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Supplementary table 1.
Crystal data and refinement details of [Fe(CO)2PPh3(eta5-C5H4Et)+][BF4-]
9BF4, local identification I1127.

Space Group and Cell Dimensions Monoclinic, P 21/c
a 11.0297(24) b 17.5912(15) c 13.774(7)
beta 70.62(3)
Volume 2521.1(14)A**3

Empirical formula : C27 H24 B F4 Fe O2 P

Cell dimensions were obtained from 25 reflections with 2Theta angle
in the range 14.63 - 34.14 degrees.

Crystal dimensions : 0.44 X 0.22 X 0.09 mm

FW = 554.10 Z = 4 F(000) = 1135.85

Dcalc 1.460Mg.m-3, mu 0.71mm-1, lambda 0.71069A, 2Theta(max) 50.0

The intensity data were collected on a Nonius diffractometer,
using the theta/2theta scan mode.
The h,k,l ranges are :-- -12 13, 0 20, 0 16
No. of reflections measured 9167
No. of unique reflections 4432
No. of reflections with Inet > 2.5sigma(Inet) 2673
Absorption corrections were made.
The minimum and maximum transmission factors are 0.914252 and 0.999177.

The last least squares cycle was calculated with
60 atoms, 326 parameters and 2673 out of 4432 reflections.
Weights based on counting-statistics were used.
The weight modifier K in KFo**2 is 0.000100

The residuals are as follows :--
For significant reflections, RF 0.040, Rw 0.044 GoF 1.69
For all reflections, RF 0.083, Rw 0.049.
where RF = Sum(Fo-Fc)/Sum(Fo),
Rw = Sqrt[Sum(w(Fo-Fc)**2)/Sum(wFo**2)] and
GoF = Sqrt[Sum(w(Fo-Fc)**2)/(No. of reflns - No. of params.)]
The maximum shift/sigma ratio was 0.019.

In the last D-map, the deepest hole was -0.310e/A**3,
and the highest peak 0.520e/A**3.

Supplementary table 2.
Final atomic fractional coordinates for [Fe(CO)2PPh3(eta5-C5H4Et)+][BF4-]
9BF4, local identification I1127.

Atom	x	y	z	Biso
FE	0.58630(6)	0.85885(3)	0.13777(5)	2.99(3)
P	0.76470(11)	0.81511(6)	0.01880(8)	2.71(5)
C1	0.4436 (4)	0.8564 (3)	0.2851 (3)	3.66(22)
C2	0.5318 (5)	0.9150 (3)	0.2794 (3)	4.12(23)
C3	0.6560 (5)	0.8836 (3)	0.2567 (3)	4.33(25)
C4	0.6442 (5)	0.8039 (3)	0.2504 (3)	4.10(24)
C5	0.5153 (5)	0.7872 (3)	0.2666 (3)	3.85(24)
C6	0.6047 (5)	0.9495 (3)	0.0776 (4)	3.88(23)
C7	0.4823 (5)	0.8217 (3)	0.0748 (4)	3.91(24)
C8	0.3009 (5)	0.8643 (3)	0.3141 (4)	5.1 (3)
C9	0.2383 (6)	0.8571 (4)	0.4287 (5)	8.5 (4)
O1	0.6153 (4)	1.00823(19)	0.0411 (3)	5.75(22)
O2	0.4121 (3)	0.79789(22)	0.0372 (3)	5.91(22)
C11	0.9050 (4)	0.83254(22)	0.0569 (3)	2.69(18)
C12	0.9722 (4)	0.77433(24)	0.0848 (3)	3.57(22)
C13	1.0748 (5)	0.7910 (3)	0.1176 (4)	4.5 (3)
C14	1.1106 (5)	0.8651 (3)	0.1231 (4)	4.7 (3)
C15	1.0432 (5)	0.9237 (3)	0.0984 (4)	4.33(25)
C16	0.9403 (4)	0.90747(24)	0.0666 (3)	3.60(22)
C21	0.8057 (4)	0.85935(22)	-0.1091 (3)	2.90(19)
C22	0.9322 (4)	0.87218(23)	-0.1682 (3)	3.42(21)
C23	0.9605 (5)	0.9029 (3)	-0.2670 (4)	4.31(24)
C24	0.8628 (6)	0.9216 (3)	-0.3043 (4)	4.7 (3)
C25	0.7378 (5)	0.9086 (3)	-0.2459 (4)	4.4 (3)
C26	0.7078 (4)	0.87837(23)	-0.1475 (3)	3.53(21)
C31	0.7697 (4)	0.71371(22)	-0.0122 (3)	3.00(20)
C32	0.8784 (5)	0.68394(25)	-0.0854 (3)	3.92(23)
C33	0.8836 (5)	0.6070 (3)	-0.1092 (4)	4.6 (3)
C34	0.7796 (6)	0.56079(25)	-0.0623 (4)	4.5 (3)
C35	0.6704 (5)	0.5899 (3)	0.0084 (4)	4.3 (3)
C36	0.6659 (4)	0.66701(23)	0.0340 (3)	3.45(22)
B	0.3093 (7)	0.6114 (4)	0.2445 (7)	5.8 (4)
F1	0.4274 (3)	0.60740(18)	0.2523 (3)	7.85(23)
F2	0.2317 (3)	0.55466(20)	0.2899 (3)	9.5 (3)
F3	0.2588 (4)	0.67839(21)	0.2635 (5)	15.0 (5)
F4	0.3266 (7)	0.5987 (4)	0.1425 (5)	17.7 (5)
H2	0.513	0.970	0.298	4.8
H3	0.735	0.914	0.248	5.3
H4	0.724	0.772	0.232	4.9
H5	0.468	0.738	0.284	4.6
H8A	0.273	0.815	0.292	5.8
H8B	0.279	0.919	0.307	5.8
H9A	0.143	0.866	0.456	9.0
H9B	0.283	0.890	0.465	9.0
H9C	0.248	0.803	0.445	9.0
H12	0.943	0.721	0.082	4.5
H13	1.122	0.748	0.136	5.6
H14	1.190	0.874	0.141	5.8
H15	1.073	0.976	0.108	5.3

H16	0.893	0.950	0.047	4.6
H22	1.007	0.859	-0.146	4.3
H23	1.054	0.915	-0.300	5.1
H24	0.883	0.937	-0.378	5.6
H25	0.664	0.923	-0.269	5.5
H26	0.620	0.860	-0.106	4.5
H32	0.951	0.718	-0.126	4.7
H33	0.960	0.584	-0.162	5.4
H34	0.794	0.505	-0.079	5.4
H35	0.598	0.556	0.048	5.3
H36	0.583	0.685	0.085	4.3

Supplementary table 3.
Anisotropic thermal parameters of non-H atoms of [Fe(CO)2PPh3(eta5-C5H4Et)+] [BF4-], 9BF4, local identification I1127. The temperature factors are of the form -2(Pi)**2(u11*h*h*astar*astar+---+2*u12*h*k*astar*bstar+---). The uij values have been multiplied by 100.

