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Table 1. Crystal data and structure refinement for W(PMe3)4H2Br2.

Identification code	ged
Empirical formula	$C_{12}H_{38}Br_2P_4W$
Formula weight	649.97
Temperature	293(2) K
Wavelength	0.71073 Å
Crystal system	Orthorhombic
Space group	Cmc2(1)
Unit cell dimensions	a = 13.273(2) Å alpha = 90° b = 13.656(2) Å beta = 90° c = 12.935(3) Å gamma = 90°
Volume, Z	2344.5(7) $Å^3$, 4
Density (calculated)	1.841 Mg/m^3
Absorption coefficient	8.599 mm^{-1}
F(000)	1256
θ range for data collection	2.14 to 25.00°
Limiting indices	$0 \le h \le 15$, $0 \le k \le 16$, $0 \le l \le 15$
Reflections collected	1129
Independent reflections	1129 (R_{int} = 0.0000)
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	1129 / 2 / 110
Goodness-of-fit on F^2	1.027
Final R indices [I>2σ(I)]	R1 = 0.0372, wR2 = 0.0806
R indices (all data)	R1 = 0.0505, wR2 = 0.0852
Absolute structure parameter	-0.09(6)
Extinction coefficient	0.0001(2)
Largest diff. peak and hole	1.186 and -1.344 $eÅ^{-3}$

Table 2. Atomic coordinates [x 10^4] and equivalent isotropic displacement parameters [$Å^2$ x 10^3] for W(PMe3)4H2Br2. U(eq) is define one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
W	0	7539(1)	1	26(1)
Br(1)	0	8151(2)	1963(2)	57(1)
Br(2)	0	5812(2)	1046(3)	61(1)
P(1)	0	6251(4)	-1312(6)	36(2)
P(2)	0	9279(4)	-486(7)	37(1)
P(3)	-1868(3)	7574(3)	324(5)	44(1)
C(11)	0	6707(16)	-2642(18)	50(6)
C(12)	-1063(11)	5409(12)	-1399(18)	66(6)
C(21)	0	10219(15)	488(22)	75(9)
C(22)	-1049(11)	9670(12)	-1339(16)	61(5)
C(31)	-2734(11)	7532(14)	-804(17)	77(6)
C(32)	-2367(12)	8692(14)	1017(21)	75(6)
C(33)	-2388(14)	6611(13)	1161(24)	92(8)

Table 3. Bond lengths [Å] and angles [°] for W(PMe3)4H2Br2.

W-P(1)	2.445(7)	W-P(2)	2.458(5)
W-P(3)#1	2.515(4)	W-P(3)	2.515(4)
W-Br(1)	2.672(3)	W-Br(2)	2.718(3)
P(1)-C(12)	1.824(13)	P(1)-C(12)#1	1.824(13)
P(1)-C(11)	1.83(2)	P(2)-C(21)	1.80(2)
P(2)-C(22)#1	1.86(2)	P(2)-C(22)	1.86(2)
P(3)-C(33)	1.84(2)	P(3)-C(31)	1.86(2)
P(3)-C(32)	1.89(2)	W-H	1.7000(11)
H-W-P(1)	58(5)	H-W-P(2)	70(5)
P(1)-W-P(2)	121.2(3)	H-W-P(3)#1	125(3)
P(1)-W-P(3)#1	97.40(11)	P(2)-W-P(3)#1	91.39(10)
H-W-P(3)	74(3)	P(1)-W-P(3)	97.40(11)
P(2)-W-P(3)	91.39(10)	P(3)#1-W-P(3)	160.8(3)
H-W-Br(1)	145(4)	P(1)-W-Br(1)	152.2(2)
P(2)-W-Br(1)	86.6(2)	P(3)#1-W-Br(1)	80.58(14)
P(3)-W-Br(1)	80.58(14)	H-W-Br(2)	123(4)
P(1)-W-Br(2)	73.8(2)	P(2)-W-Br(2)	165.0(2)
P(3)#1-W-Br(2)	86.21(11)	P(3)-W-Br(2)	86.21(11)
Br(1)-W-Br(2)	78.40(10)	C(12)-P(1)-C(12)#1	101.4(11)
C(12)-P(1)-C(11)	99.0(9)	C(12)#1-P(1)-C(11)	99.0(9)
C(12)-P(1)-W	119.8(6)	C(12)#1-P(1)-W	119.8(6)
C(11)-P(1)-W	114.1(7)	C(21)-P(2)-C(22)#1	102.2(9)
C(21)-P(2)-C(22)	102.2(9)	C(22)#1-P(2)-C(22)	97.3(10)
C(21)-P(2)-W	120.7(8)	C(22)#1-P(2)-W	115.5(6)
C(22)-P(2)-W	115.5(6)	C(33)-P(3)-C(31)	102.0(10)
C(33)-P(3)-C(32)	99.6(10)	C(31)-P(3)-C(32)	100.4(8)
C(33)-P(3)-W	117.0(7)	C(31)-P(3)-W	118.6(6)
C(32)-P(3)-W	116.1(5)		

Symmetry transformations used to generate equivalent atoms:

#1 -x,y,z

Table 4. Anisotropic displacement parameters [$Å^2$ x 10^3] for W(PMe3)4H2Br2.

The anisotropic displacement factor exponent takes the form: $-2\pi^2$ [$(ha^*)^2U_{11}$ + ... + $2hka^*b^*U_{12}$]

	U11	U22	U33	U23	U13	U12
W	36(1)	23(1)	20(1)	0(1)	0	0
Br(1)	86(2)	55(1)	31(1)	-13(1)	0	0
Br(2)	102(2)	40(1)	40(2)	20(1)	0	0
P(1)	46(3)	26(3)	38(4)	-5(3)	0	0
P(2)	36(3)	30(3)	45(4)	11(3)	0	0
P(3)	46(2)	42(2)	43(3)	-5(2)	12(2)	-9(2)
C(11)	66(15)	52(13)	32(15)	2(11)	0	0
C(12)	56(11)	62(10)	81(15)	-31(12)	12(12)	-34(8)
C(21)	120(24)	28(12)	77(22)	-9(12)	0	0
C(22)	61(12)	66(10)	57(13)	48(10)	2(10)	11(8)
C(31)	25(9)	117(16)	88(15)	-45(16)	-8(8)	12(11)
C(32)	48(11)	69(11)	109(18)	-28(13)	41(14)	-7(9)
C(33)	75(14)	66(12)	137(22)	-3(14)	59(17)	-31(10)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for W(PMe3)4H2Br2.

	x	y	z	U(eq)
H(11A)	471(101)	7237(91)	-2703(39)	75
H(11B)	-662(33)	6935(125)	-2818(51)	75
H(11C)	191(135)	6189(40)	-3104(23)	75
H(12A)	-1653(25)	5761(22)	-1614(97)	99
H(12B)	-1182(61)	5117(69)	-735(28)	99
H(12C)	-914(41)	4906(56)	-1895(73)	99
H(21A)	-563(2886)	10649(2868)	380(3086)	112
H(21B)	615(2205)	10587(3136)	446(3373)	112
H(21C)	-52(5092)	9924(268)	1160(289)	112
H(22A)	-1072(59)	9256(59)	-1938(46)	92
H(22B)	-944(49)	10336(32)	-1550(81)	92
H(22C)	-1675(15)	9621(86)	-970(32)	92
H(31A)	-2598(61)	6956(47)	-1205(53)	115
H(31B)	-2632(62)	8103(45)	-1225(51)	115
H(31C)	-3419(12)	7517(87)	-565(17)	115
H(32A)	-3090(12)	8688(64)	999(110)	113
H(32B)	-2122(100)	9272(14)	682(79)	113
H(32C)	-2143(101)	8685(61)	1723(40)	113
H(33A)	-2002(85)	6576(89)	1788(62)	139
H(33B)	-2357(124)	5993(26)	809(57)	139
H(33C)	-3077(44)	6762(69)	1324(118)	139
H	-547(53)	7688(99)	-1177(29)	85(64)

