

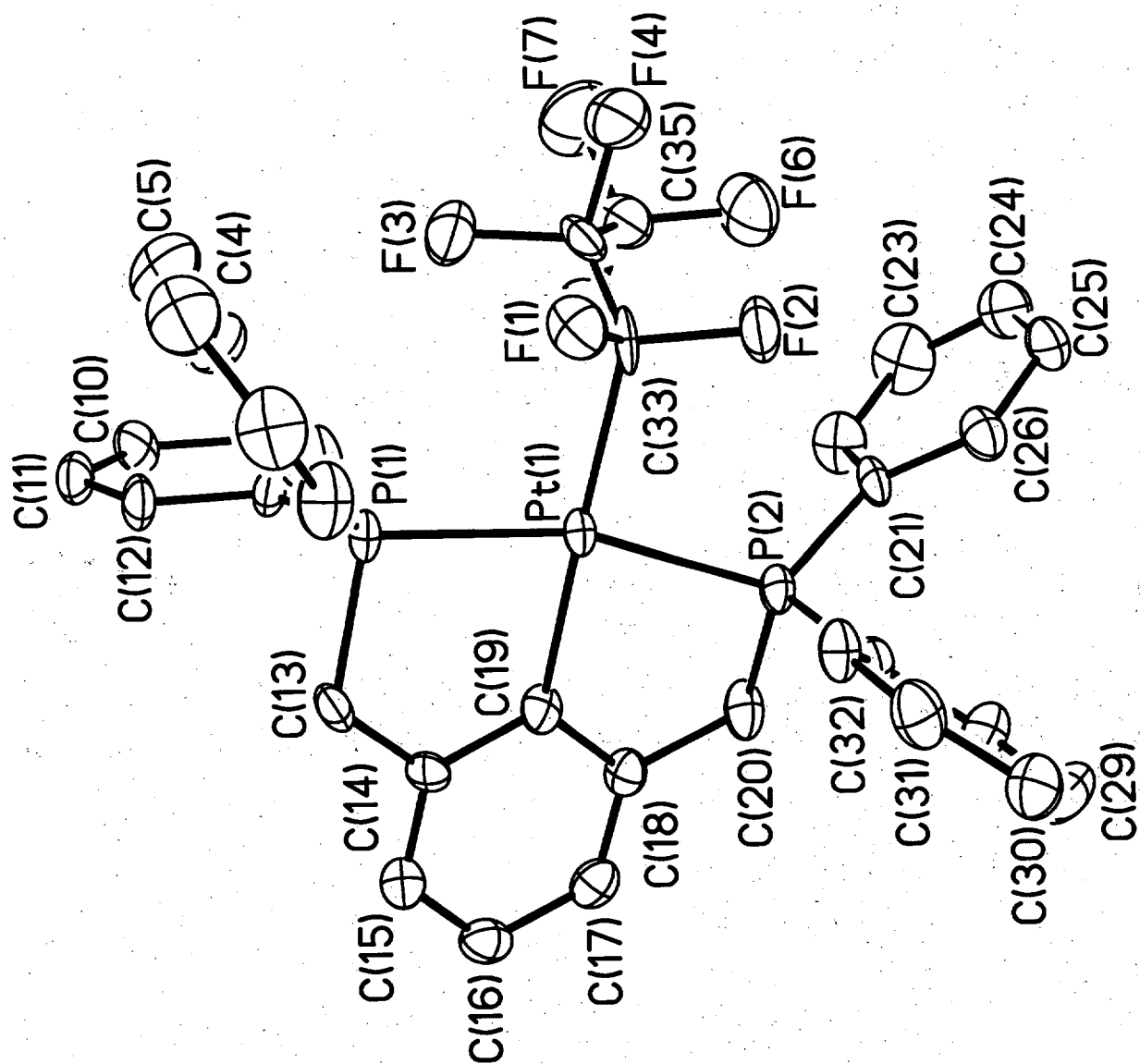


Table 1. Crystal data and structure refinement for 6.