Atom	u11(U)	u22	u33	u12	u13	u23
FE	3.87(4)	3.92(3)	3.78(3)	0.16(3)	-1.57(3)	-0.35(3)
P	3.71(6)	3.27(6)	3.60(6)	0.10(5)	-1.61(5)	0.08(5)
C1	4.4 (3)	5.9 (3)	3.27(24)	-0.2 (3)	-0.78(21)	-0.36(23)
C2	6.3 (3)	5.5 (3)	3.4 (3)	-0.4 (3)	-0.95(25)	-1.56(22)
C3	5.7 (3)	7.9 (4)	3.3 (3)	-1.6 (3)	-2.14(25)	-0.20(24)
C4	5.6 (3)	7.1 (3)	2.9 (3)	1.3 (3)	-1.41(23)	0.31(23)
C5	5.8 (3)	5.2 (3)	3.4 (3)	-0.47(24)	-1.15(24)	0.57(20)
C6	5.7 (3)	4.7 (3)	4.9 (3)	0.79(24)	-2.5 (3)	-0.94(23)
C7	4.4 (3)	5.7 (3)	4.8 (3)	0.16(24)	-1.55(25)	-0.27(24)
C8	4.6 (3)	7.5 (4)	6.6 (3)	0.2 (3)	-1.0 (3)	-0.5 (3)
C9	6.1 (4)	18.0 (7)	6.6 (4)	-0.7 (5)	0.2 (3)	-0.6 (4)
O1	10.5 (3)	4.43(20)	7.9 (3)	0.52(21)	-4.30(24)	0.71(19)
O2	5.84(25)	10.0 (3)	7.9 (3)	-1.39(21)	-3.98(22)	-0.93(21)
C11	3.38(23)	3.81(23)	3.35(23)	0.07(18)	-1.54(19)	0.10(18)
C12	4.7 (3)	4.2 (3)	4.9 (3)	0.40(21)	-1.90(24)	0.31(21)
C13	5.2 (3)	6.6 (3)	6.1 (4)	1.6 (3)	-3.1 (3)	0.2 (3)
C14	4.5 (3)	8.6 (4)	5.5 (3)	-0.6 (3)	-2.7 (3)	0.2 (3)
C15	5.9 (3)	5.5 (3)	5.5 (3)	-1.2 (3)	-2.6 (3)	-0.14(24)
C16	5.2 (3)	4.5 (3)	4.7 (3)	-0.44(22)	-2.60(25)	0.48(21)
C21	4.7 (3)	2.89(20)	3.73(23)	0.20(20)	-1.85(20)	-0.10(19)
C22	4.7 (3)	4.4 (3)	4.0 (3)	-0.43(21)	-1.63(23)	0.11(19)
C23	6.4 (3)	5.7 (3)	4.3 (3)	-1.1 (3)	-1.7 (3)	0.75(23)
C24	8.8 (4)	5.6 (3)	3.6 (3)	-0.4 (3)	-2.2 (3)	0.29(23)
C25	7.0 (4)	5.9 (3)	5.0 (3)	0.5 (3)	-3.4 (3)	0.5 (3)
C26	5.1 (3)	4.7 (3)	3.8 (3)	-0.20(21)	-1.83(23)	0.27(20)
C31	5.1 (3)	3.41(22)	3.40(24)	0.24(20)	-2.03(22)	0.11(18)
C32	5.7 (3)	4.4 (3)	4.4 (3)	0.28(24)	-1.10(24)	-0.26(22)
C33	7.9 (4)	4.9 (3)	4.6 (3)	1.7 (3)	-1.9 (3)	-0.91(23)
C34	9.6 (4)	3.6 (3)	4.2 (3)	0.4 (3)	-2.9 (3)	-0.43(22)
C35	8.1 (4)	4.4 (3)	4.4 (3)	-1.1 (3)	-3.0 (3)	0.59(22)
C36	5.3 (3)	4.09(25)	3.8 (3)	-0.30(21)	-1.63(22)	0.05(19)
B	6.7 (5)	5.2 (4)	10.7 (6)	-1.2 (4)	-3.9 (5)	1.8 (4)
F1	6.70(24)	8.54(24)	15.5 (4)	-1.02(18)	-4.92(25)	2.55(22)
F2	7.21(25)	8.8 (3)	19.6 (4)	-2.23(21)	-3.8 (3)	4.7 (3)
F3	12.2 (4)	6.1 (3)	40.7 (9)	1.6 (3)	-11.7 (5)	-3.9 (4)
F4	24.9 (8)	30.8 (8)	14.5 (5)	-11.5 (6)	-10.4 (5)	4.1 (5)

Supplementary table 4.
Bond lengths and angles of [Fe(CO)2PPh3(eta5-C5H4Et)+][BF4-], 9BF4, local identification I1127.

Atom-atom	Length, A	Atom-atom	Length, A
Fe-P	2.2380(15)	C(13)-C(14)	1.369(8)
Fe-C(1)	2.116(4)	C(13)-H(13)	1.000
Fe-C(2)	2.090(4)	C(14)-C(15)	1.378(7)
Fe-C(3)	2.074(4)	C(14)-H(14)	1.000
Fe-C(4)	2.098(4)	C(15)-C(16)	1.375(7)
Fe-C(5)	2.104(4)	C(15)-H(15)	1.000
Fe-C(6)	1.777(5)	C(16)-H(16)	1.000
Fe-C(7)	1.774(5)	C(21)-C(22)	1.381(6)
P-C(11)	1.817(4)	C(21)-C(26)	1.394(6)
P-C(21)	1.839(4)	C(22)-C(23)	1.399(6)
P-C(31)	1.831(4)	C(22)-H(22)	1.000
C(1)-C(2)	1.403(7)	C(23)-C(24)	1.379(8)
C(1)-C(5)	1.427(7)	C(23)-H(23)	1.000
C(1)-C(8)	1.496(7)	C(24)-C(25)	1.366(8)
C(2)-C(3)	1.414(7)	C(24)-H(24)	1.000
C(2)-H(2)	1.000	C(25)-C(26)	1.388(6)
C(3)-C(4)	1.411(7)	C(25)-H(25)	1.000
C(3)-H(3)	1.000	C(26)-H(26)	1.000
C(4)-C(5)	1.396(7)	C(31)-C(32)	1.388(6)
C(4)-H(4)	1.000	C(31)-C(36)	1.381(6)
C(5)-H(5)	1.000	C(32)-C(33)	1.389(6)
C(6)-O(1)	1.139(6)	C(32)-H(32)	1.000
C(7)-O(2)	1.146(6)	C(33)-C(34)	1.381(8)
C(8)-C(9)	1.505(8)	C(33)-H(33)	1.000
C(8)-H(8A)	1.000	C(34)-C(35)	1.371(8)
C(8)-H(8B)	1.000	C(34)-H(34)	1.000
C(9)-H(9A)	1.000	C(35)-C(36)	1.399(6)
C(9)-H(9B)	1.000	C(35)-H(35)	1.000
C(9)-H(9C)	1.000	C(36)-H(36)	1.000
C(11)-C(12)	1.391(6)	B-F(1)	1.345(8)
C(11)-C(16)	1.393(6)	B-F(2)	1.329(7)
C(12)-C(13)	1.382(7)	B-F(3)	1.292(8)
C(12)-H(12)	1.000	B-F(4)	1.373(11)

