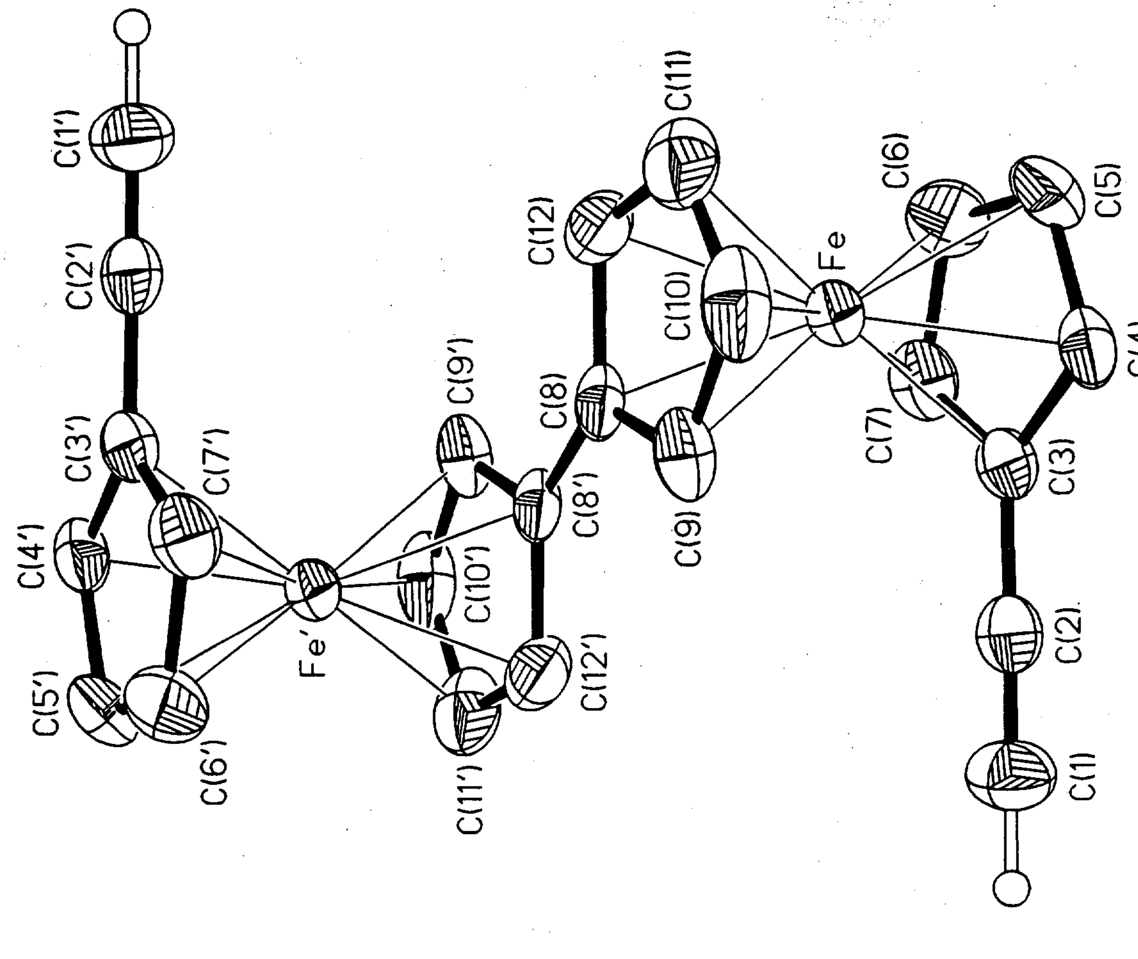

C(1')
C(2')
C(3')
C(4')
C(5')
C(6')
C(7')
Fe'
C(8')
C(9')
C(10')
C(11')
C(12')
C(8)
C(9)
C(10)
C(11)
C(12)
Fe
C(1)
C(2)
C(3)
C(4)
C(5)
C(6)
C(7)

Table 1. Crystal data and structure refinement for ~~1~~ 3.

Identification code	NL9702
Empirical formula	$C_{24}H_{18}Fe_2$
Formula weight	418.08
Temperature	203(2) K
Diffractometer Used	Siemens P4/PC
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	$P2_1/c$
Unit cell dimensions	a = 10.5679(8) Å alpha = 90°
	b = 9.2447(6) Å beta = 116.006(7)°
	c = 10.2642(11) Å gamma = 90°
Volume, Z	901.25(13) Å^3, 2
Density (calculated)	1.541 Mg/m^3
Absorption coefficient	1.613 mm^{-1}
F(000)	428
Crystal morphology/size	Orange/red rhombs, 0.37 x 0.33 x 0.23 mm
θ range for data collection	2.14 to 25.00°
Limiting indices	$-12 \le h \le 11$, $-10 \le k \le 0$, $0 \le l \le 12$
Reflections collected	1683
Independent reflections	1586 (R_{int} = 0.0224)
Observed reflections	1294 [$F > 4\sigma(F)$]
Absorption correction	Semi-empirical
Max. and min. transmission	0.7548 and 0.6021
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	1586 / 0 / 119
Goodness-of-fit on F^2	1.083
Final R indices [$I>2\sigma(I)$]	R1 = 0.0356, wR2 = 0.0784
R indices (all data)	R1 = 0.0503, wR2 = 0.0846
Extinction coefficient	0.0073(12)
Largest diff. peak and hole	0.265 and -0.276 eÅ^{-3}

Table 2. Atomic coordinates [x 10^4] and equivalent isotropic displacement parameters [$Å^2$ x 10^3] for 3. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Fe	2615(1)	5211(1)	5657(1)	29(1)
C(1)	1576(4)	9537(4)	4934(4)	48(1)
C(2)	2272(4)	8527(4)	5512(4)	36(1)
C(3)	3123(3)	7307(4)	6258(3)	32(1)
C(4)	4202(3)	6637(4)	5984(4)	37(1)
C(5)	4732(4)	5451(4)	6946(4)	48(1)
C(6)	3994(4)	5380(5)	7808(4)	51(1)
C(7)	2995(4)	6518(4)	7390(4)	40(1)
C(8)	516(3)	4688(4)	4783(4)	32(1)
C(9)	891(3)	5238(4)	3701(4)	38(1)
C(10)	1936(4)	4333(5)	3627(5)	50(1)
C(11)	2239(4)	3237(4)	4674(5)	55(1)
C(12)	1367(4)	3440(4)	5399(5)	44(1)

Table 3. Bond lengths [Å] and angles [°] for ~~1~~ 3.

