Supplementary Material (ESI) for Chemical Communications

Reactivity Patterns of Thermally Stable Terminal, Electrophilic Phosphinidene Complexes Towards Diazoalkanes: Oxidation at the Phosphorus Centre and Formation of P-bound η^1-Phosphaimine, η^1-Phosphaalkene and η^3-Phosphaallene Complexes.

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Experimental

General comments: All procedures were carried out using standard Schlenk techniques or in an Innovative Technologies glovebox under a nitrogen atmosphere. THF was distilled from Na/benzophenone. Dichloromethane and hexane were purified using solvent purification columns containing alumina (dichloromethane) or alumina and copper catalyst (hexane). $CDCl_3$ and CD_2Cl_2 were vacuum distilled from $AlCl_3$ and then CaH_2. C_6D_6 was vacuum distilled from Na/benzophenone. NMR spectra were recorded at 400 MHz (^1H) or 161.975 ($^{31}P\{^1H\}$). $Cl_2PN^iPr_2$[1] and $Ph_2C{=}N{=}N$[2] were prepared according to the literature procedures. $M(CO)_6$ (M = Cr, Mo, W) and $[Cp^\dagger Fe(CO)_2]_2$ ($Cp^\dagger$ = Cp, Cp*) were obtained from Strem Chemicals and were used as received. All other reagents were obtained from Aldrich and were used as received.

a) **$[CpFe(CO)_2(PN^iPr_2)]AlCl_4$** (**1**). Note that although this compound may be typically prepared and used *in situ* by the addition of CH_2Cl_2 to equamolar amounts of $[CpFe(CO)_2\{P(Cl)N^iPr_2\}]$ and $AlCl_3$, spectroscopically pure material was prepared as follows: 1 mL of $CHCl_3$ was added to a mixture of 83 mg (0.622 mmol) of $AlCl_3$ and 200 mg (0.582 mmol) of $[CpFe(CO)_2\{P(Cl)N^iPr_2\}]$ and the mixture was stirred for 5 min. resulting in the formation of a viscous suspension. The mixture was filtered through Celite and the crystalline yellow solid was washed with a small amount of $CHCl_3$. CH_2Cl_2 was then added to the filter until the solid was dissolved (*ca*. 2 mL); the solution was filtered and then ether was added until a slight cloudiness appeared. Cooling to –45 ºC overnight resulted in the formation of a highly crystalline solid which was dried *in vacuo*. Yield: 67 %. ^1H NMR (δ, CD_2Cl_2, 25 ºC): 5.70 (s, 5H, C_5H_5); 4.96 (br s, 1H, $CH(CH_3)_2$); 4.65 (br s, 1H, $CH(CH_3)_2$); 1.61 (br s, 6H, $CH(CH_3)_2$); 1.50 (br s, 6H, $CH(CH_3)_2$). ^{31}P NMR (δ, CD_2Cl_2, 25 ºC): 922. IR (ν_{CO}, cm^{-1}, CH_2Cl_2): 2074 (s); 2036 (s). This compound is extremely air-sensitive and correct elemental analysis could not be obtained. Mass spectrum: Calcd. M^+ m/z = 308.1; found m/z = 308.2.

b) **$[CpFe(CO)_2\{P(Cl)N^iPr_2\}]$** (**6**). 150 mg of Na/K (74 wt% K) was added to a vigorously stirred solution of 500 mg (1.413 mmol) of $[CpFe(CO)_2]_2$ in 20 mL of THF. The mixture was stirred for 3h, filtered through Celite and was then added *via* cannula to a solution of 630 mg (3.118 mmol) of $Cl_2PN^iPr_2$ in 20 mL of THF. After warming to

room temperature and stirring for 30 min., the solvent was removed *in vacuo* and the residue was extracted with pentane until the extracts were almost colorless. The extracts were filtered through Celite and concentrated *in vacuo* until precipitation occurred. After cooling to –45 °C overnight the solvent was decanted and the crystalline solid was dried *in vacuo*. Yield: 54 %. ^{1}H NMR (δ, $CDCl_3$, 25 ºC): 4.93 (s, 5H, C_5H_5); 3.79 (br s, 2H, $CH(CH_3)_2$); 1.27 (br s, 12H, $CH(CH_3)_2$). ^{31}P NMR (δ,$CDCl_3$, 25 ºC): 321. IR (ν_{CO}, cm^{-1}, CH_2Cl_2): 2019 (s); 1970 (s). Anal. Calcd. for $C_{13}H_{19}ClNO_2PFe$: C, 45.5; H, 5.6; N, 4.1. Found: C, 45.8; H, 5.9; N, 3.9.

c) **$[CpFe(CO)_2(\eta^1\text{-}P(N^iPr_2)\text{=}N\text{-}N(\text{=}CPh)_2)]AlCl_4$** (**7**). 61 mg (0.314 mmol) of Ph_2C=N=N was added to a suspension of 149 mg (0.312 mmol) of $[CpFe(CO)_2(\eta^1\text{-}PN^iPr_2)]AlCl_4$ in *ca*. 1 mL of CH_2Cl_2 at –45 ºC. The mixture was shaken vigorously and then was allowed to stand at room temperature, resulting in the formation of an orange crystalline solid over 30 min. The solvent was decanted and the solid was dried in vacuo. Yield: 78 %. ^{1}H NMR (δ, $CDCl_3$, 25 ºC): 7.67-7.65 (m, 20H, C_6H_5); 5.71 (s, 5H, C_5H_5); 5.35 (s, 2H, CH_2Cl_2); 3.99 (sept., $^{3}J_{HH}$ = 6.5 Hz, 2H, $CH(CH_3)_2$); 1.27 (d, $^{3}J_{HH}$ = 6.5 Hz, 12H, $CH(CH_3)_2$). ^{31}P NMR (δ,$CDCl_3$, 25 ºC): 291. IR (ν_{CO}, cm^{-1}, CH_2Cl_2): 2071 (s); 2032 (s). Anal. Calcd. for $C_{26}H_{29}AlCl_4N_3O_2PFe{\cdot}CH_2Cl_2$ (note that one equivalent of co-crystallized CH_2Cl_2 was shown to be present *via* X-ray crystallography): C, 42.9; H, 4.1; N, 5.6. Found: 42.6; H, 4.3; N, 5.6.

d) **$[Cp^*Fe(CO)_2(\eta^1\text{-}P(N^iPr_2)\text{=}N\text{-}N(\text{=}CPh)_2)]AlCl_4$** (**8**). 36 mg (0.270 mmol) of $AlCl_3$ was 100 mg (0.242 mmol) of $[Cp^*Fe(CO)_2\{P(Cl)N^iPr_2\}]$ and then 0.5 mL of CH_2Cl_2 was added. The mixture was cooled to –45 °C and then a cold solution of 47 mg (0.241 mmol) of Ph_2C=N=N in 0.5 mL of CH_2Cl_2 was added. After stirring for 15 min. ether was added until the solution became slightly cloudy and then the mixture was then cooled to –45 °C overnight. The solvent was decanted from the orange solid, which was then dried *in vacuo*. Yield: 85 %. ^{1}H NMR (δ, CD_2Cl_2, 25 ºC): 7.71-7.18 (m, 20H, C_6H_5); 3.86 (sept., $^{3}J_{HH}$ = 6.6 Hz, 2H, $CH(CH_3)_2$); 2.10 (s, 15H, C_5Me_5); 1.27 (d, $^{3}J_{HH}$=6.6 Hz, 12H, $CH(CH_3)_2$). ^{31}P NMR (δ, CD_2Cl_2, 25 ºC): 309. IR (ν_{CO}, cm^{-1}, CH_2Cl_2): 2051 (s); 2008 (s). Anal. Calcd. for $C_{31}H_{39}AlCl_4N_3O_2PFe$: C, 50.2; H, 5.3; N, 5.7. Found: C, 50.6; H, 5.3; N, 5.3.

e) **[CpFe(CO)$_2$(η^1-P(N^{i}Pr$_2$)=CH(SiMe$_3$)]AlCl$_4$** (**9**). 170 μL (2.0 M in hexane, 0.340 mmol) of Me_3SiCHN_2 was added at –45 ºC to a solution of 162 mg (0.340 mmol) of [CpFe(CO)$_2$(η^1-PN^{i}Pr$_2$)]AlCl$_4$ in 1 mL of CH_2Cl_2 resulting in immediate gas evolution. The mixture was warmed to room temperature, stirred for 10 min. and then pentane was added until the solution became slightly cloudy. After cooling to –45 ºC overnight the solvent was decanted and the crystalline orange solid was dried *in vacuo*. Yield: 60 %. ^{1}H NMR (δ, $CDCl_3$, 25 ºC): 6.43 (d, $^2J_{PH}$=36.8 Hz, 1H, C*H*SiMe$_3$); 5.60 (s, 5H, C_5H_5); 3.92 (sept., $^3J_{HH}$=6.6 Hz, 2H, C*H*(CH$_3$)$_2$); 1.43 (d, $^3J_{HH}$=6.6 Hz, CH(C*H*$_3$)$_2$); 0.27 (s, 9H, Si*Me*$_3$). ^{31}P NMR (δ, $CDCl_3$, 25 ºC): 242. IR (ν_{CO}, cm^{-1}, CH_2Cl_2): 2066 (s); 2027 (s). Anal. Calcd. for $C_{17}H_{29}AlCl_4NO_2PSiFe$: C, 36.3; H, 5.2; N, 2.5. Found: C, 35.9; H, 5.5; N, 2.5.

