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H32a	-0.3108(9)	0.8632(9)	0.1206(16)	0.024(6)	0.030(6)	0.077(10)	0.011(5)	0.019(7)	-0.023(7)
H32b	-0.1963(12)	0.8682(9)	0.1907(12)	0.070(10)	0.035(6)	0.021(5)	0.021(6)	0.009(6)	-0.005(5)
H32c	-0.2115(12)	0.9365(8)	0.0713(14)	0.065(9)	0.013(5)	0.053(8)	-0.001(5)	0.019(7)	0.012(5)
H33a	-0.1942(13)	0.6532(10)	0.1895(16)	0.058(10)	0.031(7)	0.055(9)	-0.006(6)	0.010(8)	0.004(7)
H33b	-0.3142(11)	0.6670(10)	0.1301(16)	0.040(8)	0.026(6)	0.088(11)	0.002(6)	0.025(8)	0.003(7)
H33c	-0.2194(10)	0.5860(8)	0.0784(15)	0.039(7)	0.015(5)	0.080(11)	-0.002(5)	0.033(7)	0.002(6)

Table 3. Selected Bond Lengths (Å)

W	-	HW	1.709(12)
W	-	P1	2.468(12)
W	-	P2	2.459(11)
W	-	P3	2.504(6)
W	-	C11	2.518(10)
W	-	C12	2.570(10)
P1	-	C11	1.848(15)
P1	-	C12	1.839(7)
P2	-	C21	1.829(13)
P2	-	C22	1.829(9)
P3	-	C31	1.828(12)
P3	-	C32	1.838(10)
P3	-	C33	1.836(11)
C11	-	H11a	1.084(18)
C11	-	H11b	1.099(13)
C12	-	H12a	1.096(16)
C12	-	H12b	1.094(15)
C12	-	H12c	1.105(13)
C21	-	H21a	1.080(17)
C21	-	H21b	1.079(15)
C22	-	H22a	1.088(15)
C22	-	H22b	1.092(12)
C22	-	H22c	1.094(16)
C31	-	H31a	1.084(17)
C31	-	H31b	1.085(16)
C31	-	H31c	1.109(15)
C32	-	H32a	1.104(14)
C32	-	H32b	1.075(17)
C32	-	H32c	1.079(14)
C33	-	H33a	1.064(22)
C33	-	H33b	1.116(16)
C33	-	H33c	1.052(15)

HW	...	HW	1.80 (2)

Table 4. Selected Bond Angles (°)

P1	- W	- P2	123.5(4)
P1	- W	- P3	97.2(2)
P2	- W	- P3	91.5(2)
P1	- W	- HW	65.6(4)
P2	- W	- HW	67.0(5)
P3	- W	- HW	131.0(5)
Cl1	- W	- Cl2	78.2(2)
Cl1	- W	- P1	151.1(4)
Cl1	- W	- P2	85.3(4)
Cl1	- W	- P3	80.5(2)
Cl1	- W	- HW	136.1(5)
Cl2	- W	- P1	73.0(4)
Cl2	- W	- P2	163.5(3)
Cl2	- W	- P3	85.8(2)
Cl2	- W	- HW	126.2(5)
W	- P1	- C11	114.4(4)
W	- P1	- C12	119.5(5)
C11	- P1	- C12	100.0(5)
W	- P2	- C21	119.4(6)
W	- P2	- C22	117.4(3)
C21	- P2	- C22	100.3(4)
W	- P3	- C31	119.5(5)
W	- P3	- C32	115.8(4)
W	- P3	- C33	116.7(4)
C31	- P3	- C33	101.9(4)
C31	- P3	- C32	100.1(4)
C32	- P3	- C33	99.7(5)
P1	- C11	- H11a	112.4(10)
P1	- C11	- H11b	108.5(9)
H11a	- C11	- H11b	108.8(10)
P1	- C12	- H12a	106.4(10)
P1	- C12	- H12b	109.6(8)
P1	- C12	- H12c	110.8(7)
H12a	- C12	- H12b	111.6(11)
H12a	- C12	- H12c	109.5(12)
H12b	- C12	- H12c	109.0(12)