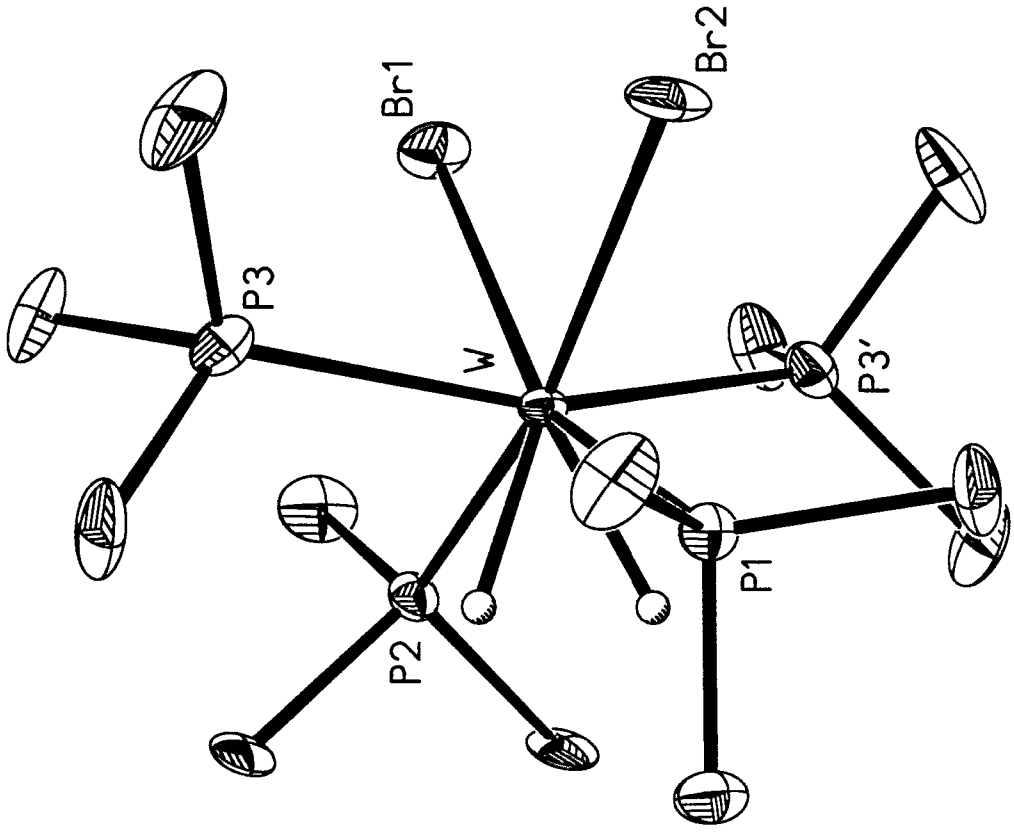

Table 1. Crystal data and structure refinement for W(PMe3)4H2Cl2.

Identification code	clshel
Empirical formula	$C_{12}H_{38}Cl_2P_4W$
Formula weight	561.05
Temperature	293(2) K
Wavelength	0.71073 Å
Crystal system	Orthorhombic
Space group	$Cmc2_1$
Unit cell dimensions	a = 13.577(2) Å alpha = 90° b = 13.395(2) Å beta = 90° c = 12.598(3) Å gamma = 90°
Volume, Z	2291.1(7) $Å^3$, 4
Density (calculated)	1.627 Mg/m^3
Absorption coefficient	5.544 mm^{-1}
F(000)	1112
Crystal size	0.2 x 0.5 x 0.5 mm
θ range for data collection	2.14 to 27.52°
Limiting indices	$-17 \le h \le 12$, $-12 \le k \le 17$, $0 \le l \le 16$
Reflections collected	2859
Independent reflections	1436 (R_{int} = 0.0366)
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	1436 / 1 / 110
Goodness-of-fit on F^2	1.060
Final R indices [I>2σ(I)]	R1 = 0.0234, wR2 = 0.0514
R indices (all data)	R1 = 0.0282, wR2 = 0.0530
Absolute structure parameter	-0.08(3)
Extinction coefficient	0.00012(7)
Largest diff. peak and hole	1.160 and -1.544 $eÅ^{-3}$

Table 2. Atomic coordinates [x 10^4] and equivalent isotropic displacement parameters [$Å^2$ x 10^3] for W(PMe3)4H2Cl2. U(eq) is define one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
W	0	7541(1)	0(1)	26(1)
Cl(1)	0	8168(2)	1884(2)	50(1)
Cl(2)	0	5904(2)	1044(3)	55(1)
P(1)	0	6205(2)	-1319(2)	34(1)
P(2)	0	9313(2)	-500(2)	32(1)
P(3)	-1819(1)	7567(1)	342(2)	40(1)
C(11)	0	6614(8)	-2680(8)	51(3)
C(12)	-1040(6)	5326(6)	-1344(7)	61(2)
C(21)	0	10277(7)	545(10)	60(3)
C(22)	-1006(5)	9760(6)	-1342(7)	57(2)
C(31)	-2672(7)	7526(7)	-763(10)	74(3)
C(32)	-2284(6)	8650(6)	1064(8)	63(2)
C(33)	-2309(7)	6575(7)	1180(9)	78(3)

Table 3. Bond lengths [Å] and angles [°] for W(PMe3)4H2Cl2.

W-P(1)	2.443(3)	W-P(2)	2.456(2)
W-P(3)	2.507(2)	W-P(3)#1	2.507(2)
W-Cl(1)	2.517(3)	W-Cl(2)	2.557(3)
P(1)-C(11)	1.800(10)	P(1)-C(12)	1.838(8)
P(1)-C(12)#1	1.838(8)	P(2)-C(22)#1	1.830(7)
P(2)-C(22)	1.830(7)	P(2)-C(21)	1.844(10)
P(3)-C(31)	1.813(11)	P(3)-C(33)	1.823(8)
P(3)-C(32)	1.825(8)		

P(1)-W-P(2)	122.27(11)	P(1)-W-P(3)	97.31(5)
P(2)-W-P(3)	91.76(4)	P(1)-W-P(3)#1	97.31(5)
P(2)-W-P(3)#1	91.76(4)	P(3)-W-P(3)#1	160.12(13)
P(1)-W-Cl(1)	152.34(10)	P(2)-W-Cl(1)	85.40(9)
P(3)-W-Cl(1)	80.40(6)	P(3)#1-W-Cl(1)	80.40(6)
P(1)-W-Cl(2)	73.82(10)	P(2)-W-Cl(2)	163.91(12)
P(3)-W-Cl(2)	85.61(5)	P(3)#1-W-Cl(2)	85.61(5)
Cl(1)-W-Cl(2)	78.51(11)	C(11)-P(1)-C(12)	100.3(4)
C(11)-P(1)-C(12)#1	100.3(4)	C(12)-P(1)-C(12)#1	100.4(6)
C(11)-P(1)-W	115.1(3)	C(12)-P(1)-W	118.7(3)
C(12)#1-P(1)-W	118.7(3)	C(22)#1-P(2)-C(22)	96.5(5)
C(22)#1-P(2)-C(21)	100.7(4)	C(22)-P(2)-C(21)	100.7(4)
C(22)#1-P(2)-W	117.7(3)	C(22)-P(2)-W	117.7(3)
C(21)-P(2)-W	119.6(4)	C(31)-P(3)-C(33)	100.9(5)
C(31)-P(3)-C(32)	100.7(4)	C(33)-P(3)-C(32)	99.5(5)
C(31)-P(3)-W	119.8(4)	C(33)-P(3)-W	116.7(3)
C(32)-P(3)-W	116.0(3)		

Symmetry transformations used to generate equivalent atoms:

#1 -x,y,z

Table 4. Anisotropic displacement parameters [$Å^2$ x 10^3] for W(PMe3)4H2Cl2.

The anisotropic displacement factor exponent takes the form: $-2\pi^2$ [$(ha^*)^2U_{11}$ + ... + $2hka^*b^*U_{12}$]

	U11	U22	U33	U23	U13	U12
W	36(1)	21(1)	21(1)	0(1)	0	0
Cl(1)	76(2)	49(1)	25(1)	-10(1)	0	0
Cl(2)	92(2)	32(1)	41(1)	13(1)	0	0
P(1)	39(1)	29(1)	33(1)	-7(1)	0	0
P(2)	36(1)	26(1)	35(1)	4(1)	0	0
P(3)	42(1)	35(1)	43(1)	-1(1)	9(1)	-7(1)
C(11)	70(7)	53(6)	32(5)	-19(5)	0	0
C(12)	67(5)	52(4)	64(5)	-20(4)	10(4)	-23(4)
C(21)	88(9)	23(4)	68(7)	-12(5)	0	0
C(22)	49(4)	43(4)	78(6)	24(4)	-8(4)	1(3)
C(31)	45(5)	92(8)	84(7)	-9(6)	-7(5)	-4(4)
C(32)	57(5)	53(5)	79(6)	-9(5)	24(5)	2(4)
C(33)	84(7)	66(6)	85(7)	20(6)	34(6)	-15(5)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for W(PMe3)4H2Cl2.

	x	y	z	U(eq)
H(11A)	555(179)	7043(260)	-2801(89)	77
H(11B)	-597(144)	6973(281)	-2825(96)	77
H(11C)	42(323)	6045(21)	-3141(10)	77
H(12A)	-1640(8)	5687(8)	-1468(46)	92
H(12B)	-1081(27)	4986(32)	-675(19)	92
H(12C)	-943(22)	4848(28)	-1902(32)	92
H(21A)	313(645)	10019(249)	1171(259)	90
H(21B)	-666(25)	10461(529)	709(551)	90
H(21C)	353(620)	10854(280)	300(292)	90
H(22A)	-1604(11)	9785(42)	-937(15)	85
H(22B)	-1090(30)	9314(26)	-1932(27)	85
H(22C)	-852(21)	10416(20)	-1601(39)	85
H(31A)	-2492(27)	8024(30)	-1276(25)	111
H(31B)	-3327(9)	7655(45)	-512(13)	111
H(31C)	-2649(33)	6878(15)	-1088(31)	111
H(32A)	-2035(38)	8640(26)	1777(17)	95
H(32B)	-2990(6)	8630(26)	1078(44)	95
H(32C)	-2070(40)	9250(6)	716(30)	95
H(33A)	-1979(40)	6583(37)	1854(24)	118
H(33B)	-2204(52)	5942(8)	842(30)	118
H(33C)	-3002(13)	6678(33)	1285(51)	118
H	-671(66)	7695(48)	-1080(75)	58(26)