f) **[Cp*M(CO)$_2$(η^3-P(N^{i}Pr$_2$)NN(CPh)$_2$)]AlCl$_4$**. (M = Cr (**13**); Mo (**14**), W (**15**) were prepared analogously as follows). 60 mg of $AlCl_3$ (0.500 mmol) was added to 200 mg (0.415 mmol) of [Cp*Mo(CO)$_3$(η^1-P(Cl)N^{i}Pr$_2$)] in 5 mL of CH_2Cl_2. The solution was cooled to -45 ºC and then a cold CH_2Cl_2 solution of 81 mg (0.415 mmol) Ph_2C=N=N was added. After stirring for 30 min. at room temperature the solvent was removed *in vacuo* and the solid was then triturated in pentane overnight. The pentane was decanted and the red solid was dried *in vacuo*. **13**: Yield 60 %. ^{1}H NMR (δ, $CDCl_3$, -30 ºC): 7.68-7.32 (m, 20H, C_6H_5); 4.04 (sept., $^3J_{HH}$ = 6.7 Hz, 1H, C*H*(CH$_3$)$_2$); 3.62 (sept., $^3J_{HH}$ = 6.8 Hz, 1H, C*H*(CH$_3$)$_2$); 1.73 (s, 15H, C_5Me_5); 1.51 (d, $^3J_{HH}$ = 6.7 Hz, 3H, CH(C*H*$_3$)$_2$), 1.31 (d, $^3J_{HH}$ = 6.8 Hz, 3H, CH(C*H*$_3$)$_2$), 1.28 (d, $^3J_{HH}$ = 6.7 Hz, 3H, CH(C*H*$_3$)$_2$), 1.17 (d, $^3J_{HH}$ = 6.7 Hz, 3H, CH(C*H*$_3$)$_2$). ^{31}P NMR (δ, $CDCl_3$, 25 ºC): 195. IR (ν_{CO}, cm^{-1}, CH_2Cl_2): 1978 (s); 1917 (s). This compound is extremely air-sensitive and correct elemental analysis could not be obtained. Mass spectrum: Calcd. M^+ m/z = 568.6; found m/z = 568.4. **14**: Yield 68 %. ^{1}H NMR (δ, $CDCl_3$, -30 ºC): 7.68-7.28 (m, 20H, C_6H_5); 3.72 (sept, $^3J_{HH}$=7.0 Hz, 2H, C*H*(CH$_3$)$_2$); 1.90 (s, 15H, C_5Me_5); 1.28 (d, $^3J_{HH}$=7.0 Hz, 12H, CH(C*H*$_3$)$_2$). ^{31}P NMR (δ, $CDCl_3$, 25 ºC): 152. IR (ν_{CO}, cm^{-1}, CH_2Cl_2): 1984 (s); 1919 (s). Anal. Calcd. for $C_{31}H_{39}AlCl_4N_3O_2PMo$: C, 47.7; H, 5.0; N, 5.4. Found: C, 47.3; H, 5.3; N, 5.1. **15**: Note that X-ray quality crystals were obtained from a CH_2Cl_2/pentane mixture at –45 ºC. Yield: 66 %. ^{1}H NMR (δ, $CDCl_3$, -30 ºC): 7.72-7.28 (m, 20H,

C_6H_5); 3.65 (sept, $^3J_{HH}$=6.7 Hz, 2H, C*H*(CH_3)$_2$); 2.02 (s, 15H, C_5Me_5); 1.28 (d, $^3J_{HH}$=6.7 Hz, 12H, CH(C*H*$_3$)$_2$). ^{31}P NMR (δ, $CDCl_3$, 25 ºC): 125. IR (ν_{CO}, cm^{-1}, CH_2Cl_2): 1975 (s); 1918 (s). Anal. Calcd. for $C_{31}H_{39}AlCl_4N_3O_2PW$: C, 40.2; H, 4.4; N, 4.4. Found: C, 40.1; H, 4.4; N, 4.3.

References

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2. L. I. Smith, K. L. Howard *Organic Syntheses* **1955**, 351.

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Crystallographic data for compounds **7**, **9** and **15**.

Table 1. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for $[CpFe(CO)_2(\eta^1\text{-}P(N^iPr_2)=N\text{-}N(=CPh)_2)]AlCl_4$ (**7**). U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Fe(1)	1025(1)	4845(1)	3341(1)	17(1)
Cl(1)	-578(1)	2988(1)	5029(1)	42(1)
Cl(2)	2759(1)	2574(1)	5434(1)	38(1)
Cl(3)	468(1)	1331(1)	5966(1)	42(1)
Cl(4)	1050(1)	3099(1)	6787(1)	28(1)
P(1)	-285(1)	5214(1)	2388(1)	15(1)
Al(1)	930(1)	2494(1)	5796(1)	23(1)
O(1)	-910(1)	5147(1)	4274(1)	32(1)
O(2)	2330(1)	6314(1)	3708(1)	32(1)
N(1)	97(1)	5758(1)	1758(1)	16(1)
N(2)	-1734(1)	4924(1)	2161(1)	20(1)
N(3)	-2212(1)	4488(1)	2685(1)	21(1)
C(1)	-191(1)	5038(1)	3896(1)	23(1)
C(2)	1813(1)	5752(1)	3557(1)	22(1)
C(8)	1476(1)	6022(1)	1798(1)	20(1)
C(9)	2060(2)	5739(1)	1157(1)	29(1)
C(10)	1590(2)	6887(1)	1892(1)	28(1)
C(11)	-859(1)	6033(1)	1123(1)	19(1)
C(12)	-1950(2)	6512(1)	1348(1)	26(1)
C(13)	-1380(1)	5388(1)	618(1)	25(1)
C(14)	-3169(1)	4039(1)	2424(1)	19(1)
C(15)	-3812(1)	3596(1)	2936(1)	21(1)
C(16)	-4831(1)	3091(1)	2682(1)	25(1)
C(17)	-5460(2)	2687(1)	3164(1)	31(1)
C(18)	-5083(2)	2784(1)	3890(1)	33(1)
C(19)	-4063(2)	3277(1)	4148(1)	32(1)
C(20)	-3427(1)	3678(1)	3675(1)	27(1)
C(21)	-3642(1)	3955(1)	1643(1)	21(1)

C(22)	-2999(2)	3477(1)	1231(1)	31(1)
C(23)	-3443(2)	3412(1)	498(1)	39(1)
C(24)	-4518(2)	3817(1)	183(1)	39(1)
C(25)	-5171(2)	4288(1)	589(1)	38(1)
C(26)	-4740(1)	4358(1)	1321(1)	29(1)
C(3)	1005(1)	3747(1)	2864(1)	35(1)
C(4)	915(1)	3677(1)	3600(1)	38(1)
C(5)	2050(1)	4015(1)	4003(1)	47(1)
C(6)	2842(1)	4294(1)	3515(1)	53(1)
C(7)	2196(1)	4129(1)	2811(1)	41(1)
C(3A)	971(1)	3695(1)	2953(1)	35(1)
C(4A)	1355(1)	3756(1)	3706(1)	38(1)
C(5A)	2562(1)	4158(1)	3840(1)	47(1)
C(6A)	2925(1)	4346(1)	3171(1)	53(1)
C(7A)	1942(1)	4059(1)	2622(1)	41(1)
Cl(1S)	-4503(1)	5563(1)	4319(1)	42(1)
Cl(2S)	-5149(1)	5830(1)	2777(1)	47(1)
C(1S)	-3895(2)	5782(1)	3528(1)	37(1)

Table 2. Bond lengths [Å] and angles [°] for $[CpFe(CO)_2(\eta^1\text{-}P(N^iPr_2)\text{=}N\text{-}N(\text{=}CPh)_2)]AlCl_4$ (**7**).

Fe(1)-C(2)	1.7970(14)
Fe(1)-C(1)	1.8002(15)
Fe(1)-C(4A)	2.0325
Fe(1)-C(5)	2.0876
Fe(1)-C(6)	2.0908
Fe(1)-C(5A)	2.0909
Fe(1)-C(4)	2.1043
Fe(1)-C(7)	2.1094
Fe(1)-C(3)	2.1177
Fe(1)-C(3A)	2.1353
Fe(1)-P(1)	2.1691(4)
Fe(1)-C(6A)	2.2246
Cl(1)-Al(1)	2.1324(6)
Cl(2)-Al(1)	2.1236(6)
Cl(3)-Al(1)	2.1217(6)
Cl(4)-Al(1)	2.1400(5)
P(1)-N(2)	1.5748(11)
P(1)-N(1)	1.6237(11)
O(1)-C(1)	1.1316(18)
O(2)-C(2)	1.1312(18)
N(1)-C(8)	1.4911(16)
N(1)-C(11)	1.5053(16)
N(2)-N(3)	1.4033(15)
N(3)-C(14)	1.2955(17)
C(8)-C(10)	1.5225(19)
C(8)-C(9)	1.526(2)
C(11)-C(13)	1.5170(19)
C(11)-C(12)	1.5225(19)
C(14)-C(15)	1.4814(18)
C(14)-C(21)	1.4871(19)
C(15)-C(20)	1.397(2)
C(15)-C(16)	1.3980(19)
C(16)-C(17)	1.397(2)
C(17)-C(18)	1.377(3)

C(18)-C(19)	1.388(2)
C(19)-C(20)	1.387(2)
C(21)-C(22)	1.387(2)
C(21)-C(26)	1.3888(15)
C(22)-C(23)	1.392(2)
C(23)-C(24)	1.369(3)
C(24)-C(25)	1.377(3)
C(25)-C(26)	1.3912(19)
C(3)-C(7)	1.4200
C(3)-C(4)	1.4200
C(4)-C(5)	1.4200
C(5)-C(6)	1.4200
C(6)-C(7)	1.4200
C(3A)-C(4A)	1.4200
C(3A)-C(7A)	1.4200
C(4A)-C(5A)	1.4200
C(5A)-C(6A)	1.4200
C(6A)-C(7A)	1.4200
Cl(1S)-C(1S)	1.7607(18)
Cl(2S)-C(1S)	1.7620(18)