Fe-C(3)	2.033(3)	Fe-C(9)	2.036(3)
Fe-C(11)	2.038(4)	Fe-C(7)	2.039(3)
Fe-C(4)	2.042(3)	Fe-C(12)	2.045(4)
Fe-C(6)	2.050(4)	Fe-C(10)	2.051(4)
Fe-C(5)	2.051(3)	Fe-C(8)	2.053(3)
C(1)-C(2)	1.176(5)	C(2)-C(3)	1.436(5)
C(3)-C(7)	1.428(5)	C(3)-C(4)	1.429(5)
C(4)-C(5)	1.417(5)	C(5)-C(6)	1.414(6)
C(6)-C(7)	1.417(5)	C(8)-C(9)	1.427(5)
C(8)-C(12)	1.429(5)	C(8)-C(8)#1	1.464(6)
C(9)-C(10)	1.413(5)	C(10)-C(11)	1.408(6)
C(11)-C(12)	1.428(5)		
C(3)-Fe-C(9)	106.89(14)	C(3)-Fe-C(11)	166.3(2)
C(9)-Fe-C(11)	68.1(2)	C(3)-Fe-C(7)	41.04(13)
C(9)-Fe-C(7)	127.0(2)	C(11)-Fe-C(7)	152.1(2)
C(3)-Fe-C(4)	41.06(13)	C(9)-Fe-C(4)	118.0(2)
C(11)-Fe-C(4)	128.8(2)	C(7)-Fe-C(4)	68.9(2)
C(3)-Fe-C(12)	150.69(14)	C(9)-Fe-C(12)	68.6(2)
C(11)-Fe-C(12)	40.9(2)	C(7)-Fe-C(12)	117.2(2)
C(4)-Fe-C(12)	167.04(14)	C(3)-Fe-C(6)	68.4(2)
C(9)-Fe-C(6)	165.4(2)	C(11)-Fe-C(6)	119.6(2)
C(7)-Fe-C(6)	40.6(2)	C(4)-Fe-C(6)	68.2(2)
C(12)-Fe-C(6)	108.3(2)	C(3)-Fe-C(10)	127.8(2)
C(9)-Fe-C(10)	40.5(2)	C(11)-Fe-C(10)	40.3(2)
C(7)-Fe-C(10)	165.5(2)	C(4)-Fe-C(10)	108.6(2)
C(12)-Fe-C(10)	68.5(2)	C(6)-Fe-C(10)	153.1(2)
C(3)-Fe-C(5)	68.5(2)	C(9)-Fe-C(5)	152.4(2)
C(11)-Fe-C(5)	109.7(2)	C(7)-Fe-C(5)	68.4(2)
C(4)-Fe-C(5)	40.5(2)	C(12)-Fe-C(5)	129.0(2)
C(6)-Fe-C(5)	40.3(2)	C(10)-Fe-C(5)	119.7(2)
C(3)-Fe-C(8)	116.61(13)	C(9)-Fe-C(8)	40.84(13)
C(11)-Fe-C(8)	68.5(2)	C(7)-Fe-C(8)	106.43(14)
C(4)-Fe-C(8)	151.15(14)	C(12)-Fe-C(8)	40.83(14)
C(6)-Fe-C(8)	127.6(2)	C(10)-Fe-C(8)	68.48(14)
C(5)-Fe-C(8)	166.2(2)	C(1)-C(2)-C(3)	178.3(4)
C(7)-C(3)-C(4)	107.9(3)	C(7)-C(3)-C(2)	125.1(3)
C(4)-C(3)-C(2)	127.0(3)	C(7)-C(3)-Fe	69.7(2)
C(4)-C(3)-Fe	69.8(2)	C(2)-C(3)-Fe	124.5(2)
C(5)-C(4)-C(3)	107.7(3)	C(5)-C(4)-Fe	70.1(2)
C(3)-C(4)-Fe	69.1(2)	C(6)-C(5)-C(4)	108.3(3)
C(6)-C(5)-Fe	69.8(2)	C(4)-C(5)-Fe	69.4(2)
C(5)-C(6)-C(7)	108.5(3)	C(5)-C(6)-Fe	69.9(2)
C(7)-C(6)-Fe	69.3(2)	C(6)-C(7)-C(3)	107.6(3)
C(6)-C(7)-Fe	70.1(2)	C(3)-C(7)-Fe	69.3(2)
C(9)-C(8)-C(12)	107.2(3)	C(9)-C(8)-C(8)#1	126.5(4)
C(12)-C(8)-C(8)#1	126.3(4)	C(9)-C(8)-Fe	69.0(2)
C(12)-C(8)-Fe	69.3(2)	C(8)#1-C(8)-Fe	125.5(3)
C(10)-C(9)-C(8)	108.8(4)	C(10)-C(9)-Fe	70.3(2)
C(8)-C(9)-Fe	70.2(2)	C(11)-C(10)-C(9)	107.8(3)
C(11)-C(10)-Fe	69.4(2)	C(9)-C(10)-Fe	69.2(2)
C(10)-C(11)-C(12)	108.7(4)	C(10)-C(11)-Fe	70.4(2)
C(12)-C(11)-Fe	69.8(2)	C(11)-C(12)-C(8)	107.5(4)
C(11)-C(12)-Fe	69.3(2)	C(8)-C(12)-Fe	69.9(2)

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

Table 4. Anisotropic displacement parameters [$Å^2 \times 10^3$] for ~~1~~ 3.

The anisotropic displacement factor exponent takes the form:

$-2\pi^2$ [$(ha^*)^2U_{11}$ + ... + $2hka^*b^*U_{12}$]

	U11	U22	U33	U23	U13	U12
Fe	24(1)	30(1)	34(1)	0(1)	13(1)	-2(1)
C(1)	50(2)	39(2)	47(2)	-1(2)	14(2)	8(2)
C(2)	34(2)	38(2)	31(2)	-9(2)	10(2)	-8(1)
C(3)	26(2)	36(2)	27(2)	-5(1)	7(1)	-5(1)
C(4)	25(2)	42(2)	43(2)	-5(2)	14(2)	-9(1)
C(5)	24(2)	52(2)	54(2)	1(2)	5(2)	4(2)
C(6)	46(2)	55(2)	35(2)	12(2)	1(2)	1(2)
C(7)	36(2)	51(2)	28(2)	-5(2)	11(2)	-6(2)
C(8)	27(1)	30(2)	39(2)	-11(1)	15(1)	-12(1)
C(9)	30(2)	52(2)	31(2)	-8(2)	11(1)	-13(2)
C(10)	45(2)	61(3)	55(2)	-28(2)	31(2)	-22(2)
C(11)	48(2)	39(2)	89(3)	-23(2)	40(2)	-8(2)
C(12)	42(2)	28(2)	69(3)	-3(2)	31(2)	-4(2)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for ~~1~~ 3.

	x	y	z	U(eq)
H(1)	1020(4)	10345(4)	4472(4)	58
H(4A)	4505(3)	6932(4)	5291(4)	45
H(5A)	5450(4)	4818(4)	7002(4)	57
H(6A)	4142(4)	4694(5)	8537(4)	62
H(7A)	2363(4)	6718(4)	7786(4)	47
H(9A)	506(3)	6065(4)	3130(4)	46
H(10A)	2354(4)	4444(5)	2991(5)	60
H(11A)	2905(4)	2495(4)	4864(5)	66
H(12A)	1355(4)	2858(4)	6145(5)	53