Identification code	rph146
Empirical formula	C ₃₅ H ₂₇ F ₇ P ₂ Pt
Formula weight	837.60
Temperature	251(2) K
Wavelength	0.71073 Å
Crystal system, space group	Monoclinic, P2(1)/c
Unit cell dimensions	a = 10.192(3) Å alpha = 90 deg. b = 18.106(8) Å beta = 91.008(17) deg. c = 17.018(3) Å gamma = 90 deg.
Volume	3140.0(17) Å ³
Z, Calculated density	4, 1.772 Mg/m ³
Absorption coefficient	4.637 mm ⁻¹
F(000)	1632
Crystal size	0.50 x 0.40 x 0.30 mm
Theta range for data collection	2.25 to 23.99 deg.
Limiting indices	-11 ≤ h ≤ 11, 0 ≤ k ≤ 20, 0 ≤ l ≤ 19
Reflections collected / unique	5671 / 4569 [R(int) = 0.0585]
Completeness to theta = 23.99	92.7 %
Absorption correction	DIFABS
Max. and min. transmission	1.00 and 0.580
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	4569 / 0 / 406
Goodness-of-fit on F ²	1.036
Final R indices [I > 2sigma(I)]	R1 = 0.0395, wR2 = 0.1003
R indices (all data)	R1 = 0.0517, wR2 = 0.1074
Largest diff. peak and hole	0.932 and -0.943 e.Å ⁻³

Table 2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 6.
 $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Pt(1)	2892(1)	8291(1)	7282(1)	32(1)
P(1)	4314(2)	8327(1)	8332(1)	36(1)
P(2)	1033(2)	8321(1)	6521(1)	38(1)
F(1)	4839(4)	7264(3)	6711(3)	61(1)
F(2)	3521(4)	7605(3)	5767(3)	63(1)
F(3)	6089(5)	8572(4)	6712(3)	77(2)
F(4)	6001(5)	7956(4)	5585(3)	84(2)
F(5)	4224(7)	9479(4)	6115(4)	94(2)
F(6)	4166(6)	8883(4)	5031(3)	92(2)
F(7)	5970(7)	9387(5)	5433(4)	129(3)
C(1)	5598(7)	7638(4)	8439(4)	39(2)
C(2)	5224(9)	6915(5)	8547(6)	63(2)
C(3)	6204(11)	6374(5)	8582(6)	71(3)
C(4)	7498(11)	6546(6)	8534(7)	82(3)
C(5)	7846(9)	7252(6)	8395(6)	73(3)
C(6)	6899(8)	7798(5)	8355(5)	61(2)
C(7)	5085(6)	9209(4)	8533(4)	39(2)
C(8)	4810(9)	9811(5)	8065(5)	63(2)
C(9)	5347(11)	10493(5)	8249(5)	78(3)
C(10)	6123(8)	10575(5)	8901(5)	59(2)
C(11)	6393(7)	9993(5)	9379(5)	51(2)
C(12)	5884(7)	9307(5)	9208(4)	49(2)
C(13)	3220(7)	8213(4)	9149(4)	42(2)
C(14)	1921(7)	8579(4)	8933(4)	37(2)
C(15)	1073(8)	8827(5)	9484(5)	52(2)
C(16)	-137(8)	9122(5)	9282(5)	51(2)
C(17)	-496(7)	9167(4)	8495(5)	48(2)
C(18)	342(7)	8924(4)	7919(4)	40(2)
C(19)	1593(6)	8630(4)	8133(4)	38(2)
C(20)	-26(7)	8964(5)	7054(4)	50(2)
C(21)	1069(7)	8652(4)	5506(4)	40(2)
C(22)	1356(9)	9378(5)	5356(6)	66(2)
C(23)	1485(10)	9626(6)	4592(6)	81(3)
C(24)	1342(9)	9150(7)	3977(6)	72(3)
C(25)	1058(8)	8432(6)	4112(5)	60(2)
C(26)	901(8)	8175(5)	4876(5)	52(2)
C(27)	184(7)	7446(4)	6496(4)	43(2)
C(28)	-1108(7)	7383(5)	6228(5)	57(2)
C(29)	-1745(9)	6710(5)	6231(7)	71(3)
C(30)	-1092(9)	6083(6)	6492(5)	65(2)
C(31)	180(9)	6138(5)	6756(5)	62(2)
C(32)	826(8)	6816(4)	6756(5)	46(2)
C(33)	4230(7)	7875(4)	6395(4)	41(2)
C(34)	5213(8)	8320(5)	6118(4)	57(3)
C(35)	4885(10)	9048(6)	5682(6)	71(3)

Table 3. Bond lengths [Å] and angles [deg] for 6.