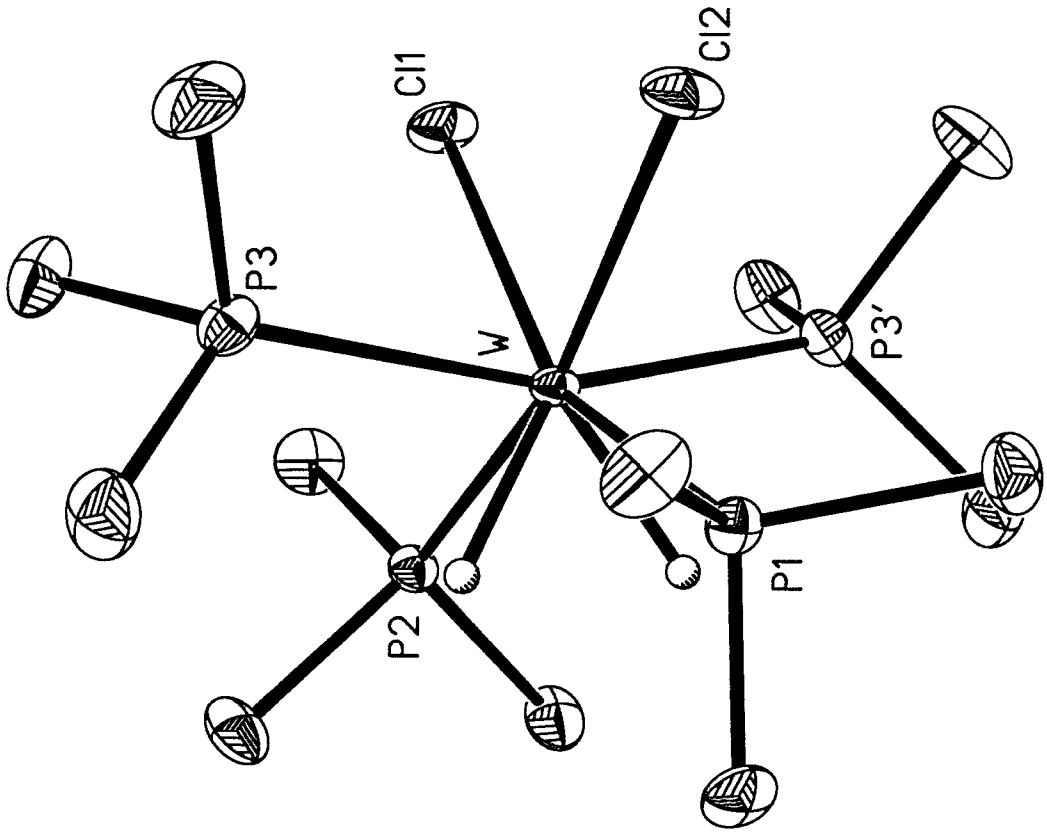

Table 1. Crystal data and structure refinement for W(PMe3)4H2Cl2 (inc polar).

Identification code	clmin1
Empirical formula	$C_{12}H_{38}Cl_2P_4W$
Formula weight	561.05
Temperature	293(2) K
Wavelength	0.71073 Å
Crystal system	Orthorhombic
Space group	$Cmc2_1$
Unit cell dimensions	a = 13.577(2) Å alpha = 90° b = 13.395(2) Å beta = 90° c = 12.598(3) Å gamma = 90°
Volume, Z	2291.1(7) $Å^3$, 4
Density (calculated)	1.627 Mg/m^3
Absorption coefficient	5.544 mm^{-1}
F(000)	1112
Crystal size	0.2 x 0.5 x 0.5 mm
θ range for data collection	2.14 to 27.52°
Limiting indices	$-17 \le h \le 12$, $-12 \le k \le 17$, $0 \le l \le 16$
Reflections collected	2859
Independent reflections	1436 (R_{int} = 0.0366)
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	1436 / 1 / 106
Goodness-of-fit on F^2	1.112
Final R indices [I>2σ(I)]	R1 = 0.0459, wR2 = 0.1242
R indices (all data)	R1 = 0.0507, wR2 = 0.1276
Absolute structure parameter	0.44(7)
Extinction coefficient	0.0001(2)
Largest diff. peak and hole	2.314 and -1.962 $eÅ^{-3}$

Table 2. Atomic coordinates [x 10^4] and equivalent isotropic displacement parameters [$Å^2$ x 10^3] for W(PMe3)4H2Cl2 (inc polar). U(e one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
W	0	7542(1)	0(1)	26(1)
Cl(1)	0	8170(4)	1856(5)	51(1)
Cl(2)	0	5902(4)	1024(7)	56(2)
P(1)	0	6204(4)	-1341(6)	37(1)
P(2)	0	9314(4)	-534(5)	34(1)
P(3)	-1815(3)	7543(2)	-310(5)	43(1)
C(11)	0	6602(21)	-2687(19)	55(6)
C(12)	-1031(15)	5327(15)	-1402(18)	63(5)
C(21)	0	10276(16)	530(24)	63(7)
C(22)	-994(12)	9751(14)	-1416(19)	57(5)
C(31)	-2647(21)	7389(23)	856(28)	112(14)
C(32)	-2210(19)	8574(21)	-1176(24)	107(12)
C(33)	-2302(24)	6504(17)	-1136(29)	116(14)

Table 3. Bond lengths [Å] and angles [°] for W(PMe3)4H2Cl2 (inc polar).

W-P(1)	2.464(7)	W-P(2)	2.467(5)
W-Cl(1)	2.485(7)	W-P(3)	2.495(5)
W-P(3)#1	2.495(5)	W-Cl(2)	2.548(6)
P(1)-C(11)	1.78(3)	P(1)-C(12)	1.83(2)
P(1)-C(12)#1	1.83(2)	P(2)-C(22)	1.84(2)
P(2)-C(22)#1	1.84(2)	P(2)-C(21)	1.86(2)
P(3)-C(32)	1.84(2)	P(3)-C(31)	1.86(3)
P(3)-C(33)	1.86(3)		

P(1)-W-P(2)	120.9(3)	P(1)-W-Cl(1)	153.1(2)
P(2)-W-Cl(1)	86.0(2)	P(1)-W-P(3)	83.87(14)
P(2)-W-P(3)	87.52(10)	Cl(1)-W-P(3)	98.5(2)
P(1)-W-P(3)#1	83.87(14)	P(2)-W-P(3)#1	87.52(10)
Cl(1)-W-P(3)#1	98.5(2)	P(3)-W-P(3)#1	162.0(3)
P(1)-W-Cl(2)	73.7(2)	P(2)-W-Cl(2)	165.4(3)
Cl(1)-W-Cl(2)	79.4(3)	P(3)-W-Cl(2)	94.57(10)
P(3)#1-W-Cl(2)	94.57(10)	C(11)-P(1)-C(12)	98.8(10)
C(11)-P(1)-C(12)#1	98.8(10)	C(12)-P(1)-C(12)#1	99.9(14)
C(11)-P(1)-W	115.8(9)	C(12)-P(1)-W	119.7(7)
C(12)#1-P(1)-W	119.7(7)	C(22)-P(2)-C(22)#1	94.1(13)
C(22)-P(2)-C(21)	102.4(10)	C(22)#1-P(2)-C(21)	102.4(10)
C(22)-P(2)-W	118.0(6)	C(22)#1-P(2)-W	118.0(6)
C(21)-P(2)-W	118.0(9)	C(32)-P(3)-C(31)	112(2)
C(32)-P(3)-C(33)	97.2(13)	C(31)-P(3)-C(33)	98(2)
C(32)-P(3)-W	112.4(8)	C(31)-P(3)-W	118.4(12)
C(33)-P(3)-W	116.0(11)		

Symmetry transformations used to generate equivalent atoms:

#1 -x,y,z

Table 4. Anisotropic displacement parameters [$Å^2$ x 10^3] for W(PMe3)4H2Cl2 (inc polar).