P2	- C21	- H21a	112.1(13)
P2	- C21	- H21b	110.5(8)
H21a	- C21	- H21b	109.0(9)
P2	- C22	- H22a	112.5(10)
P2	- C22	- H22b	111.7(8)
P2	- C22	- H22c	108.5(8)
H22a	- C22	- H22b	110.5(10)
H22a	- C22	- H22c	106.7(11)
H22b	- C22	- H22c	106.7(12)
P3	- C31	- H31a	110.0(10)
P3	- C31	- H31b	111.1(9)
P3	- C31	- H31c	111.4(13)
H31a	- C31	- H31b	109.7(15)
H31a	- C31	- H31c	108.2(13)
H31b	- C31	- H31c	106.3(13)
P3	- C32	- H32a	110.7(9)
P3	- C32	- H32b	110.3(8)
P3	- C32	- H32c	109.9(10)
H32a	- C32	- H32b	109.1(15)
H32a	- C32	- H32c	108.1(12)
H32b	- C32	- H32c	108.8(12)
P3	- C33	- H33a	108.5(9)
P3	- C33	- H33b	110.7(9)
P3	- C33	- H33c	111.0(12)
H33a	- C33	- H33b	110.2(17)
H33a	- C33	- H33c	105.0(13)
H33b	- C33	- H33c	111.2(12)

Neutron Diffraction Data for $W(PMe_3)_4H_2F(FHF)$

Table 1. Data Collection and Refinement Parameters.

name	:	W(PMe3)4H2F2HF
formula	:	W P4 C12 H39 F3
Mr	:	548.2040 au
spacegroup	:	Cmc21 (36)
Z	:	4
a	:	14.004 (4) A
b	:	12.676 (6) A
c	:	12.062 (4) A
alpha	:	90. degr
beta	:	90. degr
gamma	:	90. degr
volume	:	2141.2(23) A3
how determined	:	least-squares fit for 32 refls, 45 < 2theta < 58
density calculated	:	1.7003 g.cm-3
absorption coefficient	:	3.048 cm-1
F000	:	-95.4972 fm
forms	:	+-(111) +-(11-1) +-(001) (-2 2 1) (4 -2 -1)
shape crystal	:	irregular
color crystal	:	orange
dimension crystal	:	appr. 4.0 x 2.8 x 1.2 mm
volume crystal	:	10.5 mm3
mounted on	:	aluminum pin
mounted with	:	halocarbon grease
mounted along	:	(111)
machine	:	H6M
wavelength	:	1.0462 A
monochromator	:	Be (002)
temperature controller	:	DISPLEX Model CS-202. Air Products Chemical, Inc. helium cryostat
scattering lengths :		
W	:	4.77 fm
F	:	5.654 fm
P	:	5.13 fm

C	:	6.6460 fm
H	:	-3.7406 fm

temperature	:	15.0 (5) K
monitor reflections	:	(6 6 -5) (-10 0 4)
reflections collected	:	2433
> 3 sigma	:	1494
negative intensity	:	147
(2theta)max	:	110
(sin theta/lambda)max	:	0.79
Lp correction	:	Lorentz
decay	:	no
decay correction	:	none
psi scan	:	(1 1 1)
absorption correction	:	yes
minimum	:	1.405 0.712
maximum	:	2.124 0.471
average	:	1.610 0.621
reflections averaged	:	2
Rint	:	0.0181
Rwint	:	0.0004
collected once	:	2333
independent reflections	:	2335
without absences	:	2335
> 3 sigma	:	1396

solved structure	:	x-ray known
program used	:	UPALS
variables	:	sc xyz bij (Biso W) ext
number of variables	:	280
extinction type	:	type I, isotropic (Becker + Coppens)
extinction coefficient	:	0.2582E+04 (0.1822E+03)
max extinction corr	:	1.19 for (800)
reflections used	:	2335 (all)
ratio refls/vars	:	8.3
p	:	0.00
(delta/sigma)max	:	< 0.1

F / F2	:	F2
R(F2)	:	0.10496
Rw(F2)	:	0.07427
S(F2)	:	1.02244
R(F)	:	0.09251
Rw(F)	:	0.03883
S(F)	:	1.00308
diff. Fourier	:	residual : pos 2.0 %, neg 2.4 % of maximum