Pt(1)-C(19)	2.072(7)
Pt(1)-C(33)	2.186(8)
Pt(1)-P(2)	2.2770(18)
Pt(1)-P(1)	2.2818(18)
P(1)-C(13)	1.810(8)
P(1)-C(7)	1.811(7)
P(1)-C(1)	1.814(7)
P(2)-C(27)	1.805(8)
P(2)-C(21)	1.829(7)
P(2)-C(20)	1.839(8)
F(1)-C(33)	1.374(8)
F(2)-C(33)	1.370(7)
F(3)-C(34)	1.412(9)
F(4)-C(34)	1.388(9)
F(5)-C(35)	1.274(11)
F(6)-C(35)	1.351(11)
F(7)-C(35)	1.340(11)
C(1)-C(6)	1.367(10)
C(1)-C(2)	1.377(12)
C(2)-C(3)	1.399(13)
C(3)-C(4)	1.359(14)
C(4)-C(5)	1.348(15)
C(5)-C(6)	1.381(12)
C(7)-C(8)	1.377(11)
C(7)-C(12)	1.406(9)
C(8)-C(9)	1.384(12)
C(9)-C(10)	1.361(12)
C(10)-C(11)	1.356(12)
C(11)-C(12)	1.375(11)
C(13)-C(14)	1.520(10)
C(14)-C(15)	1.363(10)
C(14)-C(19)	1.399(9)
C(15)-C(16)	1.382(11)
C(16)-C(17)	1.386(11)
C(17)-C(18)	1.383(10)
C(18)-C(19)	1.423(9)
C(18)-C(20)	1.515(10)
C(21)-C(22)	1.372(11)
C(21)-C(26)	1.385(10)
C(22)-C(23)	1.385(13)
C(23)-C(24)	1.362(14)
C(24)-C(25)	1.351(14)
C(25)-C(26)	1.393(12)
C(27)-C(32)	1.383(10)
C(27)-C(28)	1.391(10)
C(28)-C(29)	1.381(12)
C(29)-C(30)	1.386(13)
C(30)-C(31)	1.369(11)
C(31)-C(32)	1.394(11)
C(33)-C(34)	1.376(12)
C(34)-C(35)	1.547(13)

C(19)-Pt(1)-C(33)	177.1(3)
C(19)-Pt(1)-P(2)	81.67(19)
C(33)-Pt(1)-P(2)	97.96(16)
C(19)-Pt(1)-P(1)	81.35(19)
C(33)-Pt(1)-P(1)	98.89(16)
P(2)-Pt(1)-P(1)	162.89(8)
C(13)-P(1)-C(7)	103.1(3)
C(13)-P(1)-C(1)	107.3(3)
C(7)-P(1)-C(1)	106.1(3)
C(13)-P(1)-Pt(1)	101.9(2)
C(7)-P(1)-Pt(1)	116.2(2)
C(1)-P(1)-Pt(1)	120.5(2)
C(27)-P(2)-C(21)	106.5(3)
C(27)-P(2)-C(20)	106.4(4)
C(21)-P(2)-C(20)	106.3(3)
C(27)-P(2)-Pt(1)	112.7(2)
C(21)-P(2)-Pt(1)	121.0(2)
C(20)-P(2)-Pt(1)	102.9(2)
C(6)-C(1)-C(2)	119.1(7)
C(6)-C(1)-P(1)	122.9(6)
C(2)-C(1)-P(1)	117.8(6)
C(1)-C(2)-C(3)	118.2(9)
C(4)-C(3)-C(2)	122.0(10)
C(5)-C(4)-C(3)	119.1(9)
C(4)-C(5)-C(6)	120.1(9)
C(1)-C(6)-C(5)	121.4(9)
C(8)-C(7)-C(12)	118.8(7)
C(8)-C(7)-P(1)	120.4(5)
C(12)-C(7)-P(1)	120.6(6)
C(7)-C(8)-C(9)	119.9(7)
C(10)-C(9)-C(8)	120.3(9)
C(11)-C(10)-C(9)	120.9(8)
C(10)-C(11)-C(12)	120.2(7)
C(11)-C(12)-C(7)	119.8(7)
C(14)-C(13)-P(1)	108.1(5)
C(15)-C(14)-C(19)	120.3(7)
C(15)-C(14)-C(13)	122.5(6)
C(19)-C(14)-C(13)	117.2(6)
C(14)-C(15)-C(16)	122.0(7)
C(15)-C(16)-C(17)	118.9(7)
C(16)-C(17)-C(18)	120.7(7)
C(17)-C(18)-C(19)	120.0(7)
C(17)-C(18)-C(20)	121.8(6)
C(19)-C(18)-C(20)	118.2(6)
C(14)-C(19)-C(18)	118.1(6)
C(14)-C(19)-Pt(1)	121.0(5)
C(18)-C(19)-Pt(1)	120.9(5)
C(18)-C(20)-P(2)	108.2(5)
C(22)-C(21)-C(26)	118.5(8)
C(22)-C(21)-P(2)	119.8(6)
C(26)-C(21)-P(2)	121.5(6)
C(21)-C(22)-C(23)	120.6(9)
C(24)-C(23)-C(22)	120.4(10)
C(25)-C(24)-C(23)	119.9(9)
C(24)-C(25)-C(26)	120.6(9)
C(21)-C(26)-C(25)	119.9(8)
C(32)-C(27)-C(28)	118.6(7)