The anisotropic displacement factor exponent tak $-2\pi^2$ [$(ha^*)^2U_{11}$ + ... + $2hka^*b^*U_{12}$]

	U11	U22	U33	U23	U13	U12
W	36(1)	21(1)	21(1)	2(1)	0	0
Cl(1)	76(4)	52(3)	25(2)	-9(2)	0	0
Cl(2)	88(5)	33(3)	46(3)	18(3)	0	0
P(1)	39(3)	30(3)	41(3)	-10(2)	0	0
P(2)	38(2)	30(2)	33(3)	5(2)	0	0
P(3)	39(2)	35(2)	56(3)	9(1)	-10(2)	-7(1)
C(11)	60(14)	72(16)	33(12)	-20(12)	0	0
C(12)	76(13)	50(9)	63(12)	-11(9)	-8(11)	-24(9)
C(21)	76(18)	30(11)	83(18)	-22(12)	0	0
C(22)	46(9)	48(9)	78(13)	20(9)	-24(9)	1(7)
C(31)	62(15)	183(37)	91(20)	-61(20)	35(15)	-39(15)
C(32)	84(17)	104(18)	132(23)	67(18)	-90(18)	-34(14)
C(33)	132(25)	52(11)	164(31)	16(16)	-104(25)	-2(14)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for W(PMe3)4H2Cl2 (inc polar).

	x	y	z	U(eq)
H(11A)	247(152)	6075(63)	-3130(27)	83
H(11B)	413(128)	7180(101)	-2761(38)	83
H(11C)	-660(23)	6766(157)	-2899(55)	83
H(12A)	-1097(71)	4994(82)	-731(43)	95
H(12B)	-911(53)	4843(69)	-1948(83)	95
H(12C)	-1626(24)	5685(21)	-1557(117)	95
H(21A)	629(223)	10280(466)	878(477)	95
H(21B)	-506(440)	10124(375)	1037(383)	95
H(21C)	-124(664)	10920(93)	224(96)	95
H(22A)	-1580(33)	9865(104)	-1007(25)	86
H(22B)	-1123(75)	9254(51)	-1947(72)	86
H(22C)	-797(45)	10362(62)	-1753(93)	86
H(31A)	-2511(122)	6763(85)	1197(115)	168
H(31B)	-3320(21)	7400(183)	622(38)	168
H(31C)	-2538(131)	7925(102)	1349(97)	168
H(32A)	-1875(161)	8526(124)	-1846(85)	160
H(32B)	-2052(195)	9200(21)	-846(106)	160
H(32C)	-2908(38)	8533(131)	-1289(190)	160
H(33A)	-2541(213)	5981(101)	-683(29)	174
H(33B)	-1786(56)	6249(150)	-1580(182)	174
H(33C)	-2831(146)	6746(56)	-1571(174)	174

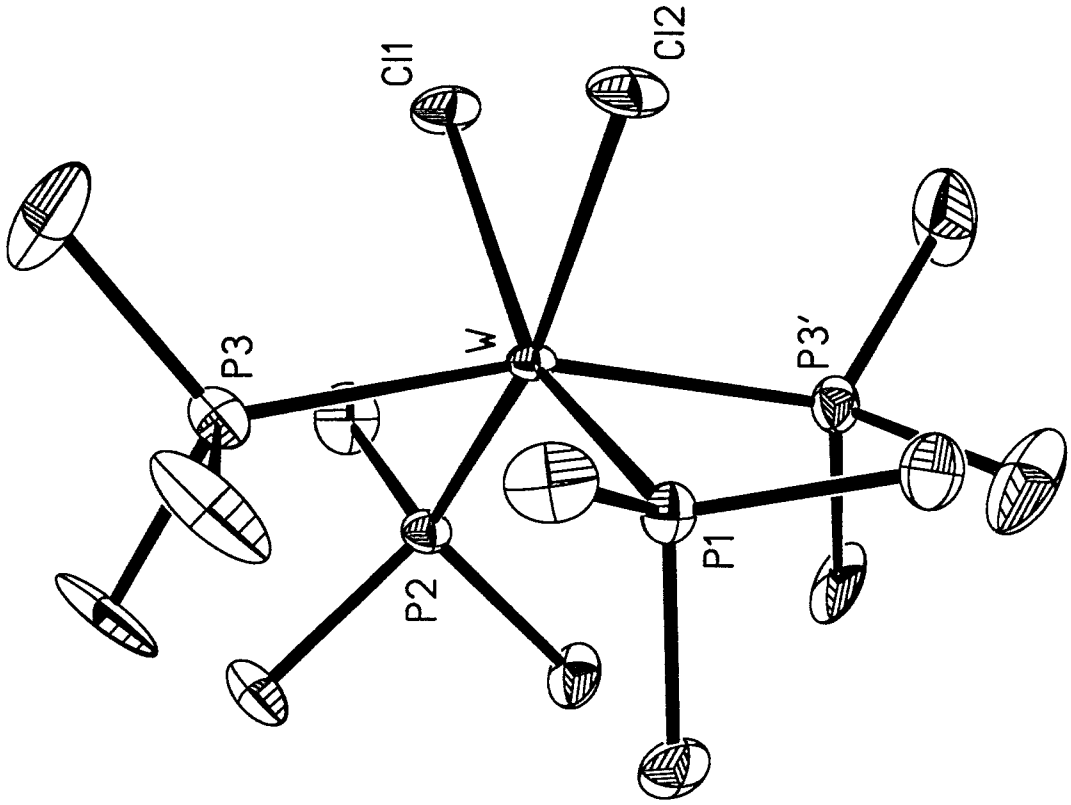

Table 1. Crystal data and structure refinement for W(PMe3)4H2F(FHF).

Identification code	gedshel
Empirical formula	$C_{12}H_{39}F_3P_4W$
Formula weight	548.16
Temperature	293(2) K
Wavelength	0.71073 Å
Crystal system	Orthorhombic
Space group	$Cmc2_1$
Unit cell dimensions	a = 14.246(3) Å alpha = 90° b = 12.917(2) Å beta = 90° c = 12.358(2) Å gamma = 90°
Volume, Z	2274.1(7) $Å^3$, 4
Density (calculated)	1.601 Mg/m^3
Absorption coefficient	5.375 mm^{-1}
F(000)	1088
Crystal size	0.3 x 0.4 x 0.5 mm
θ range for data collection	2.13 to 32.50°
Limiting indices	$0 \le h \le 21$, $0 \le k \le 19$, $-18 \le l \le 0$
Reflections collected	2227
Independent reflections	2227 (R_{int} = 0.0000)
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2225 / 2 / 116
Goodness-of-fit on F^2	1.000
Final R indices [I>2σ(I)]	R1 = 0.0364, wR2 = 0.0772
R indices (all data)	R1 = 0.0458, wR2 = 0.0803
Absolute structure parameter	0.05(4)
Extinction coefficient	0.0022(2)
Largest diff. peak and hole	1.169 and -2.550 $eÅ^{-3}$

Table 2. Atomic coordinates [x 10^4] and equivalent isotropic displacement parameters [$Å^2$ x 10^3] for W(PMe3)4H2F(FHF). U(eq) is def one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
W	0	7585(1)	0	26(1)
F(1)	0	8741(6)	-1120(7)	47(2)
F(2)	0	6810(5)	-1493(6)	40(2)
F(3)	0	7364(8)	-3335(9)	111(6)
P(1)	0	5786(2)	646(4)	35(1)
P(2)	0	9153(3)	1099(5)	40(1)
P(3)	-1718(1)	7592(1)	-392(3)	39(1)
C(11)	0	4772(8)	-364(12)	64(4)
C(12)	-985(8)	5359(8)	1503(9)	62(3)
C(21)	0	9037(13)	2524(14)	92(7)
C(22)	-954(10)	10059(8)	904(15)	115(7)
C(31)	-2589(9)	7700(8)	682(11)	70(3)
C(32)	-2161(9)	6458(9)	-1111(11)	75(3)
C(33)	-2073(9)	8594(8)	-1324(9)	65(3)

Table 3. Bond lengths [Å] and angles [°] for W(PMe3)4H2F(FHF).

W-F(1)	2.037(8)	W-F(2)	2.099(7)
W-P(2)	2.439(4)	W-P(1)	2.457(3)
W-P(3)	2.495(2)	W-P(3)#1	2.495(2)
F(2)-F(3)	2.386(13)	P(1)-C(11)	1.809(12)
P(1)-C(12)	1.842(9)	P(1)-C(12)#1	1.842(9)
P(2)-C(21)	1.77(2)	P(2)-C(22)	1.810(11)
P(2)-C(22)#1	1.810(11)	P(3)-C(33)	1.806(9)
P(3)-C(31)	1.822(12)	P(3)-C(32)	1.826(10)
W-H	1.7000(11)		
H-W-F(1)	128(2)	H-W-F(2)	141(2)
F(1)-W-F(2)	75.7(3)	H-W-P(2)	61(2)
F(1)-W-P(2)	76.7(2)	F(2)-W-P(2)	152.3(2)
H-W-P(1)	72(2)	F(1)-W-P(1)	156.1(3)
F(2)-W-P(1)	80.5(2)	P(2)-W-P(1)	127.2(2)
H-W-P(3)	75(2)	F(1)-W-P(3)	82.27(8)
F(2)-W-P(3)	80.28(8)	P(2)-W-P(3)	96.03(5)
P(1)-W-P(3)	93.81(5)	H-W-P(3)#1	128(2)
F(1)-W-P(3)#1	82.27(8)	F(2)-W-P(3)#1	80.28(8)
P(2)-W-P(3)#1	96.03(5)	P(1)-W-P(3)#1	93.81(5)
P(3)-W-P(3)#1	157.6(2)	W-F(2)-F(3)	134.1(4)
C(11)-P(1)-C(12)	100.3(4)	C(11)-P(1)-C(12)#1	100.3(4)
C(12)-P(1)-C(12)#1	99.2(7)	C(11)-P(1)-W	117.4(4)
C(12)-P(1)-W	118.0(3)	C(12)#1-P(1)-W	118.0(3)
C(21)-P(2)-C(22)	100.8(7)	C(21)-P(2)-C(22)#1	100.8(7)
C(22)-P(2)-C(22)#1	97.4(10)	C(21)-P(2)-W	119.0(6)
C(22)-P(2)-W	117.6(4)	C(22)#1-P(2)-W	117.6(4)
C(33)-P(3)-C(31)	102.7(6)	C(33)-P(3)-C(32)	99.6(7)
C(31)-P(3)-C(32)	100.4(6)	C(33)-P(3)-W	113.7(4)
C(31)-P(3)-W	121.8(5)	C(32)-P(3)-W	115.5(4)

Symmetry transformations used to generate equivalent atoms:

#1 -x,y,z

Table 4. Anisotropic displacement parameters [$Å^2$ x 10^3] for W(PMe3)4H2F(FHF).