Table 2. Atomic coordinates and displacement parameters

	x	y	z	Uiso/U11	U22	U33	U12	U13	U23
W	0.0000	0.7553(3)	0.0000	0.0017(5)					
F1	0.0000	0.8742(3)	-0.1164(4)	0.0077(13)	0.0078(13)	0.0067(13)	0.0000	0.0000	0.0025(11)
F2	0.0000	0.6766(3)	-0.1548(4)	0.0074(12)	0.0095(13)	0.0049(13)	0.0000	0.0000	0.0006(11)
F	0.0000	0.7431(3)	-0.3401(4)	0.0180(15)	0.0176(16)	0.0068(14)	0.0000	0.0000	0.0040(13)
P1	0.0000	0.5731(3)	0.0626(4)	0.0034(13)	0.0050(13)	0.0066(14)	0.0000	0.0000	0.0015(11)
P2	0.0000	0.9158(3)	0.1091(4)	0.0054(13)	0.0033(13)	0.0051(13)	0.0000	0.0000	-0.0012(11)
P3	-0.1728(1)	0.7556(2)	-0.0403(3)	0.0036(8)	0.0078(9)	0.0047(8)	-0.0005(8)	-0.0004(8)	0.0001(8)
C11	0.0000	0.4719(2)	-0.0455(4)	0.0093(11)	0.0071(11)	0.0099(12)	0.0000	0.0000	-0.0016(10)
C12	-0.0980(1)	0.5271(2)	0.1485(3)	0.0069(8)	0.0084(8)	0.0096(8)	-0.0002(7)	0.0025(7)	0.0033(7)
C21	0.0000	0.9020(2)	0.2590(4)	0.0170(14)	0.0089(12)	0.0068(12)	0.0000	0.0000	-0.0035(10)
C22	-0.0976(1)	1.0071(2)	0.0874(3)	0.0089(8)	0.0092(8)	0.0144(9)	0.0029(7)	-0.0035(8)	-0.0020(7)
C31	-0.2601(1)	0.7651(2)	0.0704(3)	0.0080(8)	0.0121(9)	0.0092(8)	0.0005(7)	0.0034(7)	0.0000(7)
C32	-0.2159(2)	0.6399(2)	-0.1142(3)	0.0074(8)	0.0102(8)	0.0097(8)	-0.0020(7)	-0.0014(7)	-0.0026(7)
C33	-0.2100(2)	0.8570(2)	-0.1373(3)	0.0105(9)	0.0094(8)	0.0091(8)	0.0013(7)	-0.0029(7)	0.0012(7)
HW	0.0641(3)	0.7404(4)	0.1189(4)	0.0189(18)	0.0213(20)	0.0192(18)	0.0026(17)	-0.0065(16)	0.0026(17)
HF	0.0000	0.7234(5)	-0.2632(6)	0.0195(27)	0.0214(29)	0.0177(28)	0.0000	0.0000	0.0042(22)
H11a	0.0000	0.3945(5)	-0.0078(8)	0.0470(43)	0.0097(25)	0.0379(40)	0.0000	0.0000	0.0006(26)
H11b	0.0626(4)	0.4814(4)	-0.0968(5)	0.0281(24)	0.0294(25)	0.0363(25)	-0.0033(19)	0.0160(21)	-0.0067(21)
H12a	-0.1012(4)	0.5755(4)	0.2226(5)	0.0357(27)	0.0285(22)	0.0190(20)	-0.0054(22)	0.0072(21)	-0.0027(18)
H12b	-0.1657(4)	0.5351(5)	0.1050(5)	0.0158(24)	0.0435(29)	0.0358(28)	-0.0004(19)	0.0000(20)	0.0058(25)
H12c	-0.0880(4)	0.4448(3)	0.1702(5)	0.0314(26)	0.0164(18)	0.0377(27)	0.0004(18)	0.0119(22)	0.0088(18)
H21a	0.0000	0.9792(5)	0.2986(7)	0.0412(41)	0.0146(27)	0.0265(34)	0.0000	0.0000	-0.0102(26)
H21b	0.0624(4)	0.8594(5)	0.2828(5)	0.0368(27)	0.0431(29)	0.0264(25)	0.0172(25)	-0.0045(22)	-0.0019(23)
H22a	-0.1004(4)	1.0264(4)	-0.0012(5)	0.0343(26)	0.0371(27)	0.0250(23)	0.0120(25)	-0.0013(23)	0.0094(21)
H22b	-0.1635(4)	0.9734(5)	0.1107(6)	0.0118(23)	0.0394(29)	0.0594(39)	-0.0047(19)	0.0011(21)	-0.0085(29)
H22c	-0.0853(4)	1.0806(4)	0.1329(6)	0.0315(27)	0.0224(21)	0.0419(28)	0.0028(20)	-0.0069(23)	-0.0143(21)
H31a	0.2486(5)	0.8364(4)	0.1171(6)	0.0370(28)	0.0331(25)	0.0345(24)	-0.0064(23)	0.0084(21)	-0.0172(22)
H31b	-0.2512(4)	0.7007(4)	0.1255(5)	0.0328(26)	0.0349(26)	0.0267(23)	0.0057(23)	0.0091(20)	0.0127(22)