Atom-atom-atom	Angle, deg	Atom-atom-atom	Angle, deg
P-Fe-C(1)	152.69(13)	C(9)-C(8)-H(8A)	99.2
P-Fe-C(2)	139.19(15)	C(9)-C(8)-H(8B)	97.9
P-Fe-C(3)	100.60(15)	H(8A)-C(8)-H(8B)	133.9
P-Fe-C(4)	88.50(13)	C(8)-C(9)-H(9A)	115.7
P-Fe-C(5)	113.74(14)	C(8)-C(9)-H(9B)	110.2
P-Fe-C(6)	91.74(15)	C(8)-C(9)-H(9C)	105.5
P-Fe-C(7)	94.00(15)	H(9A)-C(9)-H(9B)	110.6
C(1)-Fe-C(2)	38.96(18)	H(9A)-C(9)-H(9C)	104.5
C(1)-Fe-C(3)	66.40(18)	H(9B)-C(9)-H(9C)	109.9
C(1)-Fe-C(4)	66.02(18)	P-C(11)-C(12)	122.6(3)
C(1)-Fe-C(5)	39.51(18)	P-C(11)-C(16)	118.7(3)
C(1)-Fe-C(6)	113.53(19)	C(12)-C(11)-C(16)	118.6(4)
C(1)-Fe-C(7)	93.72(19)	C(11)-C(12)-C(13)	120.1(4)
C(2)-Fe-C(3)	39.70(21)	C(11)-C(12)-H(12)	118.1
C(2)-Fe-C(4)	65.88(19)	C(13)-C(12)-H(12)	121.8

C(2)-Fe-C(5)	65.45(18)	C(12)-C(13)-C(14)	120.3(4)
C(2)-Fe-C(6)	87.92(19)	C(12)-C(13)-H(13)	118.8
C(2)-Fe-C(7)	126.67(21)	C(14)-C(13)-H(13)	121.0
C(3)-Fe-C(4)	39.54(20)	C(13)-C(14)-C(15)	120.5(4)
C(3)-Fe-C(5)	65.87(19)	C(13)-C(14)-H(14)	116.7
C(3)-Fe-C(6)	99.52(20)	C(15)-C(14)-H(14)	122.7
C(3)-Fe-C(7)	158.69(20)	C(14)-C(15)-C(16)	119.6(4)
C(4)-Fe-C(5)	38.79(19)	C(14)-C(15)-H(15)	115.5
C(4)-Fe-C(6)	137.87(20)	C(16)-C(15)-H(15)	124.9
C(4)-Fe-C(7)	126.59(21)	C(11)-C(16)-C(15)	120.9(4)
C(5)-Fe-C(6)	152.04(19)	C(11)-C(16)-H(16)	119.7
C(5)-Fe-C(7)	94.10(20)	C(15)-C(16)-H(16)	119.4
C(6)-Fe-C(7)	95.43(21)	P-C(21)-C(22)	120.9(3)
Fe-P-C(11)	110.87(13)	P-C(21)-C(26)	119.4(3)
Fe-P-C(21)	115.65(14)	C(22)-C(21)-C(26)	119.7(4)
Fe-P-C(31)	117.19(15)	C(21)-C(22)-C(23)	119.5(4)
C(11)-P-C(21)	104.04(19)	C(21)-C(22)-H(22)	124.1
C(11)-P-C(31)	105.64(18)	C(23)-C(22)-H(22)	116.3
C(21)-P-C(31)	102.12(18)	C(22)-C(23)-C(24)	120.3(4)
Fe-C(1)-C(2)	69.49(24)	C(22)-C(23)-H(23)	112.4
Fe-C(1)-C(5)	69.78(23)	C(24)-C(23)-H(23)	126.8
Fe-C(1)-C(8)	129.5(3)	C(23)-C(24)-C(25)	120.1(4)
C(2)-C(1)-C(5)	106.5(4)	C(23)-C(24)-H(24)	120.4
C(2)-C(1)-C(8)	126.5(4)	C(25)-C(24)-H(24)	118.8
C(5)-C(1)-C(8)	126.8(4)	C(24)-C(25)-C(26)	120.4(4)
Fe-C(2)-C(1)	71.55(24)	C(24)-C(25)-H(25)	122.2
Fe-C(2)-C(3)	69.54(25)	C(26)-C(25)-H(25)	117.3
Fe-C(2)-H(2)	131.5	C(21)-C(26)-C(25)	119.9(4)
C(1)-C(2)-C(3)	109.1(4)	C(21)-C(26)-H(26)	116.0
C(1)-C(2)-H(2)	127.8	C(25)-C(26)-H(26)	123.1
C(3)-C(2)-H(2)	122.6	P-C(31)-C(32)	119.3(3)
Fe-C(3)-C(2)	70.8(3)	P-C(31)-C(36)	121.0(3)
Fe-C(3)-C(4)	71.2(3)	C(32)-C(31)-C(36)	119.7(4)
Fe-C(3)-H(3)	123.5	C(31)-C(32)-C(33)	119.8(4)
C(2)-C(3)-C(4)	107.4(4)	C(31)-C(32)-H(32)	121.1
C(2)-C(3)-H(3)	123.9	C(33)-C(32)-H(32)	118.9
C(4)-C(3)-H(3)	128.7	C(32)-C(33)-C(34)	120.1(4)
Fe-C(4)-C(3)	69.3(3)	C(32)-C(33)-H(33)	121.8
Fe-C(4)-C(5)	70.8(3)	C(34)-C(33)-H(33)	118.1
Fe-C(4)-H(4)	121.6	C(33)-C(34)-C(35)	120.6(4)
C(3)-C(4)-C(5)	108.0(4)	C(33)-C(34)-H(34)	115.0
C(3)-C(4)-H(4)	118.6	C(35)-C(34)-H(34)	124.2
C(5)-C(4)-H(4)	133.2	C(34)-C(35)-C(36)	119.5(4)
Fe-C(5)-C(1)	70.71(24)	C(34)-C(35)-H(35)	121.1
Fe-C(5)-C(4)	70.4(3)	C(36)-C(35)-H(35)	119.0
Fe-C(5)-H(5)	137.5	C(31)-C(36)-C(35)	120.4(4)
C(1)-C(5)-C(4)	108.9(4)	C(31)-C(36)-H(36)	123.5
C(1)-C(5)-H(5)	119.0	C(35)-C(36)-H(36)	116.1
C(4)-C(5)-H(5)	130.1	F(1)-B-F(2)	114.3(5)
Fe-C(6)-O(1)	178.5(4)	F(1)-B-F(3)	113.3(6)
Fe-C(7)-O(2)	177.9(4)	F(1)-B-F(4)	105.3(6)
C(1)-C(8)-C(9)	110.4(5)	F(2)-B-F(3)	115.0(6)
C(1)-C(8)-H(8A)	104.1	F(2)-B-F(4)	102.2(6)
C(1)-C(8)-H(8B)	109.3	F(3)-B-F(4)	105.1(7)

Supplementary table 5.
Torsion angles of [Fe(CO)2PPh3(eta5-C5H4Et)+][BF4-], 9BF4, local id. I1127.