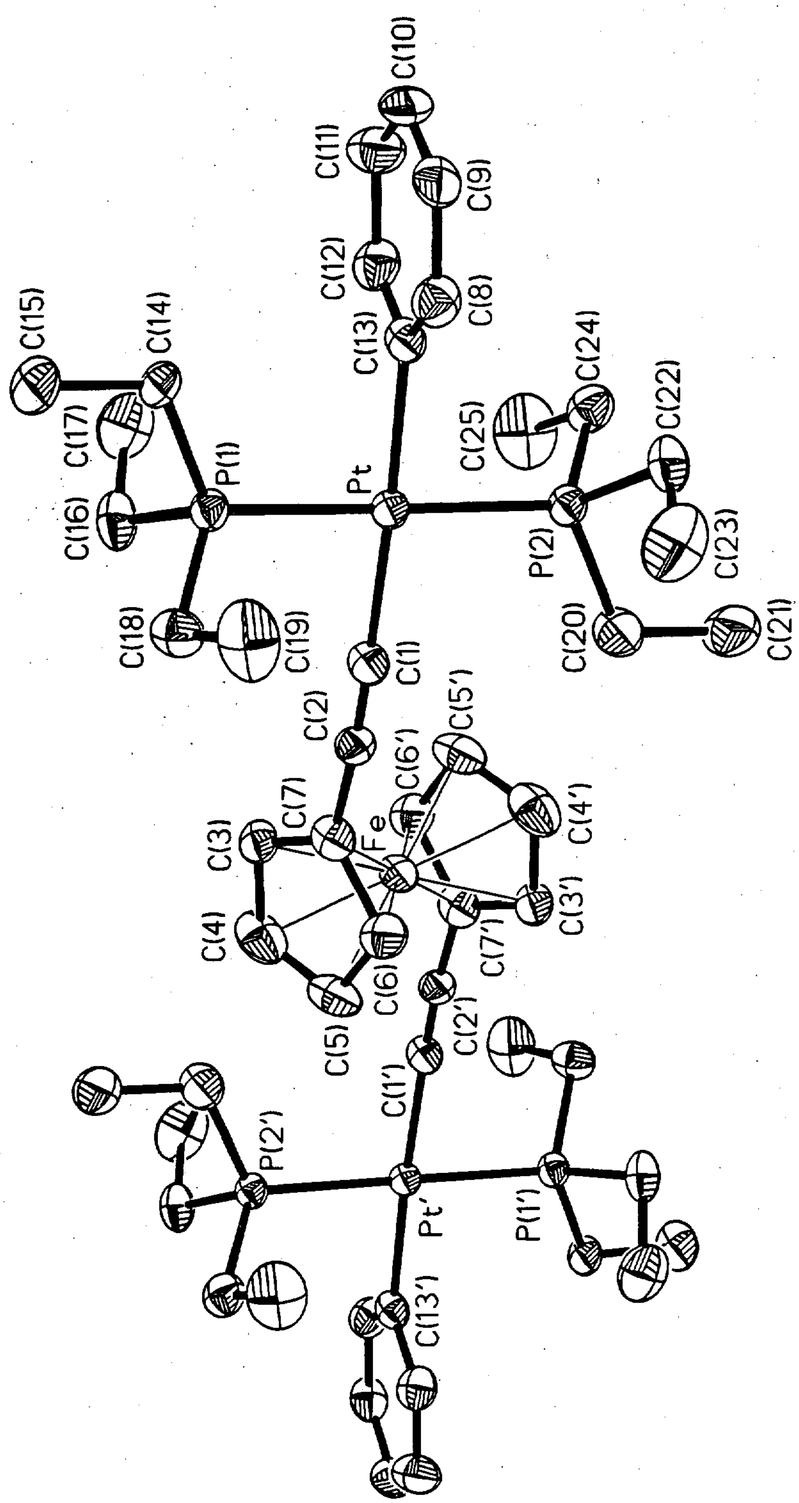

C(10)
C(11)
C(9)
C(12)
C(8)
C(15)
C(14)
C(13)
C(24)
C(17)
C(22)
C(25)
P(1)
Pt
C(16)
P(2)
C(23)
C(18)
C(19)
C(20)
C(21)
C(1)
C(2)
C(5')
C(6')
C(7)
Fe
C(3)
C(4')
C(4)
C(3')
C(7')
C(6)
C(2')
C(5)
C(1')
P(2')
Pt'
P(1')
C(13')

Table 1. Crystal data and structure refinement for ~~1~~ 5.

Identification code	NL9704
Empirical formula	$C_{50}H_{78}P_4Pt_2Fe \cdot 2CH_2Cl_2$
Formula weight	1418.89
Temperature	203(2) K
Diffractometer Used	Siemens P4/PC
Wavelength	0.71073 Å
Crystal system	Triclinic
Space group	$P\bar{1}$
Unit cell dimensions	a = 9.073(2) Å alpha = 87.857(14)° b = 11.401(2) Å beta = 75.60(2)° c = 14.753(3) Å gamma = 81.41(2)°
Volume, Z	1461.6(5) $Å^3$, 1
Density (calculated)	1.612 Mg/m^3
Absorption coefficient	5.343 mm^{-1}
F(000)	704
Crystal colour/morphology	Orange platy needles
Crystal size	0.83 x 0.48 x 0.14 mm
θ range for data collection	1.81 to 30.00°
Limiting indices	$0 \leq h \leq 12$, $-15 \leq k \leq 16$, $-20 \leq l \leq 20$
Scan type	ω-scans
Reflections collected	9012
Independent reflections	8512 (R_{int} = 0.0279)
Observed reflections [$F>4\sigma(F)$]	7113
Absorption correction	Face-indexed numerical
Max. and min. transmission	0.4790 and 0.0970
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	8511 / 0 / 274
Goodness-of-fit on F^2	1.030
Final R indices [$F>4\sigma(F)$]	R1 = 0.0379, wR2 = 0.0809
R indices (all data)	R1 = 0.0536, wR2 = 0.0882
Largest diff. peak and hole	1.749 and -1.270 $eÅ^{-3}$
Mean and maximum shift/error	0.000 and 0.001

Table 2. Atomic coordinates [x 10^4], equivalent isotropic displacement parameters [$Å^2$ x 10^3] and site occupancy factors for 5. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)	sof
Pt	4347(1)	923(1)	2643(1)	22(1)	1
Fe	5000	5000	5000	28(1)	0.50
P(1)	6618(1)	-323(1)	2557(1)	25(1)	1
P(2)	2093(1)	2133(1)	2650(1)	25(1)	1
C(1)	5279(5)	2226(4)	3106(3)	27(1)	1
C(2)	5742(6)	2970(5)	3476(3)	29(1)	1
C(3)	6719(6)	3569(5)	4846(4)	36(1)	1
C(4)	7214(7)	4591(6)	5112(5)	47(2)	1
C(5)	7114(6)	5463(6)	4430(5)	46(2)	1
C(6)	6529(7)	4996(5)	3730(4)	38(1)	1
C(7)	6297(5)	3801(5)	3974(3)	30(1)	1
C(8)	3482(4)	-800(3)	1374(2)	35(1)	1
C(9)	2907(5)	-1800(3)	1177(2)	42(1)	1
C(10)	2177(5)	-2483(3)	1904(3)	44(1)	1
C(11)	2022(5)	-2166(3)	2827(2)	46(1)	1
C(12)	2597(4)	-1167(3)	3024(2)	36(1)	1
C(13)	3327(4)	-484(3)	2297(2)	26(1)	1
C(14)	6748(6)	-1785(5)	2043(4)	38(1)	1
C(15)	8293(8)	-2596(6)	1919(5)	52(2)	1
C(16)	7038(7)	-619(6)	3694(4)	38(1)	1
C(17)	5834(9)	-1257(7)	4345(4)	55(2)	1
C(18)	8269(6)	320(5)	1880(4)	35(1)	1
C(19)	8160(9)	596(8)	879(4)	62(2)	1
C(20)	2087(7)	3692(5)	2891(5)	42(1)	1
C(21)	633(8)	4521(6)	2849(6)	58(2)	1
C(22)	1546(7)	2139(5)	1546(3)	36(1)	1
C(23)	2697(10)	2578(8)	728(4)	60(2)	1
C(24)	420(6)	1702(5)	3500(4)	36(1)	1
C(25)	576(9)	1692(8)	4496(4)	61(2)	1
C(30)	-3534(10)	4024(7)	1019(6)	65(2)	1
Cl(1)	-4659(3)	5414(2)	1268(1)	64(1)	1
Cl(2)	-1612(3)	4119(3)	464(2)	88(1)	1

Table 3. Bond lengths [Å] and angles [°] for 5.

