(2)
P(3)-C(1)#2	1.831(2)
P(4)-C(19)#3	1.820(2)
P(4)-C(19)#4	1.820(2)
C(2)-C(1)-C(5)	107.4(2)

C(2)-C(1)-P(3)	129.00(18)
C(5)-C(1)-P(3)	123.47(18)
C(2)-C(1)-Fe(1)	69.19(13)
C(5)-C(1)-Fe(1)	69.22(13)
P(3)-C(1)-Fe(1)	129.31(12)
C(3)-C(2)-C(1)	108.8(2)
C(3)-C(2)-Fe(1)	70.41(14)
C(1)-C(2)-Fe(1)	69.92(14)
C(3)-C(2)-H(2)	126.3(18)
C(1)-C(2)-H(2)	124.5(18)
Fe(1)-C(2)-H(2)	120.0(16)
C(2)-C(3)-C(4)	107.9(2)
C(2)-C(3)-Fe(1)	69.11(13)
C(4)-C(3)-Fe(1)	69.63(15)
C(2)-C(3)-H(3)	122(2)
C(4)-C(3)-H(3)	130(2)
Fe(1)-C(3)-H(3)	125(2)
C(3)-C(4)-C(5)	108.3(2)
C(3)-C(4)-Fe(1)	69.70(15)
C(5)-C(4)-Fe(1)	69.20(13)
C(3)-C(4)-H(4)	122.0(19)
C(5)-C(4)-H(4)	129.6(19)
Fe(1)-C(4)-H(4)	124.7(18)
C(4)-C(5)-C(1)	107.4(2)
C(4)-C(5)-C(22)	124.7(2)
C(1)-C(5)-C(22)	127.8(2)
C(4)-C(5)-Fe(1)	69.92(14)
C(1)-C(5)-Fe(1)	69.48(13)
C(22)-C(5)-Fe(1)	125.37(18)
C(7)-C(6)-C(10)	107.7(2)
C(7)-C(6)-Fe(1)	70.13(16)
C(10)-C(6)-Fe(1)	69.69(15)
C(7)-C(6)-H(6)	124(2)
C(10)-C(6)-H(6)	128(2)
Fe(1)-C(6)-H(6)	125(2)
C(6)-C(7)-C(8)	108.2(3)
C(6)-C(7)-Fe(1)	69.56(15)

C(8)-C(7)-Fe(1)	69.72(16)
C(6)-C(7)-H(7)	122(2)
C(8)-C(7)-H(7)	130(2)
Fe(1)-C(7)-H(7)	126(2)
C(9)-C(8)-C(7)	108.2(2)
C(9)-C(8)-Fe(1)	70.03(15)
C(7)-C(8)-Fe(1)	69.72(15)
C(9)-C(8)-H(8)	128(2)
C(7)-C(8)-H(8)	124(2)
Fe(1)-C(8)-H(8)	123.6(19)
C(10)-C(9)-C(8)	107.4(2)
C(10)-C(9)-Fe(1)	69.27(15)
C(8)-C(9)-Fe(1)	69.51(15)
C(10)-C(9)-H(9)	127.0(16)
C(8)-C(9)-H(9)	125.5(16)
Fe(1)-C(9)-H(9)	123.9(16)
C(9)-C(10)-C(6)	108.4(2)
C(9)-C(10)-Fe(1)	70.22(15)
C(6)-C(10)-Fe(1)	69.55(16)
C(9)-C(10)-H(10)	129.7(17)
C(6)-C(10)-H(10)	121.9(17)
Fe(1)-C(10)-H(10)	125.4(17)
C(12)-C(11)-C(15)	108.2(2)
C(12)-C(11)-Fe(2)	69.83(15)
C(15)-C(11)-Fe(2)	69.78(15)
C(12)-C(11)-H(11)	124(2)
C(15)-C(11)-H(11)	127(2)
Fe(2)-C(11)-H(11)	126(2)
C(11)-C(12)-C(13)	108.3(2)
C(11)-C(12)-Fe(2)	69.87(15)
C(13)-C(12)-Fe(2)	69.55(14)
C(11)-C(12)-H(12)	127(2)
C(13)-C(12)-H(12)	124(2)
Fe(2)-C(12)-H(12)	123.3(19)
C(12)-C(13)-C(14)	107.5(3)
C(12)-C(13)-Fe(2)	69.92(15)
C(14)-C(13)-Fe(2)	69.90(15)