Atom-atom-atom-atom				Angle, deg.	Atom-atom-atom-atom				Angle, deg.
C1	FE	P	C11	-68.6(2)	C1	FE	P	C21	173.3(2)
C1	FE	P	C31	52.7(2)	C2	FE	P	C11	0.9(2)
C2	FE	P	C21	-117.2(2)	C2	FE	P	C31	122.2(2)
C3	FE	P	C11	-10.3(2)	C3	FE	P	C21	-128.4(2)
C3	FE	P	C31	111.1(2)	C4	FE	P	C11	-48.1(2)
C4	FE	P	C21	-166.2(2)	C4	FE	P	C31	73.2(2)
C5	FE	P	C11	-78.4(2)	C5	FE	P	C21	163.5(2)
C5	FE	P	C31	42.9(2)	C6	FE	P	C11	89.7(2)
C6	FE	P	C21	-28.4(2)	C6	FE	P	C31	-148.9(2)
C7	FE	P	C11	-174.7(2)	C7	FE	P	C21	67.2(2)
C7	FE	P	C31	-53.3(2)	P	FE	C1	C2	103.2(3)
P	FE	C1	C5	-14.2(2)	P	FE	C1	C8	-135.8(4)
C2	FE	C1	C2	0.0(3)	C2	FE	C1	C5	-117.4(4)
C2	FE	C1	C8	121.0(4)	C3	FE	C1	C2	37.3(3)
C3	FE	C1	C5	-80.1(3)	C3	FE	C1	C8	158.3(4)
C4	FE	C1	C2	80.7(3)	C4	FE	C1	C5	-36.7(3)
C4	FE	C1	C8	-158.3(4)	C5	FE	C1	C2	117.4(4)
C5	FE	C1	C5	0.0(3)	C5	FE	C1	C8	-121.6(4)
C6	FE	C1	C2	-53.0(3)	C6	FE	C1	C5	-170.5(5)
C6	FE	C1	C8	67.9(3)	C7	FE	C1	C2	-150.7(4)
C7	FE	C1	C5	91.9(4)	C7	FE	C1	C8	-29.7(3)
P	FE	C2	C1	-136.9(4)	P	FE	C2	C3	-17.3(2)
C1	FE	C2	C1	0.0(3)	C1	FE	C2	C3	119.5(4)
C3	FE	C2	C1	-119.5(4)	C3	FE	C2	C3	0.0(3)
C4	FE	C2	C1	-81.1(3)	C4	FE	C2	C3	38.4(3)
C5	FE	C2	C1	-38.4(3)	C5	FE	C2	C3	81.2(4)
C6	FE	C2	C1	132.9(4)	C6	FE	C2	C3	-107.6(4)
C7	FE	C2	C1	37.6(3)	C7	FE	C2	C3	157.1(5)
P	FE	C3	C2	168.6(4)	P	FE	C3	C4	-74.4(3)
C1	FE	C3	C2	-36.7(3)	C1	FE	C3	C4	80.4(4)
C2	FE	C3	C2	0.0(3)	C2	FE	C3	C4	117.0(4)
C4	FE	C3	C2	-117.0(4)	C4	FE	C3	C4	0.0(3)
C5	FE	C3	C2	-80.1(4)	C5	FE	C3	C4	37.0(3)
C6	FE	C3	C2	75.0(4)	C6	FE	C3	C4	-168.0(5)
C7	FE	C3	C2	-59.0(3)	C7	FE	C3	C4	58.0(3)
P	FE	C4	C3	108.7(4)	P	FE	C4	C5	-132.5(4)
C1	FE	C4	C3	-81.4(4)	C1	FE	C4	C5	37.4(3)
C2	FE	C4	C3	-38.5(3)	C2	FE	C4	C5	80.2(4)
C3	FE	C4	C3	0.0(3)	C3	FE	C4	C5	118.8(4)
C5	FE	C4	C3	-118.8(4)	C5	FE	C4	C5	0.0(3)
C6	FE	C4	C3	17.8(3)	C6	FE	C4	C5	136.6(5)
C7	FE	C4	C3	-157.4(5)	C7	FE	C4	C5	-38.6(3)
P	FE	C5	C1	172.9(4)	P	FE	C5	C4	53.6(3)
C1	FE	C5	C1	0.0(2)	C1	FE	C5	C4	-119.3(4)
C2	FE	C5	C1	37.9(3)	C2	FE	C5	C4	-81.4(4)
C3	FE	C5	C1	81.6(3)	C3	FE	C5	C4	-37.7(3)
C4	FE	C5	C1	119.3(4)	C4	FE	C5	C4	0.0(3)
C6	FE	C5	C1	18.9(3)	C6	FE	C5	C4	-100.4(4)
C7	FE	C5	C1	-90.9(4)	C7	FE	C5	C4	149.8(5)
P	FE	C6	O1	-148.1(5)	C1	FE	C6	O1	21.2(3)