Pt-C(1)	2.031(5)	Pt-C(13)	2.105(2)
Pt-P(2)	2.2872(14)	Pt-P(1)	2.2999(14)
Fe-C(5)	2.033(6)	Fe-C(6)	2.034(5)
Fe-C(4)	2.040(6)	Fe-C(3)	2.058(5)
Fe-C(7)	2.081(4)	P(1)-C(16)	1.818(5)
P(1)-C(18)	1.819(5)	P(1)-C(14)	1.833(5)
P(2)-C(22)	1.816(5)	P(2)-C(20)	1.824(6)
P(2)-C(24)	1.830(5)	C(1)-C(2)	1.203(7)
C(2)-C(7)	1.439(7)	C(3)-C(4)	1.412(8)
C(3)-C(7)	1.435(7)	C(4)-C(5)	1.397(10)
C(5)-C(6)	1.425(8)	C(6)-C(7)	1.428(8)
C(14)-C(15)	1.534(8)	C(16)-C(17)	1.519(9)
C(18)-C(19)	1.524(8)	C(20)-C(21)	1.517(9)
C(22)-C(23)	1.511(9)	C(24)-C(25)	1.511(8)
C(30)-Cl(2)	1.750(8)	C(30)-Cl(1)	1.751(8)

C(1)-Pt-C(13)	174.4(2)	C(1)-Pt-P(2)	93.25(14)
C(13)-Pt-P(2)	87.56(10)	C(1)-Pt-P(1)	88.74(14)
C(13)-Pt-P(1)	90.67(10)	P(2)-Pt-P(1)	176.99(4)
C(5)-Fe-C(5)#1	180.0	C(5)-Fe-C(6)#1	139.0(2)
C(5)#1-Fe-C(6)#1	41.0(2)	C(5)-Fe-C(6)	41.0(2)
C(5)#1-Fe-C(6)	139.0(2)	C(6)#1-Fe-C(6)	180.0
C(5)-Fe-C(4)#1	139.9(3)	C(5)#1-Fe-C(4)#1	40.1(3)
C(6)#1-Fe-C(4)#1	68.3(3)	C(6)-Fe-C(4)#1	111.7(3)
C(5)-Fe-C(4)	40.1(3)	C(5)#1-Fe-C(4)	139.9(3)
C(6)#1-Fe-C(4)	111.7(3)	C(6)-Fe-C(4)	68.3(3)
C(4)#1-Fe-C(4)	180.0	C(5)-Fe-C(3)	67.7(3)
C(5)#1-Fe-C(3)	112.3(3)	C(6)#1-Fe-C(3)	112.0(2)
C(6)-Fe-C(3)	68.0(2)	C(4)#1-Fe-C(3)	139.7(2)
C(4)-Fe-C(3)	40.3(2)	C(5)-Fe-C(3)#1	112.3(3)
C(5)#1-Fe-C(3)#1	67.7(3)	C(6)#1-Fe-C(3)#1	68.0(2)
C(6)-Fe-C(3)#1	112.0(2)	C(4)#1-Fe-C(3)#1	40.3(2)
C(4)-Fe-C(3)#1	139.7(2)	C(3)-Fe-C(3)#1	180.0
C(5)-Fe-C(7)#1	111.6(2)	C(5)#1-Fe-C(7)#1	68.4(2)
C(6)#1-Fe-C(7)#1	40.6(2)	C(6)-Fe-C(7)#1	139.4(2)
C(4)#1-Fe-C(7)#1	68.3(2)	C(4)-Fe-C(7)#1	111.7(2)
C(3)-Fe-C(7)#1	139.5(2)	C(3)#1-Fe-C(7)#1	40.5(2)
C(5)-Fe-C(7)	68.4(2)	C(5)#1-Fe-C(7)	111.6(2)
C(6)#1-Fe-C(7)	139.4(2)	C(6)-Fe-C(7)	40.6(2)
C(4)#1-Fe-C(7)	111.7(2)	C(4)-Fe-C(7)	68.3(2)
C(3)-Fe-C(7)	40.5(2)	C(3)#1-Fe-C(7)	139.5(2)
C(7)#1-Fe-C(7)	180.0	C(16)-P(1)-C(18)	103.9(3)
C(16)-P(1)-C(14)	105.4(3)	C(18)-P(1)-C(14)	106.0(3)
C(16)-P(1)-Pt	112.9(2)	C(18)-P(1)-Pt	112.0(2)
C(14)-P(1)-Pt	115.7(2)	C(22)-P(2)-C(20)	104.8(3)
C(22)-P(2)-C(24)	103.3(3)	C(20)-P(2)-C(24)	105.3(3)
C(22)-P(2)-Pt	113.4(2)	C(20)-P(2)-Pt	115.0(2)
C(24)-P(2)-Pt	114.0(2)	C(2)-C(1)-Pt	173.0(4)
C(1)-C(2)-C(7)	175.8(6)	C(4)-C(3)-C(7)	108.7(5)
C(4)-C(3)-Fe	69.1(3)	C(7)-C(3)-Fe	70.6(3)
C(5)-C(4)-C(3)	108.4(5)	C(5)-C(4)-Fe	69.7(3)
C(3)-C(4)-Fe	70.6(3)	C(4)-C(5)-C(6)	108.2(5)
C(4)-C(5)-Fe	70.2(4)	C(6)-C(5)-Fe	69.6(3)
C(5)-C(6)-C(7)	108.4(6)	C(5)-C(6)-Fe	69.4(3)
C(7)-C(6)-Fe	71.5(3)	C(6)-C(7)-C(3)	106.2(5)
C(6)-C(7)-C(2)	128.6(5)	C(3)-C(7)-C(2)	125.2(5)
C(6)-C(7)-Fe	67.9(3)	C(3)-C(7)-Fe	68.9(3)
C(2)-C(7)-Fe	127.4(3)	C(12)-C(13)-Pt	117.9(2)

C(17)-C(16)-P(1)	111.9(4)	C(19)-C(18)-P(1)	112.0(4)
C(21)-C(20)-P(2)	115.9(5)	C(23)-C(22)-P(2)	113.8(5)
C(25)-C(24)-P(2)	113.2(5)	Cl(2)-C(30)-Cl(1)	113.0(5)