C(12)-C(13)-H(13)	127(2)
C(14)-C(13)-H(13)	126(2)
Fe(2)-C(13)-H(13)	123(2)
C(15)-C(14)-C(13)	108.3(3)
C(15)-C(14)-Fe(2)	69.79(17)
C(13)-C(14)-Fe(2)	69.45(16)
C(15)-C(14)-H(14)	125(2)
C(13)-C(14)-H(14)	126(2)
Fe(2)-C(14)-H(14)	128(2)
C(14)-C(15)-C(11)	107.7(3)
C(14)-C(15)-Fe(2)	69.79(17)
C(11)-C(15)-Fe(2)	69.74(15)
C(14)-C(15)-H(15)	127(2)
C(11)-C(15)-H(15)	125(2)
Fe(2)-C(15)-H(15)	128(2)
C(17)-C(16)-C(20)	108.4(2)
C(17)-C(16)-Fe(2)	69.74(15)
C(20)-C(16)-Fe(2)	69.32(14)
C(17)-C(16)-H(16)	121(2)
C(20)-C(16)-H(16)	130(2)
Fe(2)-C(16)-H(16)	123(2)
C(16)-C(17)-C(18)	108.3(2)
C(16)-C(17)-Fe(2)	69.88(14)
C(18)-C(17)-Fe(2)	68.89(14)
C(16)-C(17)-H(17)	128(2)
C(18)-C(17)-H(17)	124(2)
Fe(2)-C(17)-H(17)	127(2)
C(17)-C(18)-C(19)	108.0(2)
C(17)-C(18)-C(21)	125.6(2)
C(19)-C(18)-C(21)	126.4(2)
C(17)-C(18)-Fe(2)	70.15(14)
C(19)-C(18)-Fe(2)	70.06(13)
C(21)-C(18)-Fe(2)	124.43(18)
C(18)-C(19)-C(20)	106.9(2)
C(18)-C(19)-P(4)	122.89(18)
C(20)-C(19)-P(4)	130.11(19)
C(18)-C(19)-Fe(2)	68.72(13)

C(20)-C(19)-Fe(2)	69.03(13)
P(4)-C(19)-Fe(2)	129.61(12)
C(16)-C(20)-C(19)	108.4(2)
C(16)-C(20)-Fe(2)	70.17(14)
C(19)-C(20)-Fe(2)	69.82(14)
C(16)-C(20)-H(20)	125.1(18)
C(19)-C(20)-H(20)	126.4(18)
Fe(2)-C(20)-H(20)	125.1(18)
C(18)-C(21)-H(21A)	116(2)
C(18)-C(21)-H(21B)	113(2)
H(21A)-C(21)-H(21B)	105(3)
C(18)-C(21)-H(21C)	104(3)
H(21A)-C(21)-H(21C)	115(3)
H(21B)-C(21)-H(21C)	104(3)
C(5)-C(22)-H(22A)	107(3)
C(5)-C(22)-H(22B)	113(2)
H(22A)-C(22)-H(22B)	103(3)
C(5)-C(22)-H(22C)	112(3)
H(22A)-C(22)-H(22C)	111(3)
H(22B)-C(22)-H(22C)	111(3)
C(2)-Fe(1)-C(6)	108.06(11)
C(2)-Fe(1)-C(5)	69.07(10)
C(6)-Fe(1)-C(5)	151.97(11)
C(2)-Fe(1)-C(10)	127.69(10)
C(6)-Fe(1)-C(10)	40.77(13)
C(5)-Fe(1)-C(10)	117.63(12)
C(2)-Fe(1)-C(1)	40.90(9)
C(6)-Fe(1)-C(1)	118.05(10)
C(5)-Fe(1)-C(1)	41.30(9)
C(10)-Fe(1)-C(1)	107.21(10)
C(2)-Fe(1)-C(7)	119.14(11)
C(6)-Fe(1)-C(7)	40.32(13)
C(5)-Fe(1)-C(7)	165.70(11)
C(10)-Fe(1)-C(7)	67.96(12)
C(1)-Fe(1)-C(7)	152.34(11)
C(2)-Fe(1)-C(8)	153.03(11)
C(6)-Fe(1)-C(8)	68.20(11)