C2	FE	C6	O1	-9.0(	3)	C3	FE	C6	O1	-47.1(	3)
C4	FE	C6	O1	-58.4(	3)	C5	FE	C6	O1	8.2(	3)
C7	FE	C6	O1	117.7(	5)	P	FE	C7	O2	159.9(	5)
C1	FE	C7	O2	6.1(	3)	C2	FE	C7	O2	-16.5(	3)
C3	FE	C7	O2	26.5(	3)	C4	FE	C7	O2	68.8(	4)
C5	FE	C7	O2	45.7(	3)	C6	FE	C7	O2	-108.0(	5)
FE	P	C11	C12	110.7(	3)	FE	P	C11	C16	-64.0(	3)
C21	P	C11	C12	-124.3(	4)	C21	P	C11	C16	61.0(	3)
C31	P	C11	C12	-17.2(	3)	C31	P	C11	C16	168.1(	4)
FE	P	C21	C22	143.8(	4)	FE	P	C21	C26	-37.8(	2)
C11	P	C21	C22	22.0(	3)	C11	P	C21	C26	-159.6(	4)
C31	P	C21	C22	-87.8(	3)	C31	P	C21	C26	90.6(	4)
FE	P	C31	C32	-179.9(	4)	FE	P	C31	C36	1.8(	2)
C11	P	C31	C32	-55.9(	3)	C11	P	C31	C36	125.9(	4)
C21	P	C31	C32	52.7(	3)	C21	P	C31	C36	-125.6(	4)
FE	C1	C2	FE	0.0(	0)	FE	C1	C2	C3	-59.6(	3)
C5	C1	C2	FE	60.3(	3)	C5	C1	C2	C3	0.6(	3)
C8	C1	C2	FE	-124.6(	5)	C8	C1	C2	C3	175.8(	7)
FE	C1	C5	FE	0.0(	0)	FE	C1	C5	C4	60.3(	3)
C2	C1	C5	FE	-60.1(	3)	C2	C1	C5	C4	0.2(	3)
C8	C1	C5	FE	124.8(	5)	C8	C1	C5	C4	-174.9(	7)
FE	C1	C8	C9	178.8(	6)	C2	C1	C8	C9	-88.6(	6)
C5	C1	C8	C9	85.5(	5)	FE	C2	C3	FE	0.0(	0)
FE	C2	C3	C4	-62.1(	4)	C1	C2	C3	FE	60.9(	3)
C1	C2	C3	C4	-1.2(	3)	FE	C3	C4	FE	0.0(	0)
FE	C3	C4	C5	-60.5(	4)	C2	C3	C4	FE	61.8(	4)
C2	C3	C4	C5	1.3(	3)	FE	C4	C5	FE	0.0(	0)
FE	C4	C5	C1	-60.5(	3)	C3	C4	C5	FE	59.5(	3)
C3	C4	C5	C1	-0.9(	3)	P	C11	C12	C13	-177.1(	5)
C16	C11	C12	C13	-2.5(	3)	P	C11	C16	C15	177.9(	5)
C12	C11	C16	C15	3.0(	3)	C11	C12	C13	C14	0.3(	3)
C12	C13	C14	C15	1.4(	3)	C13	C14	C15	C16	-0.9(	3)
C14	C15	C16	C11	-1.4(	3)	P	C21	C22	C23	177.2(	5)
C26	C21	C22	C23	-1.2(	3)	P	C21	C26	C25	-177.0(	5)
C22	C21	C26	C25	1.4(	3)	C21	C22	C23	C24	1.2(	3)
C22	C23	C24	C25	-1.5(	3)	C23	C24	C25	C26	1.7(	3)
C24	C25	C26	C21	-1.7(	3)	P	C31	C32	C33	179.7(	6)
C36	C31	C32	C33	-2.0(	3)	P	C31	C36	C35	179.1(	5)
C32	C31	C36	C35	0.8(	3)	C31	C32	C33	C34	1.7(	3)
C32	C33	C34	C35	-0.2(	3)	C33	C34	C35	C36	-1.0(	3)
C34	C35	C36	C31	0.7(	3)	F2	B	F1	F4	111.1(	6)
F3	B	F1	F4	-114.4(	7)	F4	B	F1	F4	0.0(	4)
F1	B	F2	F4	-113.1(	6)	F3	B	F2	F4	113.2(	7)
F4	B	F2	F4	0.0(	4)	F1	B	F3	F4	114.5(	7)
F2	B	F3	F4	-111.3(	7)	F4	B	F3	F4	0.0(	4)
F1	B	F4	F1	0.0(	3)	F1	B	F4	F2	119.7(	7)
F1	B	F4	F3	-119.9(	7)	F2	B	F4	F1	-119.7(	7)
F2	B	F4	F2	0.0(	3)	F2	B	F4	F3	120.4(	8)
F3	B	F4	F1	119.9(	8)	F3	B	F4	F2	-120.4(	8)
F3	B	F4	F3	0.0(	4)	B	F1	F4	B	0.0(	5)
B	F1	F4	F2	-36.9(	5)	B	F1	F4	F3	35.3(	5)
B	F2	F4	B	0.0(	5)	B	F2	F4	F1	35.6(	5)
B	F2	F4	F3	-34.7(	5)	B	F3	F4	B	0.0(	5)
B	F3	F4	F1	-36.1(	5)	B	F3	F4	F2	36.7(	5)

Supplementary table 6.
Crystal data and refinement details of [(CO)2Fe=C(NHPh)CH2CH2(eta5-C5H4)+]
[PF6-], 12PF6, local identification I1101

Space Group and Cell Dimensions Monoclinic, P 21/n
a 10.819(10) b 15.769(5) c 10.965(4)
beta 109.17(5)
Volume 1767.0(18)A**3

Empirical formula : C16 H14 F6 Fe N O2 P

Cell dimensions were obtained from 25 reflections with 2Theta angle
in the range 15.00 - 34.50 degrees.

Crystal dimensions : 0.25 X 0.38 X 0.75 mm

FW = 453.10 Z = 4 F(000) = 911.86

Dcalc 1.703Mg.m-3, mu 1.01mm-1, lambda 0.70930A, 2Theta(max) 49.9

The intensity data were collected on a Nonius diffractometer,
using the theta/2theta scan mode.
The h,k,l ranges used during structure solution and refinement are :--
Hmin,max -12 12; Kmin,max 0 18; Lmin,max 0 13
No. of reflections measured 6381
No. of unique reflections 3097
No. of reflections with Inet > 2.5sigma(Inet) 2709
Merging R-value on intensities 0.015
Absorption corrections were made.
The minimum and maximum transmission factors are 0.914481 and 0.999229.

The last least squares cycle was calculated with
41 atoms, 245 parameters and 2709 out of 3097 reflections.
Weights based on counting-statistics were used.
The weight modifier K in KFo**2 is 0.000100

The residuals are as follows :--
For significant reflections, RF 0.056, Rw 0.080 GoF 5.19
For all reflections, RF 0.063, Rw 0.081.
where RF = Sum(Fo-Fc)/Sum(Fo),
Rw = Sqrt[Sum(w(Fo-Fc)**2)/Sum(wFo**2)] and
GoF = Sqrt[Sum(w(Fo-Fc)**2)/(No. of reflns - No. of params.)]
The maximum shift/sigma ratio was 0.003.

In the last D-map, the deepest hole was -0.710e/A**3,
and the highest peak 1.090e/A**3.

Supplementary table 7.
Final atomic fractional coordinates for [(CO)2Fe=C(NHPh)CH2CH2(eta5-C5H4)+] [PF6-], 12PF6, local identification I1011