The anisotropic displacement factor exponent takes the fo $-2\pi^2$ [$(ha^*)^2U_{11}$ + ... + $2hka^*b^*U_{12}$]

	U11	U22	U33	U23	U13	U12
W	29(1)	24(1)	26(1)	0(1)	0	0
F(1)	52(5)	40(4)	51(4)	14(4)	0	0
F(2)	56(4)	38(3)	26(3)	-4(2)	0	0
F(3)	202(19)	90(8)	41(5)	3(5)	0	0
P(1)	43(2)	28(1)	33(1)	4(1)	0	0
P(2)	43(2)	35(2)	43(2)	-11(1)	0	0
P(3)	31(1)	42(1)	43(1)	-1(1)	-3(1)	2(1)
C(11)	106(12)	30(4)	55(8)	-4(4)	0	0
C(12)	63(6)	61(5)	61(6)	24(5)	27(5)	-1(5)
C(21)	157(21)	79(11)	41(7)	-31(8)	0	0
C(22)	111(12)	60(6)	175(16)	-54(8)	-57(11)	53(7)
C(31)	46(6)	87(8)	78(8)	-16(6)	15(6)	1(5)
C(32)	67(8)	64(6)	93(9)	-21(6)	-6(7)	-15(5)
C(33)	64(7)	61(5)	69(7)	17(5)	-27(6)	13(5)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for W(PMe3)4H2F(FHF).

	x	y	z	U(eq)
H(11A)	461(58)	4925(48)	-907(53)	95
H(11B)	-609(24)	4730(61)	-693(67)	95
H(11C)	148(82)	4123(17)	-27(21)	95
H(12A)	-975(35)	5735(47)	2173(29)	93
H(12B)	-926(32)	4632(16)	1647(55)	93
H(12C)	-1567(8)	5488(58)	1135(30)	93
H(21A)	341(86)	8427(62)	2729(15)	138
H(21B)	-635(4)	8986(113)	2779(17)	138
H(21C)	294(91)	9635(54)	2837(14)	138
H(22A)	-1164(58)	10028(71)	166(28)	173
H(22B)	-742(28)	10747(15)	1065(102)	173
H(22C)	-1464(38)	9882(60)	1377(73)	173
H(31A)	-2292(14)	7588(64)	1370(12)	106
H(31B)	-3070(32)	7190(43)	575(40)	106
H(31C)	-2863(43)	8378(23)	668(44)	106
H(32A)	-2076(61)	5853(13)	-670(35)	112
H(32B)	-1823(46)	6375(43)	-1777(39)	112
H(32C)	-2816(18)	6549(33)	-1263(66)	112
H(33A)	-1781(48)	8478(38)	-2014(23)	97
H(33B)	-1884(54)	9257(10)	-1048(36)	97
H(33C)	-2743(10)	8580(44)	-1407(54)	97
H	-533(42)	7564(47)	1231(24)	44(28)

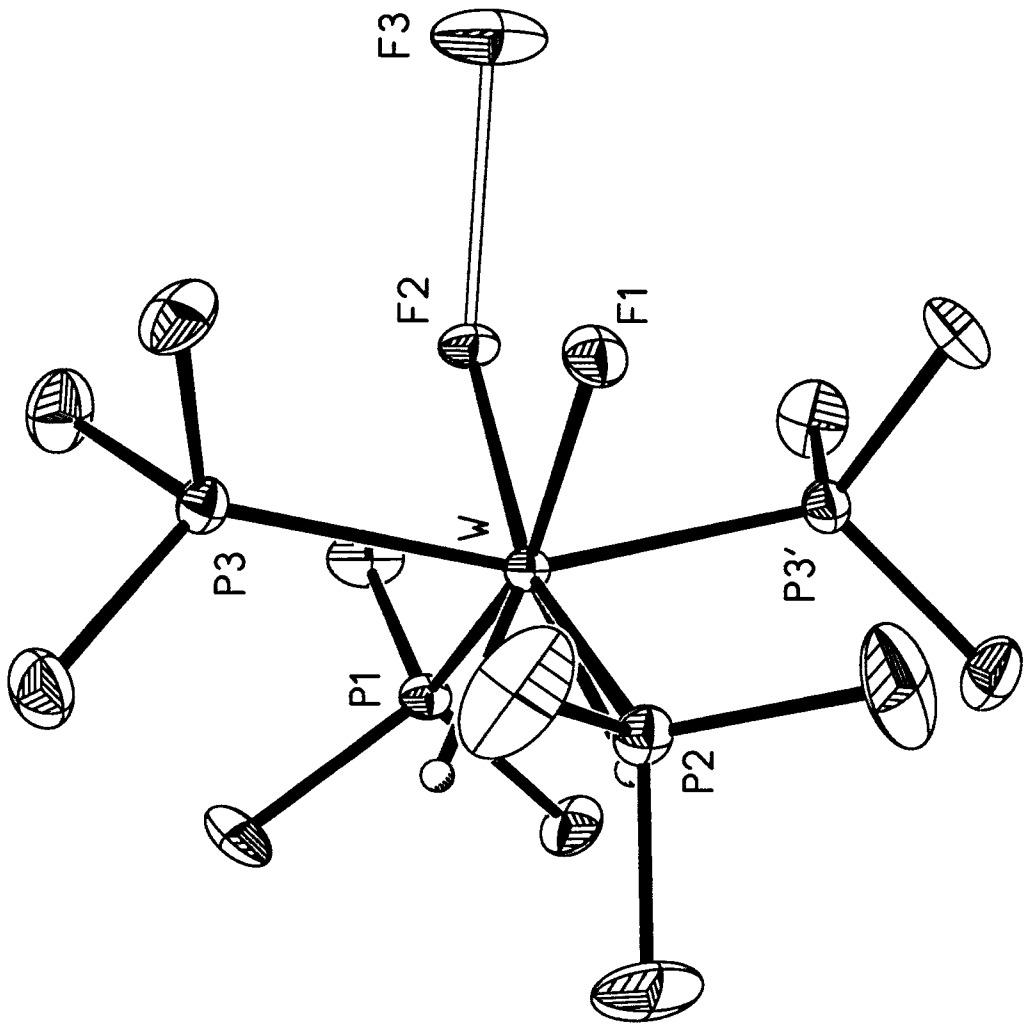

Table 1. Crystal data and structure refinement for W(PMe3)4H2F(FHF) inc polar

Identification code	gedmin1
Empirical formula	$C_{12}H_{39}F_3P_2W$
Formula weight	486.22
Temperature	293(2) K
Wavelength	0.71073 Å
Crystal system	Orthorhombic
Space group	$Cmc2_1$
Unit cell dimensions	a = 14.246(3) Å alpha = 90°
	b = 12.917(2) Å beta = 90°
	c = 12.358(2) Å gamma = 90°
Volume, Z	2274.1(7) $Å^3$, 4
Density (calculated)	1.420 Mg/m^3
Absorption coefficient	5.231 mm^{-1}
F(000)	968
Crystal size	0.3 x 0.4 x 0.5 mm
θ range for data collection	2.13 to 32.50°
Limiting indices	$0 \le h \le 21$, $0 \le k \le 19$, $-18 \le l \le 0$
Reflections collected	2227
Independent reflections	2227 (R_{int} = 0.0000)
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2225 / 1 / 112
Goodness-of-fit on F^2	1.075
Final R indices [I>2σ(I)]	R1 = 0.0500, wR2 = 0.1292
R indices (all data)	R1 = 0.0596, wR2 = 0.1346
Absolute structure parameter	0.49(7)
Extinction coefficient	0.0018(3)
Largest diff. peak and hole	1.497 and -2.619 $eÅ^{-3}$

Table 2. Atomic coordinates [x 10^4] and equivalent isotropic displacement parameters [$Å^2$ x 10^3] for W(PMe3)4H2F(FHF) inc polar. U(one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
W	0	7585(1)	0(1)	26(1)
F(1)	0	8746(10)	-1099(11)	47(3)
F(2)	0	6813(8)	-1450(9)	43(2)
F(3)	0	7378(13)	-3312(16)	116(12)
P(1)	0	5784(3)	675(6)	36(1)
P(2)	0	9154(4)	1132(7)	42(1)
P(3)	-1719(2)	7585(2)	362(4)	39(1)
C(11)	0	4776(12)	-319(21)	67(7)
C(12)	-965(12)	5348(13)	1551(15)	65(5)
C(21)	0	9043(21)	2533(23)	89(11)
C(22)	-976(17)	10049(14)	968(21)	104(9)
C(31)	-2596(16)	7620(16)	-717(25)	84(8)
C(32)	-2055(19)	6333(26)	1197(19)	137(15)
C(33)	-2108(15)	8613(16)	1179(18)	77(6)