C(2)-Fe(1)-C(1)	92.21(6)
C(2)-Fe(1)-C(4A)	134.59(5)
C(1)-Fe(1)-C(4A)	94.04(5)
C(2)-Fe(1)-C(5)	107.90(5)
C(1)-Fe(1)-C(5)	96.54(5)
C(4A)-Fe(1)-C(5)	26.7
C(2)-Fe(1)-C(6)	90.31(5)
C(1)-Fe(1)-C(6)	133.79(5)
C(4A)-Fe(1)-C(6)	54.5
C(5)-Fe(1)-C(6)	39.7
C(2)-Fe(1)-C(5A)	96.82(5)
C(1)-Fe(1)-C(5A)	113.37(5)
C(4A)-Fe(1)-C(5A)	40.3
C(5)-Fe(1)-C(5A)	19.3
C(6)-Fe(1)-C(5A)	21.0

C(2)-Fe(1)-C(4)	147.16(5)
C(1)-Fe(1)-C(4)	88.52(5)
C(4A)-Fe(1)-C(4)	13.3
C(5)-Fe(1)-C(4)	39.6
C(6)-Fe(1)-C(4)	66.4
C(5A)-Fe(1)-C(4)	53.5
C(2)-Fe(1)-C(7)	110.76(5)
C(1)-Fe(1)-C(7)	154.40(5)
C(4A)-Fe(1)-C(7)	62.0
C(5)-Fe(1)-C(7)	66.4
C(6)-Fe(1)-C(7)	39.5
C(5A)-Fe(1)-C(7)	54.6
C(4)-Fe(1)-C(7)	66.1
C(2)-Fe(1)-C(3)	149.98(5)
C(1)-Fe(1)-C(3)	117.40(5)
C(4A)-Fe(1)-C(3)	44.6
C(5)-Fe(1)-C(3)	66.2
C(6)-Fe(1)-C(3)	66.2
C(5A)-Fe(1)-C(3)	68.1
C(4)-Fe(1)-C(3)	39.3
C(7)-Fe(1)-C(3)	39.3
C(2)-Fe(1)-C(3A)	153.02(5)
C(1)-Fe(1)-C(3A)	113.31(5)
C(4A)-Fe(1)-C(3A)	39.7
C(5)-Fe(1)-C(3A)	62.4
C(6)-Fe(1)-C(3A)	66.0
C(5A)-Fe(1)-C(3A)	65.9
C(4)-Fe(1)-C(3A)	34.0
C(7)-Fe(1)-C(3A)	42.5
C(3)-Fe(1)-C(3A)	5.4
C(2)-Fe(1)-P(1)	97.23(5)
C(1)-Fe(1)-P(1)	91.70(4)
C(4A)-Fe(1)-P(1)	127.42(3)
C(5)-Fe(1)-P(1)	153.14(3)
C(6)-Fe(1)-P(1)	133.66(3)
C(5A)-Fe(1)-P(1)	150.64(3)

C(4)-Fe(1)-P(1)	115.57(2)
C(7)-Fe(1)-P(1)	96.27(2)
C(3)-Fe(1)-P(1)	87.28(2)
C(3A)-Fe(1)-P(1)	90.88(2)
C(2)-Fe(1)-C(6A)	89.89(5)
C(1)-Fe(1)-C(6A)	151.50(5)
C(4A)-Fe(1)-C(6A)	65.1
C(5)-Fe(1)-C(6A)	56.0
C(6)-Fe(1)-C(6A)	17.7
C(5A)-Fe(1)-C(6A)	38.3
C(4)-Fe(1)-C(6A)	74.8
C(7)-Fe(1)-C(6A)	26.6
C(3)-Fe(1)-C(6A)	61.9
C(3A)-Fe(1)-C(6A)	63.6
P(1)-Fe(1)-C(6A)	116.22(2)
N(2)-P(1)-N(1)	108.96(6)
N(2)-P(1)-Fe(1)	124.59(4)
N(1)-P(1)-Fe(1)	126.19(4)
Cl(3)-Al(1)-Cl(2)	110.34(3)
Cl(3)-Al(1)-Cl(1)	109.37(3)
Cl(2)-Al(1)-Cl(1)	110.18(3)
Cl(3)-Al(1)-Cl(4)	108.68(2)
Cl(2)-Al(1)-Cl(4)	109.04(2)
Cl(1)-Al(1)-Cl(4)	109.19(3)
C(8)-N(1)-C(11)	116.14(10)
C(8)-N(1)-P(1)	119.41(8)
C(11)-N(1)-P(1)	124.45(8)
N(3)-N(2)-P(1)	114.45(9)
C(14)-N(3)-N(2)	113.36(11)
O(1)-C(1)-Fe(1)	176.54(13)
O(2)-C(2)-Fe(1)	178.10(14)
N(1)-C(8)-C(10)	111.53(11)
N(1)-C(8)-C(9)	111.22(11)
C(10)-C(8)-C(9)	112.36(12)
N(1)-C(11)-C(13)	112.75(11)
N(1)-C(11)-C(12)	111.79(11)

C(13)-C(11)-C(12)	112.43(12)
N(3)-C(14)-C(15)	117.68(12)
N(3)-C(14)-C(21)	122.93(12)
C(15)-C(14)-C(21)	119.39(11)
C(20)-C(15)-C(16)	118.90(13)
C(20)-C(15)-C(14)	121.20(12)
C(16)-C(15)-C(14)	119.90(13)
C(17)-C(16)-C(15)	120.00(15)
C(18)-C(17)-C(16)	120.38(15)
C(17)-C(18)-C(19)	120.08(14)
C(20)-C(19)-C(18)	120.00(16)
C(19)-C(20)-C(15)	120.62(14)
C(22)-C(21)-C(26)	119.42(13)
C(22)-C(21)-C(14)	120.64(13)
C(26)-C(21)-C(14)	119.93(11)
C(21)-C(22)-C(23)	120.01(16)
C(24)-C(23)-C(22)	120.24(16)
C(23)-C(24)-C(25)	120.25(16)
C(24)-C(25)-C(26)	120.15(15)
C(21)-C(26)-C(25)	119.92(11)
C(7)-C(3)-C(4)	108.0
C(7)-C(3)-Fe(1)	70.1
C(4)-C(3)-Fe(1)	69.8
C(5)-C(4)-C(3)	108.0
C(5)-C(4)-Fe(1)	69.6
C(3)-C(4)-Fe(1)	70.9
C(4)-C(5)-C(6)	108.0
C(4)-C(5)-Fe(1)	70.8
C(6)-C(5)-Fe(1)	70.3
C(5)-C(6)-C(7)	108.0
C(5)-C(6)-Fe(1)	70.0
C(7)-C(6)-Fe(1)	70.9
C(6)-C(7)-C(3)	108.0
C(6)-C(7)-Fe(1)	69.5
C(3)-C(7)-Fe(1)	70.7
C(4A)-C(3A)-C(7A)	108.0

C(4A)-C(3A)-Fe(1)	66.2
C(7A)-C(3A)-Fe(1)	75.6
C(3A)-C(4A)-C(5A)	108.0
C(3A)-C(4A)-Fe(1)	74.0
C(5A)-C(4A)-Fe(1)	72.1
C(6A)-C(5A)-C(4A)	108.0
C(6A)-C(5A)-Fe(1)	76.0
C(4A)-C(5A)-Fe(1)	67.7
C(5A)-C(6A)-C(7A)	108.0
C(5A)-C(6A)-Fe(1)	65.8
C(7A)-C(6A)-Fe(1)	72.5
C(6A)-C(7A)-C(3A)	108.0
C(6A)-C(7A)-Fe(1)	70.5
C(3A)-C(7A)-Fe(1)	66.8
Cl(1S)-C(1S)-Cl(2S)	112.21(9)

Symmetry transformations used to generate equivalent atoms:

Table 3. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for $[CpFe(CO)_2(\eta^1\text{-}P(N^iPr_2)\text{=}N\text{-}N(\text{=}CPh)_2)]\text{-}AlCl_4$ (**7**). The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Fe(1)	16(1)	19(1)	16(1)	3(1)	0(1)	-1(1)
Cl(1)	40(1)	60(1)	25(1)	7(1)	0(1)	5(1)
Cl(2)	36(1)	43(1)	41(1)	-13(1)	20(1)	-6(1)
Cl(3)	63(1)	24(1)	41(1)	-5(1)	19(1)	-11(1)
Cl(4)	35(1)	29(1)	21(1)	-7(1)	8(1)	1(1)
P(1)	14(1)	17(1)	15(1)	2(1)	2(1)	-2(1)
Al(1)	28(1)	23(1)	18(1)	-3(1)	7(1)	-3(1)
O(1)	27(1)	47(1)	22(1)	0(1)	7(1)	-3(1)
O(2)	27(1)	30(1)	40(1)	-10(1)	5(1)	-6(1)
N(1)	14(1)	18(1)	16(1)	3(1)	2(1)	-1(1)
N(2)	17(1)	24(1)	18(1)	4(1)	2(1)	-5(1)
N(3)	18(1)	24(1)	19(1)	5(1)	3(1)	-3(1)
C(1)	21(1)	29(1)	18(1)	4(1)	-1(1)	-3(1)
C(2)	18(1)	28(1)	21(1)	-1(1)	2(1)	1(1)
C(8)	16(1)	22(1)	21(1)	3(1)	4(1)	-3(1)
C(9)	23(1)	37(1)	29(1)	2(1)	11(1)	1(1)
C(10)	28(1)	23(1)	33(1)	2(1)	4(1)	-9(1)
C(11)	19(1)	22(1)	16(1)	4(1)	2(1)	2(1)
C(12)	27(1)	27(1)	24(1)	4(1)	3(1)	10(1)
C(13)	27(1)	29(1)	17(1)	-1(1)	1(1)	0(1)
C(14)	15(1)	20(1)	22(1)	3(1)	4(1)	0(1)
C(15)	17(1)	20(1)	28(1)	5(1)	7(1)	1(1)
C(16)	20(1)	23(1)	34(1)	3(1)	8(1)	-2(1)
C(17)	24(1)	24(1)	49(1)	6(1)	14(1)	-4(1)
C(18)	28(1)	28(1)	45(1)	15(1)	16(1)	2(1)
C(19)	31(1)	35(1)	30(1)	12(1)	10(1)	1(1)
C(20)	23(1)	29(1)	28(1)	7(1)	6(1)	-2(1)
C(21)	18(1)	21(1)	23(1)	0(1)	3(1)	-5(1)
C(22)	29(1)	30(1)	33(1)	-4(1)	8(1)	1(1)
C(23)	48(1)	39(1)	34(1)	-13(1)	15(1)	-9(1)