C(5)-Fe(1)-C(8)	127.15(11)
C(10)-Fe(1)-C(8)	67.97(11)
C(1)-Fe(1)-C(8)	165.13(10)
C(7)-Fe(1)-C(8)	40.56(11)
C(2)-Fe(1)-C(4)	68.40(10)
C(6)-Fe(1)-C(4)	166.01(13)
C(5)-Fe(1)-C(4)	40.88(11)
C(10)-Fe(1)-C(4)	152.00(12)
C(1)-Fe(1)-C(4)	68.79(10)
C(7)-Fe(1)-C(4)	128.46(12)
C(8)-Fe(1)-C(4)	108.42(11)
C(2)-Fe(1)-C(3)	40.48(10)
C(6)-Fe(1)-C(3)	128.03(12)
C(5)-Fe(1)-C(3)	68.86(11)
C(10)-Fe(1)-C(3)	165.79(11)
C(1)-Fe(1)-C(3)	68.62(9)
C(7)-Fe(1)-C(3)	109.00(11)
C(8)-Fe(1)-C(3)	119.46(10)
C(4)-Fe(1)-C(3)	40.67(11)
C(2)-Fe(1)-C(9)	165.26(10)
C(6)-Fe(1)-C(9)	68.47(11)
C(5)-Fe(1)-C(9)	106.86(11)
C(10)-Fe(1)-C(9)	40.50(11)
C(1)-Fe(1)-C(9)	126.90(10)
C(7)-Fe(1)-C(9)	68.17(11)
C(8)-Fe(1)-C(9)	40.46(11)
C(4)-Fe(1)-C(9)	118.44(11)
C(3)-Fe(1)-C(9)	152.73(10)
C(18)-Fe(2)-C(20)	69.10(10)
C(18)-Fe(2)-C(13)	107.29(11)
C(20)-Fe(2)-C(13)	166.30(11)
C(18)-Fe(2)-C(12)	127.09(11)
C(20)-Fe(2)-C(12)	152.02(11)
C(13)-Fe(2)-C(12)	40.53(11)
C(18)-Fe(2)-C(11)	164.91(10)
C(20)-Fe(2)-C(11)	118.71(11)
C(13)-Fe(2)-C(11)	68.17(12)

C(12)-Fe(2)-C(11)	40.31(11)
C(18)-Fe(2)-C(14)	118.74(12)
C(20)-Fe(2)-C(14)	128.46(11)
C(13)-Fe(2)-C(14)	40.65(13)
C(12)-Fe(2)-C(14)	67.93(11)
C(11)-Fe(2)-C(14)	67.89(12)
C(18)-Fe(2)-C(15)	152.87(12)
C(20)-Fe(2)-C(15)	108.45(12)
C(13)-Fe(2)-C(15)	68.36(12)
C(12)-Fe(2)-C(15)	68.00(11)
C(11)-Fe(2)-C(15)	40.47(12)
C(14)-Fe(2)-C(15)	40.42(13)
C(18)-Fe(2)-C(17)	40.96(10)
C(20)-Fe(2)-C(17)	68.32(10)
C(13)-Fe(2)-C(17)	118.22(12)
C(12)-Fe(2)-C(17)	107.65(11)
C(11)-Fe(2)-C(17)	127.23(11)
C(14)-Fe(2)-C(17)	152.67(13)
C(15)-Fe(2)-C(17)	165.21(12)
C(18)-Fe(2)-C(19)	41.22(9)
C(20)-Fe(2)-C(19)	41.15(10)
C(13)-Fe(2)-C(19)	127.62(11)
C(12)-Fe(2)-C(19)	165.52(10)
C(11)-Fe(2)-C(19)	152.80(10)
C(14)-Fe(2)-C(19)	108.33(10)
C(15)-Fe(2)-C(19)	118.93(11)
C(17)-Fe(2)-C(19)	68.85(9)
C(18)-Fe(2)-C(16)	68.70(10)
C(20)-Fe(2)-C(16)	40.51(10)
C(13)-Fe(2)-C(16)	151.84(11)
C(12)-Fe(2)-C(16)	118.34(10)
C(11)-Fe(2)-C(16)	108.07(11)
C(14)-Fe(2)-C(16)	166.03(13)
C(15)-Fe(2)-C(16)	127.97(12)
C(17)-Fe(2)-C(16)	40.37(11)
C(19)-Fe(2)-C(16)	68.74(9)
C(1)#1-P(3)-C(1)	101.31(10)

C(1)#1-P(3)-C(1)#2	101.31(10)
C(1)-P(3)-C(1)#2	101.31(10)
C(19)#3-P(4)-C(19)	102.44(10)
C(19)#3-P(4)-C(19)#4	102.44(10)
C(19)-P(4)-C(19)#4	102.44(10)

Symmetry transformations used to generate equivalent atoms:

#1 $-x+y+1, -x+1, z$ #2 $-y+1, x-y, z$ #3 $-x+y, -x+1, z$

#4 $-y+1, x-y+1, z$

Table S4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$). The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12}]$