Table 3. Bond lengths [Å] and angles [°] for W(PMe3)4H2F(FHF) inc polar

W-F(1)	2.024(13)	W-F(2)	2.052(12)
W-P(2)	2.463(7)	W-P(1)	2.471(5)
W-P(3)#1	2.490(4)	W-P(3)	2.490(4)
F(2)-F(3)	2.41(2)	P(1)-C(11)	1.79(2)
P(1)-C(12)#1	1.838(14)	P(1)-C(12)	1.838(14)
P(2)-C(21)	1.74(3)	P(2)-C(22)#1	1.82(2)
P(2)-C(22)	1.82(2)	P(3)-C(33)	1.76(2)
P(3)-C(31)	1.83(2)	P(3)-C(32)	1.98(2)
F(1)-W-F(2)	76.9(5)	F(1)-W-P(2)	76.8(4)
F(2)-W-P(2)	153.7(4)	F(1)-W-P(1)	157.5(5)
F(2)-W-P(1)	80.6(3)	P(2)-W-P(1)	125.7(4)
F(1)-W-P(3)#1	96.93(11)	F(2)-W-P(3)#1	99.03(13)
P(2)-W-P(3)#1	84.15(12)	P(1)-W-P(3)#1	86.53(9)
F(1)-W-P(3)	96.93(11)	F(2)-W-P(3)	99.03(13)
P(2)-W-P(3)	84.15(12)	P(1)-W-P(3)	86.53(9)
P(3)#1-W-P(3)	159.3(3)	W-F(2)-F(3)	133.3(6)
C(11)-P(1)-C(12)#1	100.4(8)	C(11)-P(1)-C(12)	100.4(8)
C(12)#1-P(1)-C(12)	96.8(12)	C(11)-P(1)-W	117.0(7)
C(12)#1-P(1)-W	119.1(6)	C(12)-P(1)-W	119.1(6)
C(21)-P(2)-C(22)#1	99.4(10)	C(21)-P(2)-C(22)	99.4(10)
C(22)#1-P(2)-C(22)	100(2)	C(21)-P(2)-W	119.9(10)
C(22)#1-P(2)-W	117.4(7)	C(22)-P(2)-W	117.4(7)
C(33)-P(3)-C(31)	100.7(12)	C(33)-P(3)-C(32)	104(2)
C(31)-P(3)-C(32)	103.6(10)	C(33)-P(3)-W	114.4(8)
C(31)-P(3)-W	122.8(10)	C(32)-P(3)-W	109.4(10)

Symmetry transformations used to generate equivalent atoms:

#1 -x,y,z

Table 4. Anisotropic displacement parameters [$Å^2$ x 10^3] for W(PMe3)4H2F(FHF) inc polar.

The anisotropic displacement factor exponent ta $-2\pi^2$ [$(ha^*)^2U_{11}$ + ... + $2hka^*b^*U_{12}$]

	U11	U22	U33	U23	U13	U12
W	29(1)	24(1)	26(1)	0(1)	0	0
F(1)	43(7)	52(8)	45(7)	15(6)	0	0
F(2)	60(7)	38(5)	30(5)	-3(4)	0	0
F(3)	212(37)	97(15)	39(8)	2(7)	0	0
P(1)	43(2)	30(2)	34(2)	4(1)	0	0
P(2)	45(3)	38(3)	42(2)	-10(2)	0	0
P(3)	30(1)	41(1)	46(2)	-1(1)	3(1)	1(1)
C(11)	106(19)	24(6)	70(16)	-4(7)	0	0
C(12)	66(11)	63(9)	67(10)	24(8)	37(9)	2(8)
C(21)	149(32)	68(16)	49(13)	-32(12)	0	0
C(22)	125(19)	56(9)	130(20)	-39(11)	-43(16)	54(12)
C(31)	50(10)	92(14)	110(20)	35(12)	-24(12)	2(9)
C(32)	117(20)	223(33)	72(13)	72(18)	-28(14)	-134(23)
C(33)	71(13)	79(11)	81(12)	-14(10)	33(11)	10(10)

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Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for W(PMe3)4H2F(FHF) inc polar.

	x	y	z	U(eq)
H(11A)	-128(146)	4125(26)	25(34)	100
H(11B)	603(47)	4747(107)	-664(118)	100
H(11C)	-475(99)	4915(86)	-851(97)	100
H(12A)	-941(64)	5716(85)	2225(50)	98
H(12B)	-904(61)	4619(26)	1683(100)	98
H(12C)	-1554(13)	5482(108)	1200(55)	98
H(21A)	512(163)	8608(245)	2755(31)	133
H(21B)	-582(110)	8742(278)	2767(33)	133
H(21C)	70(274)	9716(40)	2852(23)	133
H(22A)	-1040(80)	10227(113)	218(31)	156
H(22B)	-858(68)	10664(64)	1382(126)	156
H(22C)	-1543(31)	9728(57)	1218(141)	156
H(31A)	-2684(111)	6936(32)	-1002(120)	126
H(31B)	-2385(68)	8073(128)	-1283(80)	126
H(31C)	-3180(42)	7872(155)	-432(44)	126
H(32A)	-1512(55)	5897(105)	1270(196)	206
H(32B)	-2541(143)	5961(123)	825(120)	206
H(32C)	-2274(187)	6531(27)	1902(86)	206
H(33A)	-1582(23)	8913(79)	1551(97)	116
H(33B)	-2552(85)	8359(27)	1699(86)	116
H(33C)	-2401(97)	9130(58)	735(25)	116

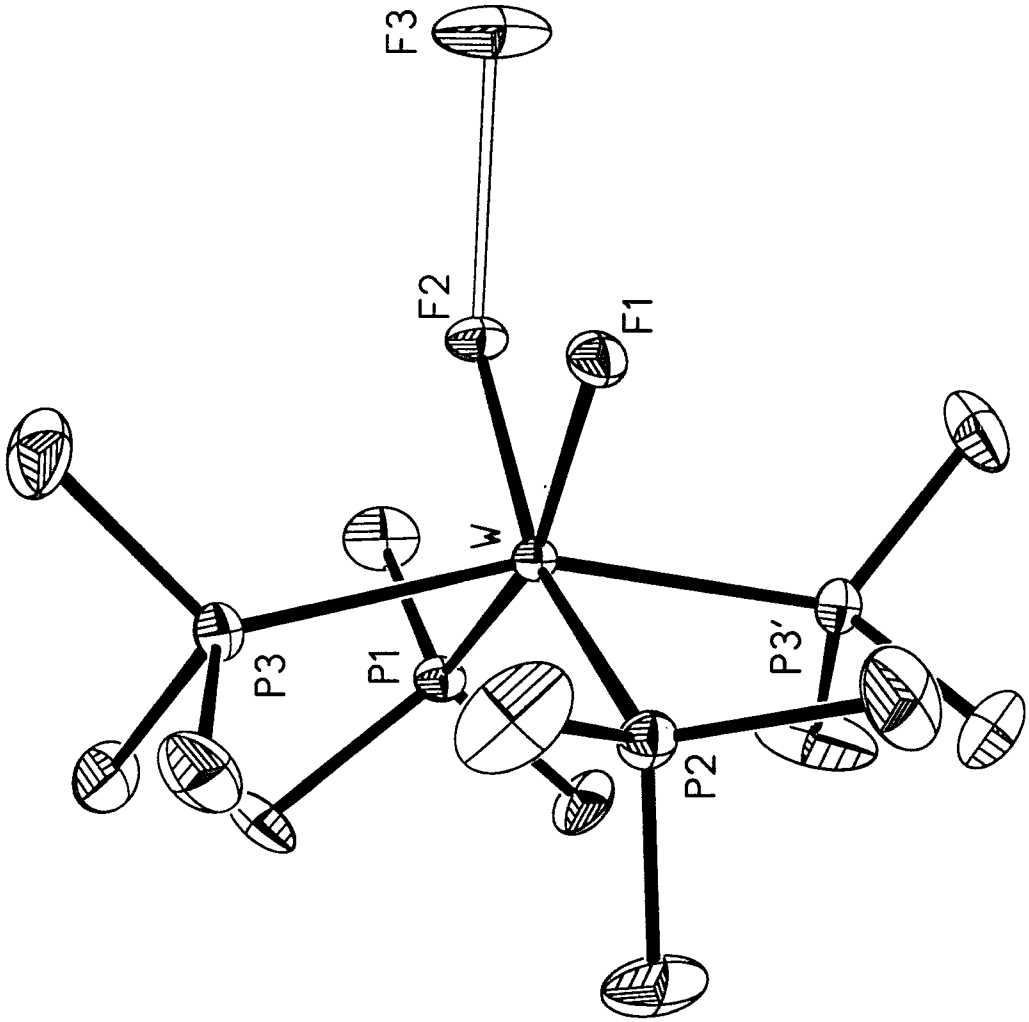


Table 1. Crystal data and structure refinement for [W(PMe3)4H2F(OH2)]F.