Atom	x	y	z	Biso
Fe	0.18177(6)	0.80766(4)	0.05031(6)	2.59(3)
P	0.13596(13)	0.69289(8)	0.44763(13)	3.75(6)
N	0.2335(4)	0.7226(2)	-0.1679(3)	3.1(2)
O1	0.4132(4)	0.7221(3)	0.2181(4)	5.2(2)
O2	0.0064(4)	0.6641(3)	0.0280(5)	6.1(2)
C1	0.3225(5)	0.7541(3)	0.1496(4)	3.5(2)
C2	0.0777(5)	0.7188(3)	0.0350(5)	3.6(2)
C3	0.2190(4)	0.7909(2)	-0.1088(4)	2.7(2)
C4	0.2308(5)	0.8717(3)	-0.1801(5)	3.7(2)
C5	0.1397(5)	0.9397(3)	-0.1603(5)	4.1(2)
C11	0.1360(5)	0.9292(3)	-0.0259(5)	3.6(2)
C12	0.2436(5)	0.9334(3)	0.0884(5)	4.0(2)
C13	0.2043(7)	0.9028(3)	0.1916(5)	5.0(3)
C14	0.0731(6)	0.8791(3)	0.1422(6)	4.8(3)
C15	0.0284(5)	0.8956(3)	0.0063(5)	4.0(2)
C21	0.2302(4)	0.6362(3)	-0.1275(4)	2.9(2)
C22	0.3367(5)	0.6007(3)	-0.0350(5)	3.8(2)
C23	0.3286(5)	0.5181(3)	0.0016(5)	4.3(2)
C24	-0.2168(5)	0.5286(3)	0.0521(5)	4.2(3)
C25	0.1135(5)	0.5065(3)	-0.1471(5)	4.3(2)
C26	0.1200(5)	0.5889(3)	-0.1858(5)	4.1(2)
F1	0.0140(4)	0.7103(3)	0.3245(3)	7.1(2)
F2	-0.2424(4)	0.8265(4)	0.0721(4)	9.3(3)
F3	0.2032(5)	0.6462(5)	0.3609(5)	13.3(4)
F4	0.5668(6)	0.7696(5)	0.0349(4)	14.6(4)
F6	0.0749(6)	0.6061(4)	0.4673(7)	14.5(4)
F5	0.2016(7)	0.7702(4)	0.4199(6)	16.4(5)
H	0.248	0.727	-0.239	4.1
H4a	0.323	0.892	-0.147	4.6
H4b	0.210	0.858	-0.274	4.6
H5a	0.051	0.933	-0.226	4.7
H5b	0.174	0.997	-0.172	4.7
H12	0.333	0.956	0.099	4.6
H13	0.260	0.894	0.284	5.7
H14	0.019	0.852	0.190	6.0
H15	-0.061	0.882	-0.054	4.8
H22	0.418	0.634	0.005	4.6
H23	-0.095	1.008	-0.432	5.0
H24	0.289	0.912	0.522	5.1
H25	-0.033	0.528	0.189	5.1
H26	0.545	0.886	0.244	4.7

Supplementary table 8.
Anisotropic termal parameters of non-H atoms of [(CO)2Fe=C(NHPh)CH2CH2(eta5 -C5H4)+][PF6-], 12PF6, local i.d. I1101. The temperature factors are of the form -2(Pi)**2(u11*h*h*astar*astar+---+2*u12*h*k*astar*bstar+---). The uij values have been multiplied by 100.

Atom	u11	u22	u33	u12	u13	u23
Fe	3.03(4)	3.06(4)	3.63(4)	-0.10(2)	0.94(3)	0.14(2)
P	4.18(8)	5.82(8)	4.39(8)	0.31(6)	1.60(6)	0.15(6)
N	4.7(2)	3.7(2)	4.0(2)	0.3(2)	2.1(2)	0.3(2)
O1	5.0(2)	8.4(3)	5.3(2)	1.6(2)	0.2(2)	1.2(2)
O2	7.8(3)	6.0(2)	11.3(4)	-3.4(2)	5.7(3)	-1.5(2)
C1	4.1(3)	4.9(3)	4.2(3)	-0.1(2)	1.1(2)	0.2(2)
C2	4.8(3)	4.5(3)	5.1(3)	-0.1(2)	2.6(2)	0.0(2)
C3	2.9(2)	3.1(2)	3.9(2)	-0.2(2)	0.7(2)	0.6(2)
C4	5.7(3)	3.7(2)	5.2(3)	0.2(2)	2.4(2)	1.3(2)
C5	5.6(3)	3.4(2)	6.0(3)	0.5(2)	1.2(3)	1.5(2)
C11	5.0(3)	2.9(2)	5.7(3)	0.6(2)	1.6(2)	0.6(2)
C12	5.4(3)	2.7(2)	6.5(3)	-0.5(2)	0.9(3)	-0.8(2)
C13	9.7(5)	4.2(3)	4.8(3)	0.4(3)	1.9(3)	-1.4(2)
C14	7.6(4)	4.8(3)	7.4(4)	0.9(3)	4.5(3)	-0.4(3)
C15	4.1(3)	3.9(3)	7.4(4)	0.8(2)	2.0(3)	0.1(2)
C21	4.5(3)	3.1(2)	3.8(2)	0.1(2)	1.8(2)	0.0(2)
C22	4.5(3)	4.3(3)	5.5(3)	-0.2(2)	1.3(2)	-0.2(2)
C23	6.2(3)	4.3(3)	5.4(3)	0.6(2)	1.4(3)	0.9(2)
C24	7.4(4)	3.6(3)	5.4(3)	-0.1(2)	2.9(3)	-0.2(2)
C25	5.5(3)	4.4(3)	6.5(3)	-1.1(2)	1.7(3)	-0.6(2)
C26	4.5(3)	4.6(3)	5.7(3)	0.0(2)	0.8(2)	-0.2(2)
F1	6.0(2)	14.0(4)	6.2(2)	1.0(2)	1.0(2)	2.0(2)
F2	5.3(2)	23.5(5)	6.1(2)	2.9(3)	1.1(2)	2.0(3)
F3	12.3(4)	29.4(8)	8.5(3)	8.5(5)	3.1(3)	-2.3(4)
F4	17.3(5)	31.6(8)	6.5(3)	16.6(6)	3.9(3)	0.3(4)
F6	16.5(6)	15.2(5)	19.2(6)	-6.2(4)	0.1(5)	7.1(5)

Supplementary table 9.
Bond lengths and angles of [(CO)2Fe=C(NHPh)CH2CH2(eta5-C5H4)+][PF6-], 12PF6, local identification I1101.

Atom-atom	Length, A	Atom-atom	Length, A
Fe-C1	1.769(5)	C5-H5a	1.000
Fe-C2	1.770(5)	C5-H5b	1.000
Fe-C3	1.933(5)	C11-C12	1.405(7)
Fe-C11	2.084(4)	C11-C15	1.424(7)
Fe-C12	2.090(4)	C12-C13	1.417(8)
Fe-C13	2.112(5)	C12-H12	1.000
Fe-C14	2.108(5)	C13-C14	1.394(9)
Fe-C15	2.093(5)	C13-H13	1.000
P-F1	1.571(4)	C14-C15	1.432(8)
P-F2	1.584(4)	C14-H14	1.000
P-F3	1.559(5)	C15-H15	1.000
P-F4	1.515(7)	C21-C22	1.380(7)
P-F6	1.565(5)	C21-C26	1.373(7)
P-F5	1.492(5)	C22-C23	1.375(7)
N-C3	1.293(6)	C22-H22	1.000
N-C21	1.436(5)	C23-C24	1.373(8)
N-H	0.850	C23-H23	1.000
O1-C1	1.139(6)	C24-C23	1.373(8)
O2-C2	1.143(6)	C24-C25	1.369(8)
C3-C4	1.522(6)	C24-H24	1.000
C4-C5	1.519(7)	C25-C24	1.369(8)
C4-H4a	1.000	C25-C26	1.377(7)
C4-H4b	1.000	C25-H25	1.000
C5-C11	1.497(7)	C26-H26	1.000