C(24)	46(1)	44(1)	24(1)	-6(1)	1(1)	-19(1)
C(25)	33(1)	46(1)	30(1)	3(1)	-7(1)	-4(1)
C(26)	25(1)	34(1)	27(1)	-1(1)	-1(1)	2(1)
C(3)	41(1)	24(1)	36(1)	-6(1)	-3(1)	8(1)
C(4)	49(1)	19(1)	52(1)	7(1)	22(1)	-2(1)
C(5)	77(2)	28(1)	28(1)	5(1)	-15(1)	19(1)
C(6)	22(1)	25(1)	103(2)	1(1)	-11(1)	7(1)
C(7)	48(1)	30(1)	51(1)	15(1)	27(1)	21(1)
C(3A)	41(1)	24(1)	36(1)	-6(1)	-3(1)	8(1)
C(4A)	49(1)	19(1)	52(1)	7(1)	22(1)	-2(1)
C(5A)	77(2)	28(1)	28(1)	5(1)	-15(1)	19(1)
C(6A)	22(1)	25(1)	103(2)	1(1)	-11(1)	7(1)
C(7A)	48(1)	30(1)	51(1)	15(1)	27(1)	21(1)
Cl(1S)	41(1)	54(1)	32(1)	-2(1)	6(1)	-11(1)
Cl(2S)	35(1)	71(1)	35(1)	5(1)	2(1)	9(1)
C(1S)	28(1)	50(1)	34(1)	-8(1)	6(1)	-10(1)

Table 4. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^{-3}) for $[CpFe(CO)_2(\eta^1\text{-}P(N^iPr_2)\text{=}N\text{-}N(\text{=}CPh)_2)]AlCl_4$ (**7**).

	x	y	z	U(eq)
H(8)	1997	5784	2235	23
H(9C)	1602	5983	720	34
H(9B)	1960	5182	1116	34
H(9A)	2991	5872	1223	34
H(10C)	1227	7040	2317	34
H(10B)	1102	7141	1468	34
H(10A)	2513	7037	1951	34
H(11)	-361	6382	847	23
H(12C)	-2485	6189	1609	31
H(12B)	-2499	6725	922	31
H(12A)	-1567	6931	1658	31
H(13C)	-1917	5043	857	29
H(13B)	-645	5101	482	29
H(13A)	-1914	5603	188	29
H(16)	-5095	3022	2182	30
H(17)	-6151	2344	2990	37
H(18)	-5522	2513	4215	39
H(19)	-3799	3340	4650	38
H(20)	-2724	4012	3854	32
H(22)	-2254	3195	1448	37
H(23)	-3000	3085	217	47
H(24)	-4813	3773	-317	46
H(25)	-5918	4567	367	45
H(26)	-5196	4680	1601	35
H(3)	379	3570	2474	42
H(4)	217	3445	3791	46
H(5)	2245	4049	4510	56
H(6)	3660	4547	3638	63
H(7)	2507	4251	2380	49
H(3A)	200	3453	2713	42

H(4A)	886	3561	4058	46
H(5A)	3043	4280	4298	56
H(6A)	3691	4615	3102	63
H(7A)	1934	4104	2122	49
H(1S2)	-3254	5386	3445	44
H(1S1)	-3433	6281	3587	44

Table 5. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for $[CpFe(CO)_2(\eta^1\text{-}P(N^iPr_2)=CH(SiMe_3)]AlCl_4$ (**9**). U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Al(1)	7690(2)	5518(3)	12541(2)	27(1)
Cl(1)	7840(2)	7282(1)	11791(2)	50(1)
Cl(2)	6264(2)	5438(3)	13798(2)	84(1)
Cl(3)	9396(2)	5084(3)	13489(3)	47(1)
Cl(4)	7411(2)	4246(2)	11132(2)	64(1)
Al(1A)	7792(13)	5524(15)	12688(14)	27(1)
Cl(1A)	7801(14)	7064(10)	11557(11)	50(1)
Cl(2A)	6418(15)	5810(20)	13930(16)	84(1)
Cl(3A)	9679(6)	5324(8)	13093(7)	47(1)
Cl(4A)	7158(10)	4084(9)	11611(9)	64(1)
Al(1B)	7996(13)	5578(15)	12528(14)	27(1)
Cl(1B)	7472(14)	4856(11)	10932(11)	50(1)
Cl(2B)	7512(14)	4416(18)	13975(13)	84(1)
Cl(3B)	9897(8)	5623(10)	12288(9)	47(1)
Cl(4B)	7057(13)	7242(13)	12895(14)	64(1)
Al(1C)	7872(14)	5425(13)	12615(14)	27(1)
Cl(1C)	7329(7)	7314(6)	12414(7)	50(1)
Cl(2C)	6766(8)	4548(12)	13941(8)	84(1)
Cl(3C)	9594(13)	5040(19)	13487(18)	47(1)
Cl(4C)	7206(14)	4536(13)	11025(13)	64(1)
Fe(1)	211(1)	5356(1)	7676(1)	29(1)
P(1)	2266(1)	5546(1)	7680(1)	25(1)
Si(1)	3026(1)	5829(1)	10498(1)	39(1)
O(1)	324(3)	3954(4)	9867(3)	69(1)
O(2)	28(3)	3242(2)	6124(3)	49(1)
N(1)	3013(2)	5520(2)	6416(2)	29(1)
C(1)	3174(3)	5682(3)	8854(2)	36(1)
C(2)	1532(4)	6568(5)	10949(3)	70(1)
C(3)	3284(5)	4324(4)	11200(4)	62(1)
C(4)	4308(5)	6850(5)	10973(4)	69(1)

C(5)	4398(2)	5550(4)	6312(3)	41(1)
C(6)	5035(4)	4416(4)	6843(4)	51(1)
C(7)	4981(5)	6736(4)	6690(9)	53(1)
C(8)	2321(3)	5412(4)	5266(2)	39(1)
C(9)	2574(4)	6523(5)	4480(4)	64(1)
C(10)	2602(4)	4204(5)	4648(4)	59(1)
C(11)	313(3)	4479(4)	9006(3)	45(1)
C(12)	171(3)	4073(3)	6729(3)	36(1)
C(13)	-40(3)	7224(3)	7960(3)	42(1)
C(14)	-209(5)	6941(4)	6727(3)	58(1)
C(15)	-1210(5)	6117(5)	6614(4)	69(1)
C(16)	-1661(4)	5871(5)	7762(4)	63(1)
C(17)	-944(3)	6574(4)	8576(3)	47(1)
Fe(1A)	-199(3)	5296(4)	7528(3)	29(1)
P(1A)	1799(4)	5647(4)	7899(4)	25(1)
Si(1A)	3654(6)	5940(6)	10288(5)	39(1)
O(1A)	-260(20)	3620(20)	9571(18)	69(1)
O(2A)	360(20)	3408(17)	5770(17)	49(1)
N(1A)	2809(11)	5714(15)	6854(10)	29(1)
C(1A)	2354(14)	5823(19)	9209(11)	36(1)
C(2A)	3070(30)	7150(30)	11382(19)	70(1)
C(3A)	3790(30)	4423(19)	10980(30)	62(1)
C(4A)	5164(17)	6440(30)	9780(20)	69(1)
C(5A)	4160(12)	5762(19)	7114(16)	41(1)
C(6A)	4860(30)	4630(30)	6640(30)	51(1)
C(7A)	4820(40)	6900(30)	6710(70)	53(1)
C(8A)	2410(20)	5754(19)	5579(13)	39(1)
C(9A)	2500(30)	6990(20)	4960(20)	64(1)
C(10A)	2800(30)	4770(30)	4740(20)	59(1)
C(11A)	-190(20)	4371(18)	8853(16)	45(1)
C(12A)	-30(20)	4015(19)	6570(20)	36(1)
C(13A)	-474(18)	7165(13)	7591(17)	42(1)
C(14A)	-690(20)	6726(18)	6396(16)	58(1)
C(15A)	-1692(19)	5910(20)	6466(17)	69(1)
C(16A)	-2065(14)	5790(20)	7650(20)	63(1)
C(17A)	-1339(17)	6581(18)	8322(17)	47(1)

Supplementary Material (ESI) for Chemical Communications

Table 6. Bond lengths [Å] and angles [°] for $[CpFe(CO)_2(\eta^1\text{-}P(N^iPr_2)=CH(SiMe_3)]AlCl_4$ (**9**).