C(32)-C(27)-P(2)	119.5(5)
C(28)-C(27)-P(2)	121.9(6)
C(29)-C(28)-C(27)	120.8(8)
C(28)-C(29)-C(30)	120.1(9)
C(31)-C(30)-C(29)	119.5(9)
C(30)-C(31)-C(32)	120.6(8)
C(27)-C(32)-C(31)	120.4(7)
F(2)-C(33)-F(1)	104.2(6)
F(2)-C(33)-C(34)	108.6(7)
F(1)-C(33)-C(34)	106.2(6)
F(2)-C(33)-Pt(1)	109.6(5)
F(1)-C(33)-Pt(1)	106.9(5)
C(34)-C(33)-Pt(1)	120.2(5)
C(33)-C(34)-F(4)	112.3(8)
C(33)-C(34)-F(3)	113.5(6)
F(4)-C(34)-F(3)	104.8(6)
C(33)-C(34)-C(35)	120.7(7)
F(4)-C(34)-C(35)	102.3(7)
F(3)-C(34)-C(35)	101.3(8)
F(5)-C(35)-F(7)	110.5(10)
F(5)-C(35)-F(6)	108.9(9)
F(7)-C(35)-F(6)	106.3(8)
F(5)-C(35)-C(34)	110.9(8)
F(7)-C(35)-C(34)	111.7(9)
F(6)-C(35)-C(34)	108.4(8)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 6.
 The anisotropic displacement factor exponent takes the form:
 $-2 \pi^2 [h^2 a^{*2} U_{11} + \dots + 2 h k a^* b^* U_{12}]$