Symmetry transformations used to generate equivalent atoms:

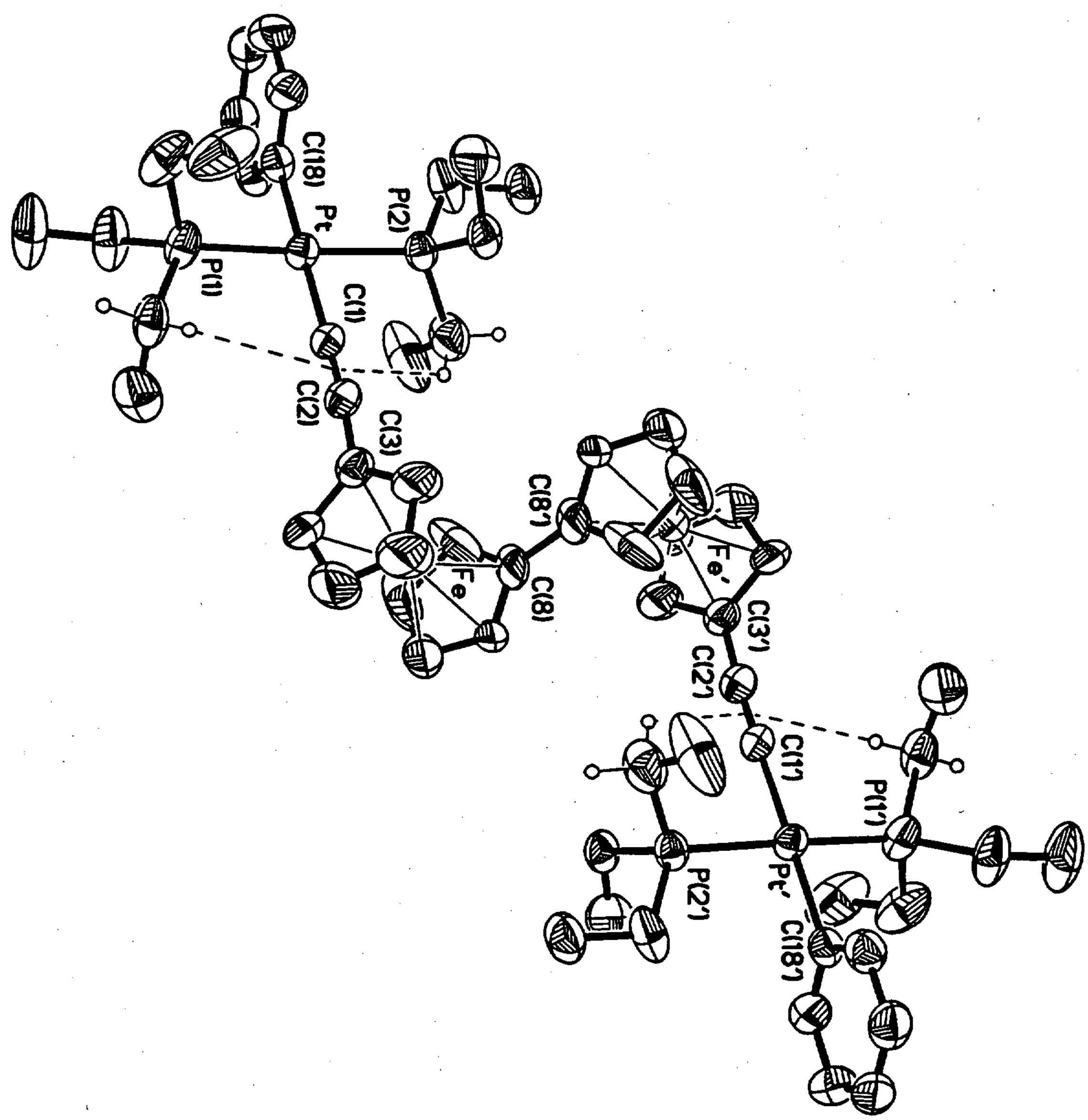
#1 -x+1,-y+1,-z+1

Table 4. Anisotropic displacement parameters [$Å^2 \times 10^3$] for 5.
The anisotropic displacement factor exponent takes the form:
$-2\pi^2$ [$(ha^*)^2U_{11}$ + ... + $2hka^*b^*U_{12}$]

	U11	U22	U33	U23	U13	U12
Pt	22(1)	21(1)	22(1)	-4(1)	-5(1)	-1(1)
Fe	24(1)	26(1)	35(1)	-12(1)	-8(1)	1(1)
P(1)	24(1)	24(1)	27(1)	-4(1)	-7(1)	0(1)
P(2)	22(1)	24(1)	26(1)	-4(1)	-5(1)	0(1)
C(1)	24(2)	28(2)	28(2)	-5(2)	-6(2)	-5(2)
C(2)	25(2)	27(2)	33(2)	-6(2)	-5(2)	-4(2)
C(3)	33(2)	33(3)	43(3)	-11(2)	-17(2)	3(2)
C(4)	34(3)	52(4)	59(3)	-28(3)	-21(3)	4(3)
C(5)	29(2)	43(3)	64(4)	-25(3)	-1(2)	-9(2)
C(6)	37(3)	33(3)	42(3)	-7(2)	0(2)	-8(2)
C(7)	23(2)	31(2)	33(2)	-12(2)	-3(2)	2(2)
C(8)	44(3)	30(3)	32(2)	-5(2)	-13(2)	-5(2)
C(9)	50(3)	38(3)	42(3)	-15(2)	-23(2)	-1(3)
C(10)	40(3)	31(3)	67(4)	-11(3)	-21(3)	-8(2)
C(11)	43(3)	41(3)	52(3)	-4(3)	-5(3)	-15(3)
C(12)	36(3)	34(3)	37(2)	-6(2)	-8(2)	-6(2)
C(13)	25(2)	22(2)	30(2)	-5(2)	-7(2)	2(2)
C(14)	33(3)	28(3)	53(3)	-14(2)	-16(2)	7(2)
C(15)	43(3)	35(3)	76(4)	-19(3)	-18(3)	13(3)
C(16)	38(3)	42(3)	35(2)	1(2)	-14(2)	2(2)
C(17)	66(4)	57(4)	39(3)	14(3)	-11(3)	-7(4)
C(18)	24(2)	40(3)	40(3)	-3(2)	-3(2)	-8(2)
C(19)	49(4)	89(6)	38(3)	13(3)	2(3)	-6(4)
C(20)	36(3)	33(3)	54(3)	-12(2)	-11(2)	1(2)
C(21)	39(3)	34(3)	98(6)	-5(3)	-12(4)	2(3)
C(22)	39(3)	39(3)	33(2)	-1(2)	-16(2)	1(2)
C(23)	75(5)	65(5)	32(3)	6(3)	-6(3)	1(4)
C(24)	28(2)	37(3)	39(2)	1(2)	-1(2)	1(2)
C(25)	58(4)	85(6)	28(3)	5(3)	4(3)	2(4)
C(30)	67(5)	45(4)	67(4)	-3(3)	5(4)	2(4)
Cl(1)	68(1)	50(1)	68(1)	-5(1)	-9(1)	2(1)
Cl(2)	58(1)	83(2)	114(2)	2(2)	-12(1)	2(1)