Al(1)-Cl(2)	2.099(3)
Al(1)-Cl(1)	2.124(3)
Al(1)-Cl(4)	2.131(3)
Al(1)-Cl(3)	2.156(3)
Al(1A)-Cl(2A)	2.068(16)
Al(1A)-Cl(3A)	2.079(14)
Al(1A)-Cl(4A)	2.102(15)
Al(1A)-Cl(1A)	2.118(16)
Al(1B)-Cl(1B)	2.030(16)
Al(1B)-Cl(3B)	2.061(14)
Al(1B)-Cl(4B)	2.134(15)
Al(1B)-Cl(2B)	2.138(16)
Al(1C)-Cl(3C)	2.119(16)
Al(1C)-Cl(4C)	2.147(16)
Al(1C)-Cl(2C)	2.148(15)
Al(1C)-Cl(1C)	2.171(15)
Fe(1)-C(12)	1.769(3)
Fe(1)-C(11)	1.780(3)
Fe(1)-C(14)	2.090(4)
Fe(1)-C(16)	2.090(4)
Fe(1)-C(15)	2.095(4)
Fe(1)-C(17)	2.096(3)
Fe(1)-C(13)	2.100(3)
Fe(1)-P(1)	2.2135(8)
P(1)-C(1)	1.633(3)
P(1)-N(1)	1.641(2)
Si(1)-C(4)	1.848(4)
Si(1)-C(3)	1.853(4)
Si(1)-C(1)	1.862(3)
Si(1)-C(2)	1.873(4)
O(1)-C(11)	1.125(4)
O(2)-C(12)	1.147(4)
N(1)-C(8)	1.484(3)
N(1)-C(5)	1.492(3)

C(5)-C(7)	1.505(7)
C(5)-C(6)	1.539(5)
C(8)-C(10)	1.532(6)
C(8)-C(9)	1.535(5)
C(13)-C(17)	1.397(5)
C(13)-C(14)	1.428(5)
C(14)-C(15)	1.410(8)
C(15)-C(16)	1.410(7)
C(16)-C(17)	1.416(5)
Fe(1A)-C(12A)	1.785(13)
Fe(1A)-C(11A)	1.803(12)
Fe(1A)-C(13A)	2.080(14)
Fe(1A)-C(17A)	2.081(14)
Fe(1A)-C(16A)	2.082(15)
Fe(1A)-C(14A)	2.085(14)
Fe(1A)-C(15A)	2.091(15)
Fe(1A)-P(1A)	2.210(5)
P(1A)-C(1A)	1.589(11)
P(1A)-N(1A)	1.612(12)
Si(1A)-C(4A)	1.810(16)
Si(1A)-C(1A)	1.837(12)
Si(1A)-C(3A)	1.847(16)
Si(1A)-C(2A)	1.927(16)
O(1A)-C(11A)	1.155(15)
O(2A)-C(12A)	1.202(17)
N(1A)-C(5A)	1.475(14)
N(1A)-C(8A)	1.489(15)
C(5A)-C(7A)	1.51(2)
C(5A)-C(6A)	1.551(19)
C(8A)-C(10A)	1.502(18)
C(8A)-C(9A)	1.533(18)
C(13A)-C(17A)	1.405(17)
C(13A)-C(14A)	1.441(18)
C(14A)-C(15A)	1.407(19)
C(15A)-C(16A)	1.399(18)
C(16A)-C(17A)	1.383(18)

Cl(2)-Al(1)-Cl(1)	111.49(16)
Cl(2)-Al(1)-Cl(4)	112.11(15)
Cl(1)-Al(1)-Cl(4)	108.50(13)
Cl(2)-Al(1)-Cl(3)	106.30(15)
Cl(1)-Al(1)-Cl(3)	109.23(15)
Cl(4)-Al(1)-Cl(3)	109.15(15)
Cl(2A)-Al(1A)-Cl(3A)	124.8(9)
Cl(2A)-Al(1A)-Cl(4A)	105.9(9)
Cl(3A)-Al(1A)-Cl(4A)	110.5(8)
Cl(2A)-Al(1A)-Cl(1A)	107.1(10)
Cl(3A)-Al(1A)-Cl(1A)	101.6(8)
Cl(4A)-Al(1A)-Cl(1A)	105.3(8)
Cl(1B)-Al(1B)-Cl(3B)	98.9(8)
Cl(1B)-Al(1B)-Cl(4B)	112.4(9)
Cl(3B)-Al(1B)-Cl(4B)	118.4(9)
Cl(1B)-Al(1B)-Cl(2B)	111.6(9)
Cl(3B)-Al(1B)-Cl(2B)	111.5(8)
Cl(4B)-Al(1B)-Cl(2B)	104.2(9)
Cl(3C)-Al(1C)-Cl(4C)	124.6(10)
Cl(3C)-Al(1C)-Cl(2C)	94.4(8)
Cl(4C)-Al(1C)-Cl(2C)	101.0(8)
Cl(3C)-Al(1C)-Cl(1C)	118.0(9)
Cl(4C)-Al(1C)-Cl(1C)	105.4(7)
Cl(2C)-Al(1C)-Cl(1C)	110.6(8)
C(12)-Fe(1)-C(11)	94.09(19)
C(12)-Fe(1)-C(14)	110.95(17)
C(11)-Fe(1)-C(14)	152.94(17)
C(12)-Fe(1)-C(16)	103.31(16)
C(11)-Fe(1)-C(16)	98.90(19)
C(14)-Fe(1)-C(16)	66.3(2)
C(12)-Fe(1)-C(15)	88.11(16)
C(11)-Fe(1)-C(15)	136.8(2)
C(14)-Fe(1)-C(15)	39.4(2)
C(16)-Fe(1)-C(15)	39.4(2)
C(12)-Fe(1)-C(17)	142.38(16)

C(11)-Fe(1)-C(17)	88.39(17)
C(14)-Fe(1)-C(17)	65.63(15)
C(16)-Fe(1)-C(17)	39.53(15)
C(15)-Fe(1)-C(17)	65.67(15)
C(12)-Fe(1)-C(13)	150.70(16)
C(11)-Fe(1)-C(13)	114.24(17)
C(14)-Fe(1)-C(13)	39.85(15)
C(16)-Fe(1)-C(13)	66.51(17)
C(15)-Fe(1)-C(13)	66.44(17)
C(17)-Fe(1)-C(13)	38.89(14)
C(12)-Fe(1)-P(1)	95.23(12)
C(11)-Fe(1)-P(1)	90.10(12)
C(14)-Fe(1)-P(1)	97.38(14)
C(16)-Fe(1)-P(1)	158.66(14)
C(15)-Fe(1)-P(1)	132.73(17)
C(17)-Fe(1)-P(1)	122.32(11)
C(13)-Fe(1)-P(1)	92.15(10)
C(1)-P(1)-N(1)	113.92(13)
C(1)-P(1)-Fe(1)	126.26(11)
N(1)-P(1)-Fe(1)	119.80(8)
C(4)-Si(1)-C(3)	108.4(2)
C(4)-Si(1)-C(1)	105.24(18)
C(3)-Si(1)-C(1)	109.18(19)
C(4)-Si(1)-C(2)	107.1(3)
C(3)-Si(1)-C(2)	113.4(2)
C(1)-Si(1)-C(2)	113.13(16)
C(8)-N(1)-C(5)	114.7(2)
C(8)-N(1)-P(1)	120.62(17)
C(5)-N(1)-P(1)	124.62(17)
P(1)-C(1)-Si(1)	138.41(18)
N(1)-C(5)-C(7)	114.0(3)
N(1)-C(5)-C(6)	112.8(3)
C(7)-C(5)-C(6)	114.5(4)
N(1)-C(8)-C(10)	111.3(3)
N(1)-C(8)-C(9)	110.2(3)
C(10)-C(8)-C(9)	113.2(3)

O(1)-C(11)-Fe(1)	176.4(4)
O(2)-C(12)-Fe(1)	173.7(3)
C(17)-C(13)-C(14)	106.8(4)
C(17)-C(13)-Fe(1)	70.4(2)
C(14)-C(13)-Fe(1)	69.7(2)
C(15)-C(14)-C(13)	108.2(3)
C(15)-C(14)-Fe(1)	70.5(2)
C(13)-C(14)-Fe(1)	70.46(19)
C(16)-C(15)-C(14)	108.3(3)
C(16)-C(15)-Fe(1)	70.1(2)
C(14)-C(15)-Fe(1)	70.1(2)
C(15)-C(16)-C(17)	107.1(4)
C(15)-C(16)-Fe(1)	70.5(2)
C(17)-C(16)-Fe(1)	70.5(2)
C(13)-C(17)-C(16)	109.6(3)
C(13)-C(17)-Fe(1)	70.71(18)
C(16)-C(17)-Fe(1)	70.0(2)
C(12A)-Fe(1A)-C(11A)	93.0(11)
C(12A)-Fe(1A)-C(13A)	144.9(10)
C(11A)-Fe(1A)-C(13A)	122.0(9)
C(12A)-Fe(1A)-C(17A)	149.4(10)
C(11A)-Fe(1A)-C(17A)	91.5(9)
C(13A)-Fe(1A)-C(17A)	39.5(5)
C(12A)-Fe(1A)-C(16A)	110.6(10)
C(11A)-Fe(1A)-C(16A)	95.0(9)
C(13A)-Fe(1A)-C(16A)	66.5(7)
C(17A)-Fe(1A)-C(16A)	38.8(5)
C(12A)-Fe(1A)-C(14A)	104.8(10)
C(11A)-Fe(1A)-C(14A)	158.0(9)
C(13A)-Fe(1A)-C(14A)	40.5(6)
C(17A)-Fe(1A)-C(14A)	66.6(7)
C(16A)-Fe(1A)-C(14A)	66.9(8)
C(12A)-Fe(1A)-C(15A)	89.6(9)
C(11A)-Fe(1A)-C(15A)	130.2(9)
C(13A)-Fe(1A)-C(15A)	66.1(8)
C(17A)-Fe(1A)-C(15A)	64.9(7)

C(16A)-Fe(1A)-C(15A)	39.2(6)
C(14A)-Fe(1A)-C(15A)	39.4(6)
C(12A)-Fe(1A)-P(1A)	98.4(9)
C(11A)-Fe(1A)-P(1A)	87.1(7)
C(13A)-Fe(1A)-P(1A)	87.6(6)
C(17A)-Fe(1A)-P(1A)	112.0(6)
C(16A)-Fe(1A)-P(1A)	150.7(7)
C(14A)-Fe(1A)-P(1A)	102.6(7)
C(15A)-Fe(1A)-P(1A)	141.5(7)
C(1A)-P(1A)-N(1A)	115.0(8)
C(1A)-P(1A)-Fe(1A)	122.9(6)
N(1A)-P(1A)-Fe(1A)	122.1(5)
C(4A)-Si(1A)-C(1A)	119.2(9)
C(4A)-Si(1A)-C(3A)	110.0(13)
C(1A)-Si(1A)-C(3A)	105.5(12)
C(4A)-Si(1A)-C(2A)	106.9(12)
C(1A)-Si(1A)-C(2A)	102.5(10)
C(3A)-Si(1A)-C(2A)	112.5(12)
C(5A)-N(1A)-C(8A)	117.3(13)
C(5A)-N(1A)-P(1A)	121.8(10)
C(8A)-N(1A)-P(1A)	120.9(11)
P(1A)-C(1A)-Si(1A)	152.5(11)
N(1A)-C(5A)-C(7A)	116(2)
N(1A)-C(5A)-C(6A)	112.4(17)
C(7A)-C(5A)-C(6A)	109(2)
N(1A)-C(8A)-C(10A)	120.2(17)
N(1A)-C(8A)-C(9A)	116.4(16)
C(10A)-C(8A)-C(9A)	109.3(18)
O(1A)-C(11A)-Fe(1A)	168(2)
O(2A)-C(12A)-Fe(1A)	158(3)
C(17A)-C(13A)-C(14A)	107.0(15)
C(17A)-C(13A)-Fe(1A)	70.3(8)
C(14A)-C(13A)-Fe(1A)	70.0(8)
C(15A)-C(14A)-C(13A)	106.0(14)
C(15A)-C(14A)-Fe(1A)	70.6(8)
C(13A)-C(14A)-Fe(1A)	69.6(8)