Identification code	gedoh
Empirical formula	$C_{12}H_{40}F_2OP_4W$
Formula weight	546.17
Temperature	293(2) K
Wavelength	0.71073 Å
Crystal system	Orthorhombic
Space group	$Cmc2_1$
Unit cell dimensions	a = 14.246(3) Å alpha = 90° b = 12.917(2) Å beta = 90° c = 12.358(2) Å gamma = 90°
Volume, Z	2274.1(7) $Å^3$, 4
Density (calculated)	1.595 Mg/m^3
Absorption coefficient	5.372 mm^{-1}
F(000)	1088
Crystal size	0.3 x 0.4 x 0.5 mm
θ range for data collection	2.13 to 32.50°
Limiting indices	$0 \le h \le 21$, $0 \le k \le 19$, $-18 \le l \le 0$
Reflections collected	2227
Independent reflections	2227 (R_{int} = 0.0000)
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	2225 / 1 / 112
Goodness-of-fit on F^2	1.054
Final R indices [I>2σ(I)]	R1 = 0.0500, wR2 = 0.1294
R indices (all data)	R1 = 0.0595, wR2 = 0.1349
Absolute structure parameter	0.49(7)
Extinction coefficient	0.0017(3)
Largest diff. peak and hole	1.482 and -2.636 $eÅ^{-3}$

Table 2. Atomic coordinates [x 10^4] and equivalent isotropic displacement parameters [$Å^2$ x 10^3] for [W(PMe3)4H2F(OH2)]F. U(eq) is one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
W	0	7585(1)	0(1)	26(1)
F(1)	0	8758(10)	-1092(11)	46(3)
F(2)	0	7364(14)	-3315(16)	115(11)
O(1)	0	6814(8)	-1455(9)	32(2)
P(1)	0	5785(3)	674(6)	36(1)
P(2)	0	9156(4)	1135(7)	42(1)
P(3)	-1719(2)	7585(2)	362(4)	39(1)
C(11)	0	4775(12)	-322(21)	66(7)
C(12)	-964(12)	5351(13)	1552(15)	65(5)
C(21)	0	9052(21)	2523(24)	95(12)
C(22)	-979(17)	10052(14)	970(21)	104(9)
C(31)	-2594(16)	7621(16)	-728(25)	82(7)
C(32)	-2058(18)	6335(26)	1189(19)	136(15)
C(33)	-2118(16)	8619(16)	1178(19)	79(6)

Table 3. Bond lengths [Å] and angles [°] for [W(PMe3)4H2F(OH2)]F.

W-F(1)	2.028(13)	W-O(1)	2.056(12)
W-P(2)	2.467(7)	W-P(1)	2.470(5)
W-P(3)#1	2.489(4)	W-P(3)	2.489(4)
F(2)-O(1)	2.41(2)	P(1)-C(11)	1.79(2)
P(1)-C(12)	1.838(14)	P(1)-C(12)#1	1.838(14)
P(2)-C(21)	1.72(3)	P(2)-C(22)#1	1.82(2)
P(2)-C(22)	1.82(2)	P(3)-C(33)	1.77(2)
P(3)-C(31)	1.84(2)	P(3)-C(32)	1.97(2)
F(1)-W-O(1)	77.3(5)	F(1)-W-P(2)	76.4(4)
O(1)-W-P(2)	153.6(4)	F(1)-W-P(1)	158.0(5)
O(1)-W-P(1)	80.7(3)	P(2)-W-P(1)	125.6(4)
F(1)-W-P(3)#1	96.86(11)	O(1)-W-P(3)#1	99.05(13)
P(2)-W-P(3)#1	84.13(12)	P(1)-W-P(3)#1	86.53(9)
F(1)-W-P(3)	96.86(11)	O(1)-W-P(3)	99.05(13)
P(2)-W-P(3)	84.13(12)	P(1)-W-P(3)	86.53(9)
P(3)#1-W-P(3)	159.3(3)	W-O(1)-F(2)	133.8(6)
C(11)-P(1)-C(12)	100.6(8)	C(11)-P(1)-C(12)#1	100.6(8)
C(12)-P(1)-C(12)#1	96.7(12)	C(11)-P(1)-W	117.0(7)
C(12)-P(1)-W	119.1(6)	C(12)#1-P(1)-W	119.1(6)
C(21)-P(2)-C(22)#1	99.3(10)	C(21)-P(2)-C(22)	99.3(10)
C(22)#1-P(2)-C(22)	100(2)	C(21)-P(2)-W	120.2(10)
C(22)#1-P(2)-W	117.3(7)	C(22)-P(2)-W	117.3(7)
C(33)-P(3)-C(31)	100.4(12)	C(33)-P(3)-C(32)	104(2)
C(31)-P(3)-C(32)	103.6(9)	C(33)-P(3)-W	114.8(8)
C(31)-P(3)-W	122.4(9)	C(32)-P(3)-W	109.5(9)

Symmetry transformations used to generate equivalent atoms:

#1 -x,y,z

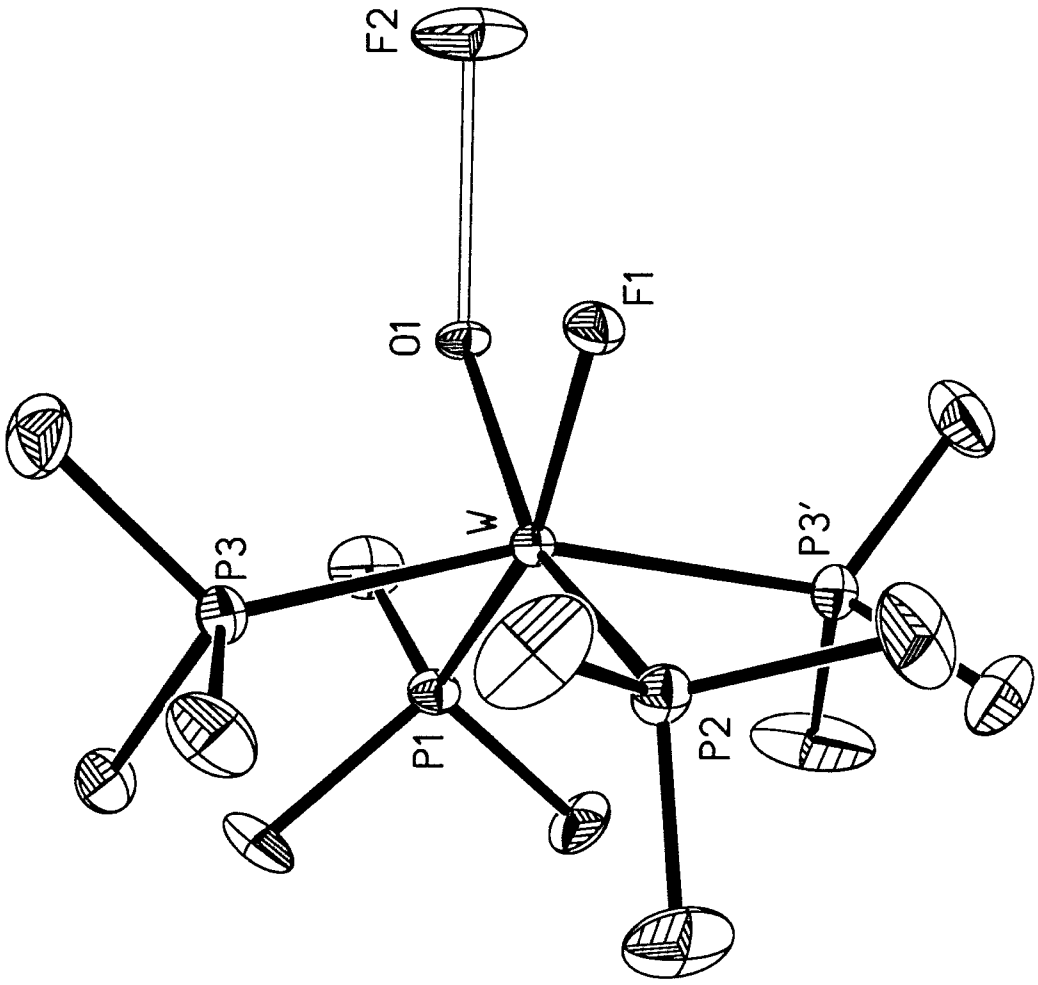
Table 4. Anisotropic displacement parameters [$Å^2$ x 10^3] for [W(PMe3)4H2F(OH2)]F.