Atom-atom-atom	Angle, deg.	Atom-atom-atom	Angle, deg.
C1-Fe-C2	94.18(23)	H4a-C4-H4b	107.8
C1-Fe-C3	95.61(20)	C4-C5-C11	106.9(4)
C1-Fe-C11	136.81(21)	C4-C5-H5a	109.5
C1-Fe-C12	100.10(21)	C4-C5-H5b	109.5
C1-Fe-C13	91.07(23)	C11-C5-H5a	111.6
C1-Fe-C14	117.60(23)	C11-C5-H5b	110.8
C1-Fe-C15	156.23(22)	H5a-C5-H5b	108.5
C2-Fe-C3	96.92(20)	Fe-C11-C5	114.6(3)
C2-Fe-C11	129.00(22)	Fe-C11-C12	70.6(3)
C2-Fe-C12	157.13(22)	Fe-C11-C15	70.4(3)
C2-Fe-C13	123.26(24)	C5-C11-C12	126.2(5)
C2-Fe-C14	91.80(23)	C5-C11-C15	125.0(5)
C2-Fe-C15	94.06(22)	C12-C11-C15	107.6(4)
C3-Fe-C11	81.75(18)	Fe-C12-C11	70.10(25)
C3-Fe-C12	99.34(19)	Fe-C12-C13	71.1(3)
C3-Fe-C13	138.67(21)	Fe-C12-H12	126.8
C3-Fe-C14	144.95(20)	C11-C12-C13	108.6(5)
C3-Fe-C15	105.47(20)	C11-C12-H12	127.1
C11-Fe-C12	39.33(20)	C13-C12-H12	124.3
C11-Fe-C13	66.18(20)	Fe-C13-C12	69.5(3)
C11-Fe-C14	66.66(20)	Fe-C13-C14	70.6(3)
C11-Fe-C15	39.87(20)	Fe-C13-H13	122.0
C12-Fe-C13	39.42(23)	C12-C13-C14	108.4(5)

C12-Fe-C14	65.76(22)	C12-C13-H13	127.7
C12-Fe-C15	66.14(20)	C14-C13-H13	123.7
C13-Fe-C14	38.6(3)	Fe-C14-C13	70.9(3)
C13-Fe-C15	65.85(23)	Fe-C14-C15	69.5(3)
C14-Fe-C15	39.85(23)	Fe-C14-H14	122.8
F1-P-F2	178.8(3)	C13-C14-C15	108.0(5)
F1-P-F3	89.24(25)	C13-C14-H14	127.6
F1-P-F4	91.4(3)	C15-C14-H14	124.4
F1-P-F6	89.9(3)	Fe-C15-C11	69.7(3)
F1-P-F5	90.2(3)	Fe-C15-C14	70.6(3)
F2-P-F3	90.7(3)	Fe-C15-H15	121.7
F2-P-F4	88.5(3)	C11-C15-C14	107.5(5)
F2-P-F6	88.9(3)	C11-C15-H15	127.2
F2-P-F5	91.0(3)	C14-C15-H15	125.1
F3-P-F4	174.7(4)	N-C21-C22	120.8(4)
F3-P-F6	88.5(5)	N-C21-C26	118.5(4)
F3-P-F5	85.0(5)	C22-C21-C26	120.7(4)
F4-P-F6	86.3(4)	C21-C22-C23	118.8(4)
F4-P-F5	100.2(5)	C21-C22-H22	120.7
F6-P-F5	173.5(5)	C23-C22-H22	120.6
C3-N-C21	128.0(4)	C22-C23-C24	121.0(5)
C3-N-H	119.1	C22-C23-H23	119.5
C21-N-H	112.9	C24-C23-H23	119.5
Fe-C1-O1	176.8(4)	C23-C24-C25	119.6(4)
Fe-C2-O2	176.2(5)	C23-C24-H24	120.3
Fe-C3-N	131.5(3)	C25-C24-H24	120.2
Fe-C3-C4	115.3(3)	C24-C25-C26	120.4(5)
N-C3-C4	113.3(4)	C24-C25-H25	119.8
C3-C4-C5	110.5(4)	C26-C25-H25	119.8
C3-C4-H4a	108.7	C21-C26-C25	119.6(4)
C3-C4-H4b	109.0	C21-C26-H26	120.2
C5-C4-H4a	110.0	C25-C26-H26	120.2
C5-C4-H4b	110.9		

Supplementary table 10.
Torsion angles of [(CO)2Fe=C(NHPh)CH2CH2(eta5-C5H4)+][PF6-], 12PF6,
local identification I1101