C(16A)-C(15A)-C(14A)	109.9(15)
C(16A)-C(15A)-Fe(1A)	70.1(8)
C(14A)-C(15A)-Fe(1A)	70.1(8)
C(17A)-C(16A)-C(15A)	107.2(16)
C(17A)-C(16A)-Fe(1A)	70.6(8)
C(15A)-C(16A)-Fe(1A)	70.8(9)
C(16A)-C(17A)-C(13A)	109.8(15)
C(16A)-C(17A)-Fe(1A)	70.6(8)
C(13A)-C(17A)-Fe(1A)	70.2(8)

Symmetry transformations used to generate equivalent atoms:

Table 7. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for $[CpFe(CO)_2(\eta^1\text{-}P(N^iPr_2)=CH(SiMe_3)]AlCl_4$ (**9**). The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Al(1)	24(1)	27(1)	30(1)	-2(1)	1(1)	0(1)
Cl(1)	60(1)	32(1)	56(1)	10(1)	-17(1)	-10(1)
Cl(2)	56(1)	135(2)	63(1)	18(1)	36(1)	7(1)
Cl(3)	39(1)	46(1)	56(1)	3(1)	-13(1)	9(1)
Cl(4)	71(1)	54(1)	69(1)	-37(1)	-14(1)	13(1)
Al(1A)	24(1)	27(1)	30(1)	-2(1)	1(1)	0(1)
Cl(1A)	60(1)	32(1)	56(1)	10(1)	-17(1)	-10(1)
Cl(2A)	56(1)	135(2)	63(1)	18(1)	36(1)	7(1)
Cl(3A)	39(1)	46(1)	56(1)	3(1)	-13(1)	9(1)
Cl(4A)	71(1)	54(1)	69(1)	-37(1)	-14(1)	13(1)
Al(1B)	24(1)	27(1)	30(1)	-2(1)	1(1)	0(1)
Cl(1B)	60(1)	32(1)	56(1)	10(1)	-17(1)	-10(1)
Cl(2B)	56(1)	135(2)	63(1)	18(1)	36(1)	7(1)
Cl(3B)	39(1)	46(1)	56(1)	3(1)	-13(1)	9(1)
Cl(4B)	71(1)	54(1)	69(1)	-37(1)	-14(1)	13(1)
Al(1C)	24(1)	27(1)	30(1)	-2(1)	1(1)	0(1)
Cl(1C)	60(1)	32(1)	56(1)	10(1)	-17(1)	-10(1)
Cl(2C)	56(1)	135(2)	63(1)	18(1)	36(1)	7(1)
Cl(3C)	39(1)	46(1)	56(1)	3(1)	-13(1)	9(1)
Cl(4C)	71(1)	54(1)	69(1)	-37(1)	-14(1)	13(1)
Fe(1)	30(1)	34(1)	24(1)	1(1)	-3(1)	0(1)
P(1)	29(1)	24(1)	21(1)	-2(1)	-4(1)	0(1)
Si(1)	43(1)	52(1)	23(1)	-1(1)	-5(1)	6(1)
O(1)	70(2)	86(2)	49(2)	30(2)	-2(1)	-18(2)
O(2)	63(2)	29(1)	55(2)	-5(1)	-16(1)	-9(1)
N(1)	26(1)	38(1)	22(1)	-2(1)	-2(1)	3(1)
C(1)	35(1)	48(2)	25(1)	-3(1)	-6(1)	-3(1)
C(2)	69(2)	107(4)	32(2)	-15(2)	-4(2)	30(3)
C(3)	74(3)	66(3)	45(2)	20(2)	-5(2)	1(2)
C(4)	84(3)	70(3)	50(2)	-6(2)	-34(2)	-18(2)
C(5)	27(1)	60(2)	36(1)	4(1)	0(1)	2(1)

C(6)	40(2)	57(2)	57(2)	7(2)	-6(2)	18(2)
C(7)	41(2)	57(2)	62(2)	12(2)	0(2)	-5(2)
C(8)	33(1)	64(2)	21(1)	-6(1)	-5(1)	2(2)
C(9)	46(2)	115(4)	32(2)	31(2)	-2(2)	-4(2)
C(10)	42(2)	90(4)	46(2)	-36(2)	2(2)	6(2)
C(11)	37(2)	61(2)	39(2)	13(1)	-3(1)	-8(2)
C(12)	33(2)	31(1)	43(2)	3(1)	-14(1)	-5(1)
C(13)	44(2)	37(1)	45(2)	-3(1)	3(1)	11(1)
C(14)	83(3)	59(2)	33(2)	14(2)	12(2)	45(2)
C(15)	78(3)	75(3)	52(2)	-25(2)	-38(2)	45(3)
C(16)	35(2)	74(3)	79(3)	-27(2)	-12(2)	9(2)
C(17)	41(2)	62(2)	38(2)	-9(1)	7(1)	6(2)
Fe(1A)	30(1)	34(1)	24(1)	1(1)	-3(1)	0(1)
P(1A)	29(1)	24(1)	21(1)	-2(1)	-4(1)	0(1)
Si(1A)	43(1)	52(1)	23(1)	-1(1)	-5(1)	6(1)
O(1A)	70(2)	86(2)	49(2)	30(2)	-2(1)	-18(2)
O(2A)	63(2)	29(1)	55(2)	-5(1)	-16(1)	-9(1)
N(1A)	26(1)	38(1)	22(1)	-2(1)	-2(1)	3(1)
C(1A)	35(1)	48(2)	25(1)	-3(1)	-6(1)	-3(1)
C(2A)	69(2)	107(4)	32(2)	-15(2)	-4(2)	30(3)
C(3A)	74(3)	66(3)	45(2)	20(2)	-5(2)	1(2)
C(4A)	84(3)	70(3)	50(2)	-6(2)	-34(2)	-18(2)
C(5A)	27(1)	60(2)	36(1)	4(1)	0(1)	2(1)
C(6A)	40(2)	57(2)	57(2)	7(2)	-6(2)	18(2)
C(7A)	41(2)	57(2)	62(2)	12(2)	0(2)	-5(2)
C(8A)	33(1)	64(2)	21(1)	-6(1)	-5(1)	2(2)
C(9A)	46(2)	115(4)	32(2)	31(2)	-2(2)	-4(2)
C(10A)	42(2)	90(4)	46(2)	-36(2)	2(2)	6(2)
C(11A)	37(2)	61(2)	39(2)	13(1)	-3(1)	-8(2)
C(12A)	33(2)	31(1)	43(2)	3(1)	-14(1)	-5(1)
C(13A)	44(2)	37(1)	45(2)	-3(1)	3(1)	11(1)
C(14A)	83(3)	59(2)	33(2)	14(2)	12(2)	45(2)
C(15A)	78(3)	75(3)	52(2)	-25(2)	-38(2)	45(3)
C(16A)	35(2)	74(3)	79(3)	-27(2)	-12(2)	9(2)
C(17A)	41(2)	62(2)	38(2)	-9(1)	7(1)	6(2)

Table 8. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for [$CpFe(CO)_2(\eta^1$-$P(N^iPr_2)$=$CH(SiMe_3)$]$AlCl_4$ (**9**).

	x	y	z	U(eq)
H(1)	4026	5687	8634	43
H(2A)	862	5963	10944	83
H(2B)	1322	7220	10386	83
H(2C)	1632	6908	11751	83
H(3A)	3945	3893	10780	74
H(3B)	2512	3849	11152	74
H(3C)	3532	4434	12037	74
H(4A)	4414	6811	11841	82
H(4B)	4108	7685	10735	82
H(4C)	5082	6596	10594	82
H(5)	4549	5497	5437	49
H(6A)	4962	4426	7712	62
H(6B)	5918	4413	6633	62
H(6C)	4630	3685	6523	62
H(7A)	4529	7409	6309	64
H(7B)	5854	6753	6448	64
H(7C)	4938	6817	7557	64
H(8)	1411	5417	5449	47
H(9A)	2401	7266	4928	77
H(9B)	2034	6492	3768	77
H(9C)	3449	6520	4242	77
H(10A)	3460	4212	4362	71
H(10B)	2023	4091	3973	71
H(10C)	2502	3536	5216	71
H(13)	569	7754	8298	50
H(14)	271	7253	6092	70
H(15)	-1527	5785	5889	82
H(16)	-2322	5334	7953	75
H(17)	-1059	6599	9413	56
H(1A)	1635	5917	9684	43

H(2A1)	3723	7328	11979	83
H(2A2)	2324	6854	11781	83
H(2A3)	2863	7899	10943	83
H(3A1)	4522	4005	10671	74
H(3A2)	3038	3948	10792	74
H(3A3)	3877	4512	11847	74
H(4A1)	5556	5786	9330	82
H(4A2)	5694	6647	10473	82
H(4A3)	5060	7155	9272	82
H(5A)	4254	5736	8001	49
H(6A1)	5044	4077	7299	62
H(6A2)	5638	4890	6271	62
H(6A3)	4333	4218	6042	62
H(7A1)	5393	6701	6071	64
H(7A2)	5295	7247	7388	64
H(7A3)	4206	7495	6427	64
H(8A)	1484	5625	5623	47
H(9A1)	2359	7639	5535	77
H(9A2)	1864	7038	4318	77
H(9A3)	3328	7079	4615	77
H(10D)	3601	4994	4385	71
H(10E)	2170	4677	4104	71
H(10F)	2895	4006	5173	71
H(13A)	139	7739	7838	50
H(14A)	-249	6946	5703	70
H(15A)	-2061	5490	5807	82
H(16A)	-2699	5271	7936	75
H(17A)	-1415	6709	9155	56