	U ¹¹	U ²²	U ³³	U ²³	U ¹³	U ¹²
C(1)	13(1)	12(1)	17(1)	0(1)	2(1)	7(1)
C(2)	18(1)	14(1)	16(1)	0(1)	-2(1)	9(1)
C(3)	21(1)	19(1)	21(1)	-6(1)	-4(1)	11(1)
C(4)	15(1)	13(1)	31(1)	-1(1)	1(1)	5(1)
C(5)	14(1)	12(1)	23(1)	3(1)	6(1)	6(1)
C(6)	22(1)	29(1)	40(2)	13(1)	12(1)	19(1)
C(7)	40(2)	39(2)	22(1)	5(1)	8(1)	32(1)
C(8)	31(1)	19(1)	28(1)	3(1)	0(1)	17(1)
C(9)	25(1)	24(1)	23(1)	2(1)	-1(1)	16(1)
C(10)	20(1)	21(1)	40(2)	1(1)	-6(1)	13(1)
C(11)	25(1)	26(1)	27(2)	2(1)	-4(1)	18(1)
C(12)	29(1)	21(1)	30(1)	-2(1)	-1(1)	17(1)
C(13)	40(2)	36(2)	24(1)	-2(1)	5(1)	29(1)
C(14)	26(1)	26(1)	42(2)	8(1)	16(1)	17(1)
C(15)	17(1)	26(1)	41(2)	-6(1)	-3(1)	13(1)
C(16)	20(1)	20(1)	21(1)	7(1)	6(1)	11(1)
C(17)	20(1)	14(1)	28(1)	2(1)	0(1)	8(1)
C(18)	19(1)	14(1)	18(1)	0(1)	-1(1)	9(1)
C(19)	15(1)	16(1)	16(1)	1(1)	0(1)	9(1)
C(20)	20(1)	19(1)	17(1)	-1(1)	0(1)	12(1)
C(21)	33(1)	22(1)	20(1)	-5(1)	-11(1)	13(1)
C(22)	27(1)	21(1)	24(1)	6(1)	11(1)	12(1)
Fe(1)	17(1)	13(1)	17(1)	1(1)	1(1)	9(1)
Fe(2)	18(1)	15(1)	16(1)	1(1)	0(1)	9(1)
P(3)	12(1)	12(1)	12(1)	0	0	6(1)
P(4)	14(1)	14(1)	13(1)	0	0	7(1)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$).

	x	y	z	U(eq)
H(2)	6960(17)	4174(17)	1420(20)	13(6)
H(3)	7940(20)	5620(20)	1680(30)	31(9)
H(4)	8503(19)	6320(20)	-20(20)	22(7)
H(6)	5340(20)	4290(20)	1010(30)	37(9)
H(7)	6210(20)	5740(20)	1570(30)	38(9)
H(8)	6934(19)	6640(20)	30(30)	22(8)
H(9)	6484(17)	5754(16)	-1570(20)	12(6)
H(10)	5466(17)	4272(18)	-940(20)	17(7)
H(11)	3660(20)	4100(20)	-190(30)	34(9)
H(12)	2920(20)	3250(20)	-1770(30)	28(8)
H(13)	3460(20)	4240(20)	-3270(30)	40(10)
H(14)	4510(20)	5630(20)	-2620(30)	41(10)
H(15)	4620(20)	5550(20)	-720(30)	34(9)
H(16)	1980(20)	4240(20)	-40(30)	31(9)
H(17)	1440(20)	3700(20)	-1790(30)	30(8)
H(20)	3007(18)	5794(19)	-140(20)	21(7)
H(21A)	1710(20)	5000(20)	-3750(30)	45(10)
H(21B)	2630(20)	5180(20)	-3850(30)	29(8)
H(21C)	1990(20)	4330(30)	-3600(30)	44(10)
H(22A)	8010(30)	5770(30)	-1960(30)	52(11)
H(22B)	7430(20)	4900(20)	-2180(30)	33(9)
H(22C)	8300(30)	5140(20)	-2020(30)	44(10)

^1H NMR of 2-methyl-1-diphenylphosphinoferrocene **11**.

^{31}P NMR of 2-methyl-1-diphenylphosphinoferrocene **11**.

^1H NMR of 2-methyl-1-dicyclohexylphosphinoferrocene **12**.

^{31}P NMR of 2-methyl-1-dicyclohexylphosphinoferrocene **12**.

^1H NMR of 2-methyl-1-di-tert-butylphosphinoferrocene **13**.

^{31}P NMR of 2-methyl-1-di-tert-butylphosphinoferrocene **13**.