Atom-atom-atom-atom				Angle, deg.	Atom-atom-atom-atom				Angle, deg.
C2	Fe	C1	O1	-113.8(4)	C3	Fe	C1	O1	148.8(4)
C11	Fe	C1	O1	64.9(3)	C12	Fe	C1	O1	48.3(3)
C13	Fe	C1	O1	9.7(2)	C14	Fe	C1	O1	-19.6(3)
C15	Fe	C1	O1	-3.8(2)	C1	Fe	C2	O2	121.3(4)
C3	Fe	C2	O2	-142.6(4)	C11	Fe	C2	O2	-57.6(3)
C12	Fe	C2	O2	-7.5(3)	C13	Fe	C2	O2	27.2(3)
C14	Fe	C2	O2	3.4(3)	C15	Fe	C2	O2	-36.4(3)
C1	Fe	C3	N	59.8(3)	C1	Fe	C3	C4	-121.8(3)
C2	Fe	C3	N	-35.1(2)	C2	Fe	C3	C4	143.3(3)
C11	Fe	C3	N	-163.7(3)	C11	Fe	C3	C4	14.8(2)
C12	Fe	C3	N	161.0(3)	C12	Fe	C3	C4	-20.5(2)
C13	Fe	C3	N	157.8(3)	C13	Fe	C3	C4	-23.7(2)
C14	Fe	C3	N	-138.3(3)	C14	Fe	C3	C4	40.1(2)
C15	Fe	C3	N	-131.3(3)	C15	Fe	C3	C4	47.1(2)
C1	Fe	C11	C5	95.4(3)	C1	Fe	C11	C12	-26.4(2)
C1	Fe	C11	C15	-144.1(4)	C2	Fe	C11	C5	-86.2(3)
C2	Fe	C11	C12	151.9(4)	C2	Fe	C11	C15	34.2(3)
C3	Fe	C11	C5	6.0(2)	C3	Fe	C11	C12	-115.8(3)
C3	Fe	C11	C15	126.4(3)	C12	Fe	C11	C5	121.8(3)
C12	Fe	C11	C12	0.0(2)	C12	Fe	C11	C15	-117.7(3)
C13	Fe	C11	C5	159.3(4)	C13	Fe	C11	C12	37.5(3)
C13	Fe	C11	C15	-80.3(3)	C14	Fe	C11	C5	-158.5(4)
C14	Fe	C11	C12	79.7(3)	C14	Fe	C11	C15	-38.0(3)
C15	Fe	C11	C5	-120.4(3)	C15	Fe	C11	C12	117.7(3)
C15	Fe	C11	C15	0.0(2)	C1	Fe	C12	C11	162.0(4)
C1	Fe	C12	C13	-79.2(3)	C2	Fe	C12	C11	-70.2(3)
C2	Fe	C12	C13	48.6(3)	C3	Fe	C12	C11	64.5(3)
C3	Fe	C12	C13	-176.7(4)	C11	Fe	C12	C11	0.0(2)
C11	Fe	C12	C13	118.8(4)	C13	Fe	C12	C11	-118.8(3)
C13	Fe	C12	C13	0.0(3)	C14	Fe	C12	C11	-82.2(3)
C14	Fe	C12	C13	36.6(3)	C15	Fe	C12	C11	-38.3(2)
C15	Fe	C12	C13	80.4(3)	C1	Fe	C13	C12	104.7(4)
C1	Fe	C13	C14	-136.0(4)	C2	Fe	C13	C12	-159.6(4)
C2	Fe	C13	C14	-40.3(3)	C3	Fe	C13	C12	4.9(2)
C3	Fe	C13	C14	124.2(4)	C11	Fe	C13	C12	-37.4(2)
C11	Fe	C13	C14	81.9(3)	C12	Fe	C13	C12	0.0(2)
C12	Fe	C13	C14	119.3(4)	C14	Fe	C13	C12	-119.3(4)
C14	Fe	C13	C14	0.0(3)	C15	Fe	C13	C12	-81.2(3)
C15	Fe	C13	C14	38.1(3)	C1	Fe	C14	C13	51.6(3)
C1	Fe	C14	C15	170.2(4)	C2	Fe	C14	C13	147.2(4)
C2	Fe	C14	C15	-94.2(4)	C3	Fe	C14	C13	-108.0(4)
C3	Fe	C14	C15	10.6(2)	C11	Fe	C14	C13	-80.5(3)
C11	Fe	C14	C15	38.1(3)	C12	Fe	C14	C13	-37.4(3)
C12	Fe	C14	C15	81.2(3)	C13	Fe	C14	C13	0.0(3)
C13	Fe	C14	C15	118.6(4)	C15	Fe	C14	C13	-118.6(4)
C15	Fe	C14	C15	0.0(2)	C1	Fe	C15	C11	95.9(3)
C1	Fe	C15	C14	-22.1(3)	C2	Fe	C15	C11	-154.0(4)
C2	Fe	C15	C14	87.9(3)	C3	Fe	C15	C11	-55.7(3)
C3	Fe	C15	C14	-173.7(4)	C11	Fe	C15	C11	0.0(2)

C11	Fe	C15	C14	-118.0(	4)	C12	Fe	C15	C11	37.8(	2)
C12	Fe	C15	C14	-80.2(	3)	C13	Fe	C15	C11	81.2(	3)
C13	Fe	C15	C14	-36.9(	3)	C14	Fe	C15	C11	118.0(	3)
C14	Fe	C15	C14	0.0(	3)	F3	P	F1	F3	0.0(	3)
F3	P	F1	F5	-85.0(	3)	F6	P	F1	F3	-88.5(	3)
F6	P	F1	F5	-173.5(	4)	F5	P	F1	F3	85.0(	3)
F5	P	F1	F5	0.0(	3)	F1	P	F3	F1	0.0(	2)
F1	P	F3	F6	-89.9(	3)	F1	P	F3	F5	90.2(	3)
F6	P	F3	F1	89.9(	3)	F6	P	F3	F6	0.0(	3)
F6	P	F3	F5	-179.9(	5)	F5	P	F3	F1	-90.2(	4)
F5	P	F3	F6	179.9(	5)	F5	P	F3	F5	0.0(	3)
F1	P	F6	F3	89.2(	3)	F3	P	F6	F3	0.0(	3)
F5	P	F6	F3	-1.2(	3)	F1	P	F5	F1	0.0(	2)
F1	P	F5	F3	-89.2(	4)	F3	P	F5	F1	89.2(	4)
F3	P	F5	F3	0.0(	3)	F6	P	F5	F1	90.5(	4)
F6	P	F5	F3	1.2(	3)	C21	N	C3	Fe	-2.4(	2)
C21	N	C3	C4	179.1(	4)	C3	N	C21	C22	-78.4(	4)
C3	N	C21	C26	103.5(	4)	Fe	C3	C4	C5	-32.8(	2)
N	C3	C4	C5	145.9(	5)	C3	C4	C5	C11	35.0(	3)
C4	C5	C11	Fe	-24.2(	2)	C4	C5	C11	C12	59.0(	3)
C4	C5	C11	C15	-106.8(	5)	Fe	C11	C12	Fe	0.0(	0)
Fe	C11	C12	C13	-61.0(	3)	C5	C11	C12	Fe	-106.8(	4)
C5	C11	C12	C13	-167.9(	6)	C15	C11	C12	Fe	61.0(	3)
C15	C11	C12	C13	0.0(	3)	Fe	C11	C15	Fe	0.0(	0)
Fe	C11	C15	C14	60.8(	3)	C5	C11	C15	Fe	106.9(	4)
C5	C11	C15	C14	167.8(	6)	C12	C11	C15	Fe	-61.1(	3)
C12	C11	C15	C14	-0.3(	3)	Fe	C12	C13	Fe	0.0(	0)
Fe	C12	C13	C14	-60.1(	3)	C11	C12	C13	Fe	60.4(	3)
C11	C12	C13	C14	0.3(	3)	Fe	C13	C14	Fe	0.0(	0)
Fe	C13	C14	C15	-59.8(	3)	C12	C13	C14	Fe	59.4(	3)
C12	C13	C14	C15	-0.5(	3)	Fe	C14	C15	Fe	0.0(	0)
Fe	C14	C15	C11	-60.3(	3)	C13	C14	C15	Fe	60.7(	3)
C13	C14	C15	C11	0.5(	3)	N	C21	C22	C23	179.4(	5)
C26	C21	C22	C23	-2.6(	3)	N	C21	C26	C25	-178.8(	5)
C22	C21	C26	C25	3.1(	3)	P	F1	F3	P	0.0(	1)
P	F1	F3	F6	55.3(	3)	P	F1	F3	F5	-55.4(	3)
F5	F1	F3	P	55.4(	3)	F5	F1	F3	F6	110.7(	4)
F5	F1	F3	F5	0.0(	2)	P	F1	F5	P	0.0(	1)
P	F1	F5	F3	58.1(	3)	F3	F1	F5	P	-58.1(	3)
F3	F1	F5	F3	0.0(	2)	P	F3	F6	P	0.0(	1)
F1	F3	F6	P	-55.0(	3)	F5	F3	F6	P	0.1(	2)
P	F3	F5	P	0.0(	1)	P	F3	F5	F1	-54.7(	3)
F1	F3	F5	P	54.7(	3)	F1	F3	F5	F1	0.0(	1)
F6	F3	F5	P	-0.1(	2)	F6	F3	F5	F1	-54.8(	3)