Table 5. Hydrogen coordinates (x 10^4), isotropic displacement parameters ($Å^2$ x 10^3) and site occupancy factors for ~~1~~5.

	x	y	z	U(eq)	sof
H(3A)	6673(6)	2854(5)	5184(4)	43	1
H(4A)	7554(7)	4671(6)	5655(5)	56	1
H(5A)	7386(6)	6227(6)	4433(5)	55	1
H(6A)	6329(7)	5404(5)	3199(4)	46	1
H(8A)	3975(4)	-339(3)	883(2)	42	1
H(9A)	3012(7)	-2014(5)	553(2)	50	1
H(10A)	1789(7)	-3159(4)	1771(4)	53	1
H(11A)	1529(7)	-2628(4)	3319(3)	55	1
H(12A)	2492(6)	-953(5)	3648(2)	43	1
H(14A)	5946(6)	-2198(5)	2437(4)	45	1
H(14B)	6519(6)	-1668(5)	1428(4)	45	1
H(15A)	8236(8)	-3342(6)	1643(5)	78	1
H(15B)	8524(8)	-2745(6)	2525(5)	78	1
H(15C)	9098(8)	-2214(6)	1512(5)	78	1
H(16A)	8048(7)	-1105(6)	3609(4)	46	1
H(16B)	7081(7)	133(6)	3980(4)	46	1
H(17A)	6097(9)	-1398(7)	4942(4)	82	1
H(17B)	5801(9)	-2009(7)	4069(4)	82	1
H(17C)	4835(9)	-771(7)	4440(4)	82	1
H(18A)	8340(6)	1052(5)	2185(4)	42	1
H(18B)	9209(6)	-235(5)	1871(4)	42	1
H(19A)	9059(9)	937(8)	543(4)	92	1
H(19B)	7242(9)	1157(8)	885(4)	92	1
H(19C)	8110(9)	-129(8)	571(4)	92	1
H(20A)	2261(7)	3750(5)	3516(5)	50	1
H(20B)	2955(7)	3970(5)	2441(5)	50	1
H(21A)	744(8)	5323(6)	2986(6)	88	1
H(21B)	-234(8)	4274(6)	3305(6)	88	1
H(21C)	461(8)	4495(6)	2227(6)	88	1
H(22A)	1413(7)	1332(5)	1412(3)	44	1
H(22B)	551(7)	2643(5)	1611(3)	44	1
H(23A)	2334(10)	2558(8)	164(4)	90	1
H(23B)	3680(10)	2072(8)	648(4)	90	1
H(23C)	2817(10)	3385(8)	847(4)	90	1
H(24A)	-495(6)	2254(5)	3454(4)	44	1
H(24B)	269(6)	908(5)	3341(4)	44	1
H(25A)	-341(9)	1458(8)	4914(4)	92	1
H(25B)	702(9)	2479(8)	4664(4)	92	1
H(25C)	1466(9)	1133(8)	4551(4)	92	1
H(30A)	-3575(10)	3579(7)	1604(6)	78	1
H(30B)	-3968(10)	3582(7)	616(6)	78	1


C(18)
Pt
P(2)
P(1)
C(1)
C(2)
C(3)
C(8')
Fe
C(8)
Fe'
C(3')
C(2')
C(1')
P(1')
P(2')
Pt'
C(18')

E

Table 1. Crystal data and structure refinement for 8.

Identification code	NL9807
Empirical formula	$C_{60}H_{86}P_4Fe_2Pt_2$
Formula weight	1433.05
Temperature	203(2) K
Diffractometer Used	Siemens P4/PC
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	$P2_1/c$
Unit cell dimensions	*a* = 9.240(3) Å alpha = 90° *b* = 9.3360(12) Å beta = 93.55(2)° *c* = 34.801(6) Å gamma = 90°
Volume, Z	2996.2(10) $Å^3$, 2
Density (calculated)	1.588 Mg/m^3
Absorption coefficient	5.271 mm^{-1}
F(000)	1428
Crystal colour/morphology	Orange prisms
Crystal size	0.60 x 0.53 x 0.53 mm
θ range for data collection	2.21 to 25.00°
Limiting indices	$0 \le h \le 10$, $0 \le k \le 11$, $-41 \le l \le 41$
Scan type	ω-scans
Reflections collected	5620
Independent reflections	5267 (R_{int} = 0.0654)
Observed reflections [$F>4\sigma(F)$]	3829
Absorption correction	Ellipsoidal
Max. and min. transmission	0.0593 and 0.0283
Structure solution method	Direct
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4819 / 0 / 296
Goodness-of-fit on F^2	1.043
Final R indices [$F>4\sigma(F)$]	R1 = 0.0523, wR2 = 0.1209
R indices (all data)	R1 = 0.0818, wR2 = 0.1396
Extinction coefficient	0.0001(2)
Largest diff. peak and hole	1.902 and -1.244 $eÅ^{-3}$
Mean and maximum shift/error	0.000 and 0.001

Table 2. Atomic coordinates [x 10^4], equivalent isotropic displacement parameters [$Å^2$ x 10^3] and site occupancy factors for 1. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)	sof
Pt	3885(1)	5118(1)	3574(1)	40(1)	1
Fe	6912(3)	1899(2)	4963(1)	91(1)	1
P(1)	5693(3)	6654(3)	3420(1)	54(1)	1
P(2)	2179(3)	3426(3)	3685(1)	44(1)	1
C(1)	5246(11)	4011(10)	3937(3)	40(2)	1
C(2)	6035(11)	3371(11)	4166(3)	44(2)	1
C(3)	7100(12)	2680(11)	4421(3)	48(2)	1
C(4)	8085(14)	3395(15)	4692(3)	62(3)	1
C(5)	8971(22)	2340(19)	4875(6)	108(7)	1
C(6)	8584(25)	990(19)	4705(6)	115(8)	1
C(7)	7417(19)	1212(15)	4436(5)	85(5)	1
C(8)	5310(32)	562(26)	5116(4)	147(12)	1
C(9)	4794(25)	2020(32)	5068(4)	139(12)	1
C(10)	5703(32)	2886(29)	5343(5)	163(15)	1
C(11)	6683(36)	2025(27)	5533(5)	178(17)	1
C(12)	6364(34)	644(24)	5408(5)	193(17)	1
C(13)	2252(9)	5929(8)	2821(2)	62(3)	1
C(14)	1272(10)	6687(9)	2580(2)	78(4)	1
C(15)	465(9)	7793(8)	2727(2)	70(4)	1
C(16)	637(8)	8141(7)	3115(2)	64(3)	1
C(17)	1616(8)	7383(8)	3357(2)	56(3)	1
C(18)	2423(7)	6277(7)	3210(2)	45(2)	1
C(19)	6123(17)	6415(19)	2920(5)	87(5)	1
C(20)	6530(25)	4878(21)	2844(5)	114(7)	1
C(21)	5270(13)	8581(13)	3451(6)	81(5)	1
C(22)	6421(16)	9604(17)	3332(7)	113(8)	1
C(23)	7451(12)	6461(13)	3684(4)	61(3)	1
C(24)	7519(16)	6993(16)	4086(5)	85(5)	1
C(25)	1926(17)	3183(17)	4190(4)	75(4)	1
C(26)	1374(23)	4531(23)	4379(7)	133(10)	1
C(27)	2732(12)	1678(10)	3528(4)	51(2)	1
C(28)	2899(18)	1592(15)	3099(4)	77(4)	1
C(29)	371(12)	3673(12)	3460(5)	69(4)	1
C(30)	-731(14)	2508(14)	3544(5)	72(4)	1

Table 3. Bond lengths [Å] and angles [°] for ~~1~~ 8.