	U11	U22	U33	U23	U13	U12
Pt(1)	35(1)	35(1)	26(1)	-2(1)	-11(1)	1(1)
P(1)	39(1)	38(1)	29(1)	-1(1)	-13(1)	-1(1)
P(2)	39(1)	40(1)	35(1)	-2(1)	-15(1)	5(1)
F(1)	69(3)	56(3)	56(3)	4(2)	-5(2)	23(2)
F(2)	65(3)	77(4)	47(3)	-21(3)	-18(2)	2(3)
F(3)	55(3)	112(4)	65(3)	6(3)	-14(2)	-13(3)
F(4)	59(3)	127(5)	66(4)	8(4)	5(3)	30(3)
F(5)	142(5)	64(4)	75(4)	2(3)	15(4)	-7(4)
F(6)	100(4)	110(5)	66(4)	16(3)	-14(3)	11(4)
F(7)	108(5)	149(7)	131(6)	46(6)	16(4)	-50(5)
C(1)	50(4)	38(4)	29(4)	-6(3)	-17(3)	5(3)
C(2)	77(6)	42(5)	70(6)	0(5)	-19(5)	-2(4)
C(3)	99(8)	41(5)	74(7)	5(5)	-14(6)	14(5)
C(4)	82(8)	70(8)	94(9)	4(6)	-5(6)	32(6)
C(5)	57(5)	61(7)	102(8)	19(6)	-3(5)	17(5)
C(6)	46(5)	59(6)	78(6)	4(5)	-8(4)	4(4)
C(7)	36(4)	45(4)	34(4)	-4(4)	-8(3)	-2(3)
C(8)	100(7)	45(5)	42(5)	2(4)	-35(5)	-15(5)
C(9)	130(9)	48(6)	56(6)	6(5)	-23(6)	-18(6)
C(10)	69(5)	56(6)	51(5)	-13(5)	-8(4)	-20(4)
C(11)	47(4)	57(6)	49(5)	-13(4)	-16(4)	-3(4)
C(12)	46(4)	60(5)	40(4)	1(4)	-18(4)	-1(4)
C(13)	50(4)	45(5)	29(4)	0(3)	-12(3)	-8(3)
C(14)	44(4)	36(4)	31(4)	5(3)	-1(3)	-12(3)
C(15)	55(5)	66(6)	36(4)	-2(4)	-4(4)	-4(4)
C(16)	54(5)	52(5)	46(5)	-5(4)	14(4)	-7(4)
C(17)	43(4)	41(5)	61(6)	2(4)	0(4)	-2(3)
C(18)	48(4)	36(4)	34(4)	5(3)	-3(3)	-2(3)
C(19)	36(4)	37(4)	40(4)	-4(4)	0(3)	-1(3)
C(20)	50(4)	53(5)	47(5)	-5(4)	-17(4)	11(4)
C(21)	43(4)	46(5)	31(4)	-1(3)	-12(3)	9(3)
C(22)	78(6)	53(6)	66(6)	13(5)	-12(5)	-4(5)
C(23)	102(8)	70(7)	71(7)	32(6)	-11(6)	3(6)
C(24)	64(6)	103(9)	48(6)	22(6)	-11(5)	9(6)
C(25)	62(5)	82(7)	37(5)	0(5)	-14(4)	-1(5)
C(26)	59(5)	57(5)	40(5)	-5(4)	-13(4)	10(4)
C(27)	43(4)	48(5)	37(4)	-3(4)	-12(3)	0(3)
C(28)	44(4)	60(6)	66(6)	-2(5)	-15(4)	0(4)
C(29)	41(5)	77(8)	97(8)	-12(6)	0(5)	-11(5)
C(30)	71(6)	61(6)	64(6)	-11(5)	-1(5)	-17(5)
C(31)	85(6)	49(5)	50(5)	-8(4)	-7(5)	-2(5)
C(32)	50(4)	44(5)	44(5)	0(4)	-15(4)	-2(4)
C(33)	54(4)	32(4)	36(4)	-1(3)	-36(4)	5(3)
C(34)	58(5)	90(7)	24(4)	-7(4)	-6(4)	33(5)
C(35)	77(6)	76(7)	60(6)	-6(6)	8(6)	-8(6)

Table 5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for 6.

	x	y	z	U(eq)
H(2A)	4335	6788	8596	76
H(3A)	5960	5877	8640	86
H(4A)	8142	6178	8597	99
H(5A)	8733	7374	8326	88
H(6A)	7155	8289	8267	73
H(8A)	4257	9759	7620	76
H(9A)	5174	10901	7921	94
H(10A)	6477	11041	9023	71
H(11A)	6929	10058	9828	62
H(12A)	6069	8905	9540	59
H(13A)	3084	7687	9255	50
H(13B)	3599	8442	9622	50
H(15A)	1320	8797	10018	62
H(16A)	-707	9289	9673	61
H(17A)	-1319	9364	8350	58
H(20A)	97	9468	6859	60
H(20B)	-950	8828	6975	60
H(22A)	1467	9710	5777	79
H(23A)	1672	10126	4496	97
H(24A)	1441	9319	3459	86
H(25A)	966	8104	3687	73
H(26A)	681	7677	4964	62
H(28A)	-1553	7805	6042	68
H(29A)	-2622	6678	6056	86
H(30A)	-1520	5623	6487	78
H(31A)	622	5714	6940	74
H(32A)	1703	6846	6934	56