The anisotropic displacement factor exponent takes the $-2\pi^2$ [$(ha^*)^2U_{11}$ + ... + $2hka^*b^*U_{12}$]

	U11	U22	U33	U23	U13	U12
W	29(1)	24(1)	26(1)	0(1)	0	0
F(1)	44(7)	51(8)	42(6)	15(6)	0	0
F(2)	207(35)	101(15)	37(8)	2(8)	0	0
O(1)	47(7)	29(4)	20(4)	-4(4)	0	0
P(1)	43(2)	30(2)	34(2)	4(1)	0	0
P(2)	46(3)	38(3)	42(3)	-11(2)	0	0
P(3)	30(1)	41(1)	45(2)	-1(1)	3(1)	1(1)
C(11)	105(19)	25(7)	70(16)	-2(7)	0	0
C(12)	66(11)	63(9)	64(10)	22(8)	36(9)	1(8)
C(21)	165(35)	66(16)	55(14)	-33(12)	0	0
C(22)	126(19)	57(9)	128(20)	-41(11)	-42(16)	55(12)
C(31)	49(10)	94(15)	103(19)	34(12)	-20(12)	2(9)
C(32)	108(19)	230(32)	71(12)	73(18)	-25(13)	-131(22)
C(33)	80(13)	74(12)	84(13)	-10(10)	36(11)	11(10)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for [W(PMe3)4H2F(OH2)]F.

	x	y	z	U(eq)
H(11A)	138(290)	4125(50)	21(57)	100
H(11B)	468(201)	4920(166)	-860(184)	100
H(11C)	-606(89)	4738(216)	-659(240)	100
H(12A)	-939(64)	5719(85)	2226(50)	97
H(12B)	-903(61)	4622(26)	1685(100)	97
H(12C)	-1554(13)	5485(108)	1203(55)	97
H(21A)	578(89)	8742(216)	2758(30)	143
H(21B)	-518(125)	8627(194)	2748(29)	143
H(21C)	-60(214)	9728(31)	2839(24)	143
H(22A)	-1032(80)	10245(113)	222(34)	155
H(22B)	-870(69)	10660(66)	1400(123)	155
H(22C)	-1549(29)	9724(54)	1201(143)	155
H(31A)	-2683(83)	6936(26)	-1011(89)	123
H(31B)	-2378(51)	8070(97)	-1295(60)	123
H(31C)	-3179(33)	7877(113)	-449(37)	123
H(32A)	-1525(62)	5881(97)	1229(190)	204
H(32B)	-2567(131)	5986(121)	835(124)	204
H(32C)	-2246(184)	6530(30)	1907(74)	204
H(33A)	-1599(26)	8904(79)	1575(94)	119
H(33B)	-2583(82)	8369(29)	1676(88)	119
H(33C)	-2389(97)	9145(56)	728(22)	119



Neutron Diffraction Data for $W(PMe_3)_4H_2Cl_2$

Table 1. Data Collection and Refinement Parameters.

name	:	W(PMe3)4Cl2H2
formula	:	W P4 C12 H38 Cl2
code	:	WPHCl
Mr	:	561.1100 au
spacegroup	:	Cmc21
Z	:	4
a	:	13.489 (4) A
b	:	13.287 (5) A
c	:	12.426 (3) A
alpha	:	90. degr
beta	:	90. degr
gamma	:	90. degr
volume	:	2227.1(20) A3
how determined	:	least-squares fit for 32 refls, 51 < 2theta < 60
density calculated	:	1.6732 g.cm-3
absorption coefficient	:	3.116 cm-1
F000	:	-71.7016 fm
forms	:	+-(31-2) (001) +-(011) +-(01-1)
shape crystal	:	irregular
color crystal	:	dark red
dimension crystal	:	about 4.4 x 2.5 x 1.5 mm
volume crystal	:	14.1 mm3
mounted on	:	aluminum pin
mounted with	:	halocarbon grease
mounted along	:	+- (0-11)
machine	:	H6S
wavelength	:	1.16395(10) A
monochromator	:	Ge (220)
temperature controller	:	DISPLEX Model CS-202. Air Products Chemical, Inc. helium cryostat
scattering lengths :		
W	:	4.77 fm
Cl	:	9.5770 fm

P	: 5.13	fm
C	: 6.6460	fm
H	: -3.7406	fm

temperature	: 15.00(1)	K
monitor reflections	: (4 0 10) (4 -4 -8)	
reflections collected	: 1743	
> 3 sigma	: 1403	
negative intensity	: 25	
(2theta)max	: 108	
(sin theta/lambda)max	: 0.71	
Lp correction	: Lorentz	
decay	: no	
decay correction	: none	
psi scan	: (0 -4 1) (0 -2 1)	
absorption correction	: yes	
minimum	: 1.524	0.656
maximum	: 2.329	0.429
average	: 1.789	0.559
reflections averaged	: 2 (standards)	
Rint	: 0.0111	
Rwint	: 0.0006	
collected once	: 1705	
independent reflections	: 1707	
without absences	: 1707	
> 3 sigma	: 1367	

solved structure	: x-ray known	
program used	: UPALS	
variables	: sc xyz bij ext	
number of variables	: 271	
extinction type	: type I, isotropic (Becker + Coppens)	
extinction coefficient	: 0.4077E+04 (0.5831E+03)	
max extinction corr	: 1.39 for 800	
reflections used	: 1707	
ratio refls/vars	: 6.3	
p	: 0.02	

(delta/sigma)max	:	< 0.1
F / F2	:	F2
R(F2)	:	0.14426
Rw(F2)	:	0.16578
S	:	2.60822
diff. Fourier	:	residual : pos 2.6 %, neg 4.4 % of maximum (Cl1)

Table 2. Atomic coordinates and displacement parameters

	x	y	z	Uiso/U11	U22	U33	U12	U13	U23
W	0.0000(0)	0.7575(6)	0.0000(0)	0.010(3)	0.004(4)	0.006(3)	0.000(0)	0.000(0)	0.000(3)
Cl1	0.0000(0)	0.8145(3)	0.1932(8)	0.031(3)	0.006(2)	0.004(2)	0.000(0)	0.000(0)	-0.004(2)
Cl2	0.0000(0)	0.5889(3)	0.1014(7)	0.015(2)	0.008(2)	0.002(2)	0.000(0)	0.000(0)	0.002(2)
P1	0.0000(0)	0.6231(6)	-0.1371(10)	0.009(3)	0.005(3)	0.010(3)	0.000(0)	0.000(0)	0.003(3)
P2	0.0000(0)	0.9380(6)	-0.0439(9)	0.009(4)	0.005(3)	0.007(4)	0.000(0)	0.000(0)	0.001(3)
P3	-0.1829(5)	0.7595(5)	0.0342(8)	0.014(3)	0.006(3)	0.021(3)	-0.003(2)	0.004(2)	0.000(2)
C11	0.0000(0)	0.6689(5)	-0.2775(8)	0.017(3)	0.012(3)	0.002(2)	0.000(0)	0.000(0)	0.002(2)
C12	-0.1043(4)	0.5342(3)	-0.1430(7)	0.012(2)	0.009(2)	0.012(2)	0.001(2)	-0.001(2)	-0.002(2)
C21	0.0000(0)	1.0305(5)	0.0651(8)	0.020(3)	0.009(3)	0.004(3)	0.000(0)	0.000(0)	0.001(2)
C22	-0.1026(4)	0.9855(3)	-0.1256(8)	0.012(2)	0.011(2)	0.010(2)	0.003(2)	-0.004(2)	0.001(2)
C31	-0.2686(4)	0.7625(4)	-0.0798(8)	0.012(2)	0.015(2)	0.041(3)	0.003(2)	-0.005(2)	-0.009(3)
C32	-0.2295(4)	0.8672(3)	0.1121(8)	0.022(3)	0.006(2)	0.020(3)	0.002(2)	0.009(2)	-0.002(2)
C33	-0.2333(5)	0.6560(4)	0.1152(9)	0.022(3)	0.007(2)	0.049(4)	-0.002(2)	0.020(3)	0.002(3)
HW	0.0666(8)	0.7850(8)	-0.1132(10)	0.029(5)	0.027(5)	0.022(5)	-0.005(4)	0.007(4)	0.003(4)
H11a	0.0000(0)	0.6078(11)	-0.3354(14)	0.034(8)	0.019(7)	0.021(7)	0.000(0)	0.000(0)	-0.008(6)
H11b	0.0667(9)	0.7150(10)	-0.2900(12)	0.032(6)	0.049(7)	0.030(6)	-0.025(6)	0.006(5)	0.007(5)
H12a	-0.1090(11)	0.4988(10)	-0.0635(11)	0.050(7)	0.040(6)	0.019(5)	-0.015(6)	-0.001(5)	0.008(4)
H12b	-0.0907(9)	0.4785(9)	-0.2062(12)	0.033(6)	0.030(6)	0.031(5)	-0.009(5)	0.004(5)	-0.024(5)
H12c	-0.1744(8)	0.5739(9)	-0.1605(13)	0.014(5)	0.037(6)	0.061(9)	0.011(5)	-0.008(5)	0.006(6)
H21a	0.0000(0)	1.1068(11)	0.0353(16)	0.059(11)	0.015(7)	0.025(7)	0.000(0)	0.000(0)	0.002(6)
H21b	0.0636(10)	1.0199(9)	0.1165(11)	0.044(6)	0.042(7)	0.021(5)	0.005(5)	-0.018(5)	-0.016(5)
H22a	-0.1740(9)	0.9768(10)	-0.0860(13)	0.022(6)	0.042(7)	0.046(7)	0.000(5)	0.013(5)	0.009(6)
H22b	-0.0910(9)	1.0638(8)	-0.1492(12)	0.031(6)	0.026(5)	0.038(6)	-0.001(5)	-0.018(5)	0.011(5)
H22c	-0.1061(10)	0.9416(9)	-0.1999(11)	0.037(6)	0.033(5)	0.023(5)	0.012(5)	-0.011(5)	-0.004(4)
H31a	-0.2573(11)	0.6971(10)	-0.1304(15)	0.046(8)	0.036(7)	0.067(10)	0.005(6)	-0.013(7)	-0.030(7)
H31b	-0.2589(11)	0.8305(9)	-0.1269(13)	0.044(7)	0.032(6)	0.048(8)	0.000(5)	-0.027(6)	0.006(6)
H31c	-0.3469(9)	0.7625(12)	-0.0525(17)	0.024(6)	0.054(9)	0.092(13)	-0.002(6)	0.015(7)	-0.007(9)