Pt-C(1)	2.011(9)	Pt-C(18)	2.096(5)
Pt-P(2)	2.281(3)	Pt-P(1)	2.291(3)
Fe-C(5)	1.99(2)	Fe-C(10)	2.01(3)
Fe-C(11)	2.01(2)	Fe-C(9)	2.02(2)
Fe-C(6)	2.02(2)	Fe-C(7)	2.03(2)
Fe-C(12)	2.03(2)	Fe-C(8)	2.03(2)
Fe-C(4)	2.034(12)	Fe-C(3)	2.038(11)
P(1)-C(19)	1.82(2)	P(1)-C(23)	1.824(12)
P(1)-C(21)	1.845(12)	P(2)-C(25)	1.80(2)
P(2)-C(27)	1.806(10)	P(2)-C(29)	1.815(12)
C(1)-C(2)	1.206(14)	C(2)-C(3)	1.437(14)
C(3)-C(7)	1.40(2)	C(3)-C(4)	1.43(2)
C(4)-C(5)	1.41(2)	C(5)-C(6)	1.43(2)
C(6)-C(7)	1.40(2)	C(8)-C(12)	1.36(3)
C(8)-C(8)#1	1.42(3)	C(8)-C(9)	1.45(4)
C(9)-C(10)	1.47(2)	C(10)-C(11)	1.35(4)
C(11)-C(12)	1.39(3)	C(19)-C(20)	1.51(2)
C(21)-C(22)	1.51(2)	C(23)-C(24)	1.48(2)
C(25)-C(26)	1.52(2)	C(27)-C(28)	1.51(2)
C(29)-C(30)	1.53(2)		
C(1)-Pt-C(18)	178.3(4)	C(1)-Pt-P(2)	87.1(3)
C(18)-Pt-P(2)	91.9(2)	C(1)-Pt-P(1)	91.8(3)
C(18)-Pt-P(1)	89.3(2)	P(2)-Pt-P(1)	174.14(11)
C(5)-Fe-C(10)	125.7(8)	C(5)-Fe-C(11)	107.4(10)
C(10)-Fe-C(11)	39.3(13)	C(5)-Fe-C(9)	164.8(10)
C(10)-Fe-C(9)	43.0(7)	C(11)-Fe-C(9)	69.8(11)
C(5)-Fe-C(6)	41.7(8)	C(10)-Fe-C(6)	163.2(9)
C(11)-Fe-C(6)	126.3(12)	C(9)-Fe-C(6)	151.8(8)
C(5)-Fe-C(7)	69.5(8)	C(10)-Fe-C(7)	155.7(10)
C(11)-Fe-C(7)	163.0(10)	C(9)-Fe-C(7)	117.6(6)
C(6)-Fe-C(7)	40.5(6)	C(5)-Fe-C(12)	121.5(10)
C(10)-Fe-C(12)	65.6(12)	C(11)-Fe-C(12)	40.1(8)
C(9)-Fe-C(12)	66.6(12)	C(6)-Fe-C(12)	109.2(12)
C(7)-Fe-C(12)	126.2(9)	C(5)-Fe-C(8)	152.4(11)
C(10)-Fe-C(8)	70.4(9)	C(11)-Fe-C(8)	69.8(7)
C(9)-Fe-C(8)	41.9(12)	C(6)-Fe-C(8)	116.6(11)
C(7)-Fe-C(8)	104.8(8)	C(12)-Fe-C(8)	39.2(8)
C(5)-Fe-C(4)	40.9(6)	C(10)-Fe-C(4)	108.9(7)
C(11)-Fe-C(4)	120.5(6)	C(9)-Fe-C(4)	126.6(9)
C(6)-Fe-C(4)	68.8(7)	C(7)-Fe-C(4)	68.8(6)
C(12)-Fe-C(4)	156.1(6)	C(8)-Fe-C(4)	163.9(8)
C(5)-Fe-C(3)	69.3(6)	C(10)-Fe-C(3)	121.9(9)
C(11)-Fe-C(3)	155.7(8)	C(9)-Fe-C(3)	106.7(7)
C(6)-Fe-C(3)	68.2(6)	C(7)-Fe-C(3)	40.4(5)
C(12)-Fe-C(3)	162.0(5)	C(8)-Fe-C(3)	124.6(6)
C(4)-Fe-C(3)	41.2(5)	C(19)-P(1)-C(23)	103.2(7)
C(19)-P(1)-C(21)	103.6(8)	C(23)-P(1)-C(21)	104.6(6)
C(19)-P(1)-Pt	110.6(6)	C(23)-P(1)-Pt	117.4(4)
C(21)-P(1)-Pt	115.9(4)	C(25)-P(2)-C(27)	103.8(7)
C(25)-P(2)-C(29)	105.3(7)	C(27)-P(2)-C(29)	104.7(5)
C(25)-P(2)-Pt	112.6(5)	C(27)-P(2)-Pt	111.3(4)
C(29)-P(2)-Pt	117.8(5)	C(2)-C(1)-Pt	177.4(9)
C(1)-C(2)-C(3)	174.1(11)	C(7)-C(3)-C(4)	108.0(11)
C(7)-C(3)-C(2)	126.5(11)	C(4)-C(3)-C(2)	125.5(10)
C(7)-C(3)-Fe	69.4(9)	C(4)-C(3)-Fe	69.2(6)
C(2)-C(3)-Fe	129.7(8)	C(5)-C(4)-C(3)	107.4(13)
C(5)-C(4)-Fe	67.8(10)	C(3)-C(4)-Fe	69.5(7)
C(4)-C(5)-C(6)	107.9(14)	C(4)-C(5)-Fe	71.2(10)

C(6)-C(5)-Fe	70.3(14)	C(7)-C(6)-C(5)	108(2)
C(7)-C(6)-Fe	69.9(13)	C(5)-C(6)-Fe	68.0(14)
C(6)-C(7)-C(3)	108.6(14)	C(6)-C(7)-Fe	69.6(13)
C(3)-C(7)-Fe	70.3(9)	C(12)-C(8)-C(8)#1	135(4)
C(12)-C(8)-C(9)	104(2)	C(8)#1-C(8)-C(9)	121(3)
C(12)-C(8)-Fe	70.3(11)	C(8)#1-C(8)-Fe	125(2)
C(9)-C(8)-Fe	68.4(9)	C(8)-C(9)-C(10)	106(2)
C(8)-C(9)-Fe	70(2)	C(10)-C(9)-Fe	68.1(14)
C(11)-C(10)-C(9)	109(3)	C(11)-C(10)-Fe	71(2)
C(9)-C(10)-Fe	68.8(13)	C(10)-C(11)-C(12)	106(2)
C(10)-C(11)-Fe	70.2(11)	C(12)-C(11)-Fe	70.7(12)
C(8)-C(12)-C(11)	114(3)	C(8)-C(12)-Fe	70.5(8)
C(11)-C(12)-Fe	69.1(10)	C(17)-C(18)-Pt	120.1(4)
C(13)-C(18)-Pt	119.9(4)	C(20)-C(19)-P(1)	110.9(10)
C(22)-C(21)-P(1)	116.5(11)	C(24)-C(23)-P(1)	115.2(9)
C(26)-C(25)-P(2)	112.7(14)	C(28)-C(27)-P(2)	113.3(8)
C(30)-C(29)-P(2)	115.7(10)		

Symmetry transformations used to generate equivalent atoms:

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

Table 4. Anisotropic displacement parameters [$Å^2 \times 10^3$] for ~~1~~ 8.