Table 9. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for [Cp*W(CO)$_2$(η^3-P(N^iPr$_2$)NN(CPh)$_2$)]AlCl$_4$ (**15**). U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
W(1)	3259(1)	-3225(1)	-3315(1)	21(1)
Cl(1)	8074(1)	-2053(1)	-815(1)	43(1)
Cl(2)	7505(1)	-1047(1)	356(1)	55(1)
Cl(3)	5167(1)	-1606(1)	-794(1)	59(1)
Cl(4)	6760(1)	-3396(1)	43(1)	48(1)
P(1)	2228(1)	-1489(1)	-3336(1)	21(1)
Al(1)	6874(1)	-2036(1)	-302(1)	27(1)
O(1)	5288(2)	-2860(2)	-2226(1)	33(1)
O(2)	4802(2)	-1742(1)	-3749(1)	36(1)
N(1)	1864(2)	-3010(1)	-2951(1)	20(1)
N(2)	1499(2)	-2542(1)	-3476(1)	21(1)
N(3)	1980(2)	-993(1)	-3954(1)	22(1)
C(1)	4520(2)	-2971(2)	-2620(1)	24(1)
C(2)	4218(2)	-2272(2)	-3589(1)	26(1)
C(3)	2424(2)	-4748(2)	-3516(1)	26(1)
C(4)	2373(2)	-4327(2)	-4038(1)	26(1)
C(5)	3564(2)	-4114(2)	-4056(1)	30(1)
C(6)	4357(2)	-4425(2)	-3541(1)	32(1)
C(7)	3649(2)	-4814(2)	-3203(1)	31(1)
C(8)	1364(3)	-5125(2)	-3348(1)	37(1)
C(9)	1255(3)	-4199(2)	-4494(1)	38(1)
C(10)	3927(3)	-3772(3)	-4558(1)	47(1)
C(11)	5690(3)	-4466(3)	-3405(2)	51(1)
C(12)	4097(3)	-5337(2)	-2661(1)	46(1)
C(13)	1200(2)	-3191(2)	-2619(1)	21(1)
C(14)	1803(2)	-3709(2)	-2100(1)	23(1)
C(15)	1311(2)	-4531(2)	-1949(1)	29(1)
C(16)	1924(3)	-5031(2)	-1481(1)	39(1)
C(17)	3012(3)	-4708(2)	-1156(1)	41(1)
C(18)	3487(3)	-3875(2)	-1292(1)	36(1)

C(19)	2892(2)	-3375(2)	-1765(1)	26(1)
C(20)	-68(2)	-2926(2)	-2728(1)	22(1)
C(21)	-541(2)	-2790(2)	-2272(1)	25(1)
C(22)	-1726(2)	-2519(2)	-2350(1)	30(1)
C(23)	-2445(2)	-2397(2)	-2885(1)	31(1)
C(24)	-1996(2)	-2557(2)	-3344(1)	30(1)
C(25)	-815(2)	-2820(2)	-3268(1)	25(1)
C(26)	2036(2)	62(2)	-3966(1)	25(1)
C(27)	3260(3)	423(2)	-3659(2)	47(1)
C(28)	1046(3)	502(2)	-3755(2)	46(1)
C(29)	1596(2)	-1510(2)	-4491(1)	29(1)
C(30)	259(3)	-1442(2)	-4735(1)	46(1)
C(31)	2285(3)	-1193(2)	-4902(1)	42(1)
Cl(1A)	1111(1)	-1729(1)	-950(1)	52(1)
Cl(2A)	1577(1)	-875(1)	-1941(1)	48(1)
C(1A)	2028(3)	-997(4)	-1214(2)	63(1)

Table 10. Bond lengths [Å] and angles [°] for $[Cp^*W(CO)_2(\eta^3\text{-}P(N^iPr_2)NN(CPh)_2)]AlCl_4$ (**15**).

W(1)-C(1)	1.981(2)
W(1)-C(2)	1.981(3)
W(1)-N(1)	2.076(2)
W(1)-N(2)	2.2011(19)
W(1)-C(6)	2.281(3)
W(1)-C(7)	2.298(3)
W(1)-C(5)	2.333(2)
W(1)-C(3)	2.363(2)
W(1)-C(4)	2.397(2)
W(1)-P(1)	2.7289(9)
Cl(1)-Al(1)	2.1206(11)
Cl(2)-Al(1)	2.1309(12)
Cl(3)-Al(1)	2.1253(13)
Cl(4)-Al(1)	2.1259(12)
P(1)-N(3)	1.642(2)
P(1)-N(2)	1.704(2)
O(1)-C(1)	1.147(3)
O(2)-C(2)	1.150(3)
N(1)-C(13)	1.294(3)
N(1)-N(2)	1.424(3)
N(3)-C(29)	1.482(3)
N(3)-C(26)	1.497(3)
C(3)-C(4)	1.414(4)
C(3)-C(7)	1.434(4)
C(3)-C(8)	1.498(4)
C(4)-C(5)	1.429(3)
C(4)-C(9)	1.492(4)
C(5)-C(6)	1.435(4)
C(5)-C(10)	1.496(4)
C(6)-C(7)	1.430(4)
C(6)-C(11)	1.498(4)
C(7)-C(12)	1.503(4)
C(13)-C(20)	1.474(3)
C(13)-C(14)	1.487(3)

C(14)-C(15)	1.391(3)
C(14)-C(19)	1.400(4)
C(15)-C(16)	1.387(4)
C(16)-C(17)	1.386(5)
C(17)-C(18)	1.381(5)
C(18)-C(19)	1.390(4)
C(20)-C(21)	1.396(3)
C(20)-C(25)	1.400(3)
C(21)-C(22)	1.393(3)
C(22)-C(23)	1.382(4)
C(23)-C(24)	1.392(4)
C(24)-C(25)	1.385(3)
C(26)-C(27)	1.514(4)
C(26)-C(28)	1.517(4)
C(29)-C(30)	1.513(4)
C(29)-C(31)	1.523(4)
Cl(1A)-C(1A)	1.734(4)
Cl(2A)-C(1A)	1.751(4)

C(1)-W(1)-C(2)	79.75(10)
C(1)-W(1)-N(1)	94.41(9)
C(2)-W(1)-N(1)	128.61(9)
C(1)-W(1)-N(2)	121.11(9)
C(2)-W(1)-N(2)	102.56(9)
N(1)-W(1)-N(2)	38.76(7)
C(1)-W(1)-C(6)	90.95(10)
C(2)-W(1)-C(6)	91.23(11)
N(1)-W(1)-C(6)	140.12(9)
N(2)-W(1)-C(6)	146.65(8)
C(1)-W(1)-C(7)	89.75(10)
C(2)-W(1)-C(7)	126.71(10)
N(1)-W(1)-C(7)	104.05(9)
N(2)-W(1)-C(7)	126.63(9)
C(6)-W(1)-C(7)	36.40(10)
C(1)-W(1)-C(5)	123.67(10)
C(2)-W(1)-C(5)	83.12(10)

N(1)-W(1)-C(5)	136.16(8)
N(2)-W(1)-C(5)	114.89(9)
C(6)-W(1)-C(5)	36.21(10)
C(7)-W(1)-C(5)	60.05(10)
C(1)-W(1)-C(3)	121.21(9)
C(2)-W(1)-C(3)	141.77(10)
N(1)-W(1)-C(3)	84.36(8)
N(2)-W(1)-C(3)	93.03(8)
C(6)-W(1)-C(3)	59.56(9)
C(7)-W(1)-C(3)	35.79(9)
C(5)-W(1)-C(3)	58.69(9)
C(1)-W(1)-C(4)	147.59(9)
C(2)-W(1)-C(4)	110.81(10)
N(1)-W(1)-C(4)	101.04(8)
N(2)-W(1)-C(4)	87.44(8)
C(6)-W(1)-C(4)	59.23(9)
C(7)-W(1)-C(4)	58.99(9)
C(5)-W(1)-C(4)	35.13(8)
C(3)-W(1)-C(4)	34.54(9)
C(1)-W(1)-P(1)	94.20(7)
C(2)-W(1)-P(1)	70.32(7)
N(1)-W(1)-P(1)	59.17(6)
N(2)-W(1)-P(1)	38.61(5)
C(6)-W(1)-P(1)	159.55(8)
C(7)-W(1)-P(1)	162.97(7)
C(5)-W(1)-P(1)	128.89(7)
C(3)-W(1)-P(1)	131.63(6)
C(4)-W(1)-P(1)	118.19(6)
N(3)-P(1)-N(2)	103.20(10)
N(3)-P(1)-W(1)	111.78(8)
N(2)-P(1)-W(1)	53.70(7)
Cl(1)-Al(1)-Cl(3)	108.66(5)
Cl(1)-Al(1)-Cl(4)	110.58(5)
Cl(3)-Al(1)-Cl(4)	110.08(5)
Cl(1)-Al(1)-Cl(2)	108.67(5)
Cl(3)-Al(1)-Cl(2)	109.46(6)