The anisotropic displacement factor exponent takes the form:

$-2\pi^2$ [$(ha^*)^2U_{11}$ + ... + $2hka^*b^*U_{12}$]

	U11	U22	U33	U23	U13	U12
Pt	36(1)	37(1)	48(1)	4(1)	3(1)	4(1)
Fe	144(2)	73(1)	51(1)	28(1)	-38(1)	-63(1)
P(1)	40(1)	47(1)	76(2)	17(1)	12(1)	4(1)
P(2)	38(1)	37(1)	56(2)	-2(1)	4(1)	0(1)
C(1)	44(5)	36(4)	40(5)	3(4)	6(4)	1(4)
C(2)	43(5)	47(5)	44(5)	3(4)	11(4)	0(4)
C(3)	48(6)	44(5)	52(6)	7(4)	1(5)	3(4)
C(4)	67(7)	69(7)	50(6)	22(6)	-5(6)	-13(6)
C(5)	112(14)	80(10)	122(15)	21(10)	-65(13)	-10(10)
C(6)	151(19)	67(9)	117(15)	15(10)	-61(14)	12(11)
C(7)	112(13)	55(7)	82(10)	12(7)	-38(9)	14(8)
C(8)	246(27)	147(17)	46(7)	28(10)	-10(11)	-160(20)
C(9)	140(18)	234(29)	44(9)	-26(12)	16(10)	-141(20)
C(10)	254(32)	187(24)	53(10)	-37(13)	49(15)	-180(25)
C(11)	320(41)	163(21)	44(9)	29(11)	-42(15)	-173(26)
C(12)	338(37)	155(18)	70(10)	70(11)	-109(17)	-191(23)
C(13)	72(8)	53(6)	58(7)	2(5)	-4(6)	2(5)
C(14)	102(12)	71(8)	58(8)	10(7)	-19(8)	-1(8)
C(15)	57(7)	60(7)	90(10)	19(7)	-24(7)	-6(6)
C(16)	50(6)	53(6)	88(9)	8(6)	-4(6)	3(5)
C(17)	47(6)	55(6)	66(7)	-1(5)	0(5)	-4(5)
C(18)	38(5)	39(5)	58(6)	-1(4)	1(4)	-1(4)
C(19)	68(9)	108(12)	89(11)	43(10)	29(8)	9(8)
C(20)	177(21)	107(14)	62(8)	11(10)	48(11)	48(14)
C(21)	42(6)	41(6)	160(16)	26(8)	-1(8)	8(5)
C(22)	56(8)	65(9)	218(24)	45(12)	4(11)	-15(7)
C(23)	38(5)	55(6)	92(9)	15(6)	15(6)	-7(5)
C(24)	57(8)	72(9)	123(14)	4(9)	-22(9)	8(7)
C(25)	74(9)	84(9)	70(9)	-9(7)	21(7)	-29(7)
C(26)	126(16)	140(18)	139(18)	-81(15)	68(14)	-77(15)
C(27)	51(6)	33(5)	70(7)	-3(4)	1(5)	4(4)
C(28)	97(11)	56(7)	78(9)	-13(7)	-2(8)	16(7)
C(29)	40(6)	42(5)	122(12)	-19(6)	-4(7)	0(5)
C(30)	49(7)	62(7)	105(11)	3(7)	-7(7)	-14(5)

Table 5. Hydrogen coordinates (x 10^4), isotropic displacement parameters ($Å^2$ x 10^3) and site occupancy factors for ~~1~~. 8

	x	y	z	U(eq)	sof
H(4A)	8112(14)	4435(15)	4748(3)	74	1
H(5A)	9755(22)	2510(19)	5077(6)	129	1
H(6A)	9037(25)	56(19)	4774(6)	138	1
H(7A)	6898(19)	458(15)	4282(5)	102	1
H(9A)	3989(25)	2361(32)	4890(4)	167	1
H(10A)	5628(32)	3935(29)	5377(5)	196	1
H(11A)	7433(36)	2314(27)	5733(5)	213	1
H(12A)	6948(34)	-196(24)	5496(5)	231	1
H(13A)	2798(9)	5181(8)	2722(2)	74	1
H(14A)	1156(15)	6452(13)	2317(2)	94	1
H(15A)	-197(12)	8306(12)	2564(3)	84	1
H(16A)	90(11)	8889(10)	3215(3)	77	1
H(17A)	1732(12)	7618(11)	3620(2)	67	1
H(19A)	5281(17)	6683(19)	2750(5)	105	1
H(19B)	6930(17)	7045(19)	2863(5)	105	1
H(20A)	6754(25)	4775(21)	2576(5)	171	1
H(20B)	5726(25)	4255(21)	2896(5)	171	1
H(20C)	7373(25)	4617(21)	3009(5)	171	1
H(21A)	4382(13)	8766(13)	3290(6)	98	1
H(21B)	5062(13)	8799(13)	3718(6)	98	1
H(22A)	6086(16)	10581(17)	3360(7)	170	1
H(22B)	6619(16)	9429(17)	3066(7)	170	1
H(22C)	7301(16)	9461(17)	3495(7)	170	1
H(23A)	7717(12)	5445(13)	3687(4)	73	1
H(23B)	8178(12)	6974(13)	3543(4)	73	1
H(24A)	8488(16)	6848(16)	4203(5)	128	1
H(24B)	6825(16)	6474(16)	4231(5)	128	1
H(24C)	7287(16)	8007(16)	4087(5)	128	1
H(25A)	1231(17)	2405(17)	4221(4)	90	1
H(25B)	2850(17)	2900(17)	4321(4)	90	1
H(26A)	1256(23)	4345(23)	4650(7)	199	1
H(26B)	448(23)	4806(23)	4254(7)	199	1
H(26C)	2067(23)	5301(23)	4355(7)	199	1
H(27A)	3659(12)	1427(10)	3663(4)	61	1
H(27B)	2012(12)	970(10)	3598(4)	61	1
H(28A)	3196(18)	632(15)	3032(4)	116	1
H(28B)	3627(18)	2274(15)	3028(4)	116	1
H(28C)	1980(18)	1816(15)	2963(4)	116	1
H(29A)	-4(12)	4595(12)	3545(5)	82	1
H(29B)	445(12)	3729(12)	3181(5)	82	1
H(30A)	-1658(14)	2735(14)	3412(5)	108	1
H(30B)	-842(14)	2460(14)	3819(5)	108	1
H(30C)	-392(14)	1592(14)	3454(5)	108	1