Cl(4)-Al(1)-Cl(2)	109.36(5)
C(13)-N(1)-N(2)	126.28(19)
C(13)-N(1)-W(1)	155.94(17)
N(2)-N(1)-W(1)	75.39(11)
N(1)-N(2)-P(1)	102.07(14)
N(1)-N(2)-W(1)	65.85(11)
P(1)-N(2)-W(1)	87.69(8)
C(29)-N(3)-C(26)	118.56(19)
C(29)-N(3)-P(1)	124.52(16)
C(26)-N(3)-P(1)	116.63(15)
O(1)-C(1)-W(1)	176.3(2)
O(2)-C(2)-W(1)	177.7(2)
C(4)-C(3)-C(7)	108.7(2)
C(4)-C(3)-C(8)	124.5(2)
C(7)-C(3)-C(8)	126.7(3)
C(4)-C(3)-W(1)	74.03(14)
C(7)-C(3)-W(1)	69.62(13)
C(8)-C(3)-W(1)	126.03(17)
C(3)-C(4)-C(5)	108.2(2)
C(3)-C(4)-C(9)	124.4(2)
C(5)-C(4)-C(9)	127.4(3)
C(3)-C(4)-W(1)	71.43(13)
C(5)-C(4)-W(1)	70.02(13)
C(9)-C(4)-W(1)	127.24(18)
C(4)-C(5)-C(6)	107.8(2)
C(4)-C(5)-C(10)	125.6(3)
C(6)-C(5)-C(10)	125.9(3)
C(4)-C(5)-W(1)	74.85(14)
C(6)-C(5)-W(1)	69.91(14)
C(10)-C(5)-W(1)	128.0(2)
C(7)-C(6)-C(5)	108.0(2)
C(7)-C(6)-C(11)	125.0(3)
C(5)-C(6)-C(11)	126.5(3)
C(7)-C(6)-W(1)	72.44(14)
C(5)-C(6)-W(1)	73.88(14)
C(11)-C(6)-W(1)	125.85(19)

C(6)-C(7)-C(3)	107.4(2)
C(6)-C(7)-C(12)	126.7(3)
C(3)-C(7)-C(12)	125.3(3)
C(6)-C(7)-W(1)	71.16(15)
C(3)-C(7)-W(1)	74.58(14)
C(12)-C(7)-W(1)	126.92(19)
N(1)-C(13)-C(20)	124.5(2)
N(1)-C(13)-C(14)	115.2(2)
C(20)-C(13)-C(14)	120.4(2)
C(15)-C(14)-C(19)	119.5(2)
C(15)-C(14)-C(13)	120.8(2)
C(19)-C(14)-C(13)	119.6(2)
C(16)-C(15)-C(14)	119.8(3)
C(15)-C(16)-C(17)	120.5(3)
C(18)-C(17)-C(16)	120.1(3)
C(17)-C(18)-C(19)	120.0(3)
C(18)-C(19)-C(14)	120.0(3)
C(21)-C(20)-C(25)	119.0(2)
C(21)-C(20)-C(13)	118.2(2)
C(25)-C(20)-C(13)	122.8(2)
C(22)-C(21)-C(20)	120.8(2)
C(23)-C(22)-C(21)	119.5(2)
C(22)-C(23)-C(24)	120.4(2)
C(25)-C(24)-C(23)	120.3(2)
C(24)-C(25)-C(20)	120.0(2)
N(3)-C(26)-C(27)	111.5(2)
N(3)-C(26)-C(28)	111.2(2)
C(27)-C(26)-C(28)	112.5(3)
N(3)-C(29)-C(30)	111.3(2)
N(3)-C(29)-C(31)	111.8(2)
C(30)-C(29)-C(31)	112.2(2)
Cl(1A)-C(1A)-Cl(2A)	113.68(18)

Symmetry transformations used to generate equivalent atoms:

Table 11. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for $[Cp^*W(CO)_2(\eta^3\text{-}P(N^iPr_2)NN(CPh)_2)]AlCl_4$ (**15**). The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + \ldots + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
W(1)	20(1)	20(1)	21(1)	0(1)	5(1)	0(1)
Cl(1)	54(1)	34(1)	50(1)	5(1)	32(1)	3(1)
Cl(2)	91(1)	39(1)	36(1)	-10(1)	18(1)	-10(1)
Cl(3)	37(1)	58(1)	75(1)	14(1)	3(1)	9(1)
Cl(4)	73(1)	31(1)	46(1)	10(1)	24(1)	-4(1)
P(1)	23(1)	20(1)	18(1)	1(1)	5(1)	1(1)
Al(1)	34(1)	24(1)	25(1)	2(1)	10(1)	1(1)
O(1)	27(1)	39(1)	28(1)	0(1)	1(1)	-3(1)
O(2)	28(1)	36(1)	46(1)	10(1)	14(1)	-2(1)
N(1)	21(1)	20(1)	20(1)	2(1)	4(1)	0(1)
N(2)	20(1)	22(1)	19(1)	4(1)	4(1)	-1(1)
N(3)	26(1)	20(1)	18(1)	2(1)	3(1)	-1(1)
C(1)	24(1)	23(1)	26(1)	1(1)	7(1)	0(1)
C(2)	21(1)	27(1)	29(1)	3(1)	6(1)	2(1)
C(3)	30(1)	20(1)	29(1)	-6(1)	10(1)	-3(1)
C(4)	28(1)	25(1)	25(1)	-7(1)	7(1)	-3(1)
C(5)	33(1)	29(1)	32(1)	-11(1)	15(1)	-6(1)
C(6)	24(1)	27(1)	44(2)	-12(1)	8(1)	2(1)
C(7)	33(1)	21(1)	34(1)	-3(1)	3(1)	3(1)
C(8)	44(2)	28(1)	45(2)	-11(1)	23(1)	-13(1)
C(9)	37(1)	39(2)	32(1)	-8(1)	-3(1)	-2(1)
C(10)	61(2)	50(2)	43(2)	-15(1)	34(2)	-19(2)
C(11)	25(1)	45(2)	82(3)	-28(2)	11(1)	2(1)
C(12)	59(2)	25(1)	45(2)	4(1)	-4(2)	5(1)
C(13)	23(1)	18(1)	21(1)	-1(1)	7(1)	-1(1)
C(14)	27(1)	22(1)	22(1)	2(1)	10(1)	4(1)
C(15)	35(1)	25(1)	31(1)	3(1)	15(1)	0(1)
C(16)	58(2)	28(1)	40(2)	12(1)	27(1)	10(1)
C(17)	50(2)	48(2)	29(1)	15(1)	15(1)	22(1)
C(18)	35(1)	47(2)	24(1)	4(1)	6(1)	12(1)

C(19)	29(1)	29(1)	21(1)	2(1)	8(1)	4(1)
C(20)	22(1)	20(1)	24(1)	-1(1)	7(1)	-2(1)
C(21)	25(1)	27(1)	23(1)	-2(1)	7(1)	-3(1)
C(22)	27(1)	34(1)	31(1)	-6(1)	12(1)	-1(1)
C(23)	22(1)	34(1)	37(1)	-2(1)	8(1)	0(1)
C(24)	23(1)	37(1)	29(1)	1(1)	4(1)	-3(1)
C(25)	24(1)	29(1)	24(1)	0(1)	7(1)	-2(1)
C(26)	30(1)	19(1)	25(1)	3(1)	6(1)	-1(1)
C(27)	44(2)	28(1)	55(2)	9(1)	-12(1)	-11(1)
C(28)	64(2)	30(1)	55(2)	8(1)	34(2)	12(1)
C(29)	39(1)	25(1)	19(1)	1(1)	2(1)	-5(1)
C(30)	41(2)	45(2)	40(2)	5(1)	-11(1)	-11(1)
C(31)	68(2)	37(2)	24(1)	-2(1)	18(1)	-7(1)
Cl(1A)	55(1)	62(1)	31(1)	1(1)	0(1)	-9(1)
Cl(2A)	48(1)	50(1)	46(1)	-2(1)	10(1)	-15(1)
C(1A)	45(2)	105(3)	39(2)	-28(2)	12(1)	-32(2)

Table 12. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for $[Cp^*W(CO)_2(\eta^3\text{-}P(N^iPr_2)NN(CPh)_2)]AlCl_4$ (**15**).

	x	y	z	U(eq)
H(8C)	1090	-5708	-3555	55(11)
H(8B)	1585	-5257	-2947	42(9)
H(8A)	721	-4656	-3435	53(11)
H(9C)	639	-3917	-4340	68(13)
H(9B)	1411	-3782	-4781	88(16)
H(9A)	979	-4814	-4658	58(11)
H(10C)	3349	-3303	-4756	110(20)
H(10B)	4720	-3482	-4439	50(10)
H(10A)	3949	-4305	-4806	54(11)
H(11C)	5943	-5118	-3441	62(12)
H(11B)	5972	-4061	-3664	37(9)
H(11A)	6030	-4246	-3022	56(11)
H(12C)	4904	-5120	-2474	75(14)
H(12B)	3566	-5216	-2421	103(19)
H(12A)	4114	-6016	-2736	53(11)
H(15)	559	-4750	-2166	32(8)
H(16)	1595	-5599	-1382	41(9)
H(17)	3432	-5061	-840	46(10)
H(18)	4220	-3644	-1062	46(10)
H(19)	3223	-2805	-1860	34(8)
H(21)	-47	-2881	-1905	32(8)
H(22)	-2038	-2419	-2037	26(7)
H(23)	-3251	-2204	-2940	31(8)
H(24)	-2500	-2484	-3711	27(7)
H(25)	-513	-2930	-3583	17(6)
H(26)	1896	254	-4366	22(7)
H(27C)	3863	142	-3821	39(9)
H(27B)	3280	1112	-3693	35(8)
H(27A)	3428	248	-3264	73(15)
H(28C)	1165	340	-3361	50(10)

H(28B)	1065	1190	-3796	52(11)
H(28A)	272	260	-3972	110(20)
H(29)	1788	-2191	-4408	30(8)
H(30C)	22	-776	-4774	51(10)
H(30B)	38	-1746	-5102	42(10)
H(30A)	-147	-1759	-4486	63(13)
H(31C)	3143	-1241	-4726	53(11)
H(31B)	2076	-1598	-5234	69(14)
H(31A)	2081	-536	-5012	51(10)
H(1A1)	2850	-1252	-1105	76
H(1A2)	2045	-364	-1042	76