H31c	-0.3319(3)	0.7633(5)	0.0395(5)	0.0134(19)	0.0515(34)	0.0348(26)	-0.0003(22)	0.0023(18)	-0.0034(26)	
H32a	-0.2899(4)	0.6490(4)	-0.1384(5)	0.0150(20)	0.0328(24)	0.0410(30)	-0.0012(18)	-0.0092(20)	-0.0077(23)	
H32b	-0.2098(4)	0.5710(4)	-0.0624(6)	0.0380(29)	0.0215(22)	0.0426(30)	-0.0034(21)	-0.0149(26)	0.0086(21)	
H32c	-0.1727(4)	0.6277(4)	-0.1872(5)	0.0373(27)	0.0329(26)	0.0283(24)	-0.0076(22)	0.0138(23)	-0.0145(22)	
H33a	-0.1955(4)	0.9341(4)	-0.1041(6)	0.0448(32)	0.0160(19)	0.0401(27)	0.0004(20)	-0.0186(26)	-0.0012(20)	
H33b	-0.2854(4)	0.8491(4)	-0.1568(6)	0.0150(21)	0.0399(28)	0.0424(29)	-0.0015(19)	-0.0113(22)	0.0111(26)	
H33c	-0.1669(4)	0.8490(4)	-0.2120(5)	0.0339(27)	0.0372(27)	0.0228(22)	0.0086(22)	0.0136(22)	0.0090(22)	

50

Table 3. Selected Bond Lengths (Å)

W	-	HW	1.702(5)
W	-	HW'	1.702(5)
W	-	F1	2.060(5)
W	-	F2	2.117(5)
W	-	P1	2.431(5)
W	-	P2	2.422(5)
W	-	P3	2.468(2)
W	-	P3'	2.468(2)
F2	...	HF	1.436(9)
F	-	HF	0.961(9)
P1	-	C11	1.829(6)
P1	-	C12	1.816(4)
P1	-	C12'	1.816(4)
P2	-	C21	1.815(6)
P2	-	C22	1.811(3)
P2	-	C22'	1.811(3)
P3	-	C31	1.814(4)
P3	-	C32	1.820(4)
P3	-	C33	1.814(4)
C11	-	H11a	1.081(8)
C11	-	H11b	1.080(6)
C11	-	H11b'	1.080(6)
C12	-	H12a	1.085(7)
C12	-	H12b	1.089(6)
C12	-	H12c	1.085(5)
C21	-	H21a	1.089(8)
C21	-	H21b	1.067(6)
C21	-	H21b'	1.067(6)
C22	-	H22a	1.098(7)
C22	-	H22b	1.055(6)
C22	-	H22c	1.094(6)
C31	-	H31a	1.076(7)
C31	-	H31b	1.061(6)
C31	-	H31c	1.073(5)
C32	-	H32a	1.083(6)
C32	-	H32b	1.077(6)

C32	- H32c	1.079(7)	
C33	- H33a	1.076(6)	
C33	- H33b	1.086(6)	
C33	- H33c	1.090(7)	
HW	... HW	1.796(8)	

F1	... H21a	2.122(8)	
F2	... HF	1.436(9)	
HF	- F	0.961(9)	170.6(7)

H...H > 2.35 except :

H12b	... H32b	55501	2.159(9)
H12c	... H32c	56504	2.283(9)
H21b	... H32a	56508	2.279(8)
H22a	... H33a	55501	2.164(8)
H22b	... H31a	55501	2.108(8)
H32b	... H33a	44506	2.240(8)

53

Table 4. Selected Bond Angles (°)

F1	- W	- F2		75.2(2)
F1	- W	- P1		155.1(2)
F1	- W	- P2		75.9(2)
F1	- W	- P3		82.2(1)
F1	- W	- HW		131.0(2)
F2	- W	- P1		80.0(2)
F2	- W	- P2		151.1(2)
F2	- W	- P3		80.0(1)
F2	- W	- HW		133.7(2)
P1	- W	- P2		129.0(2)
P1	- W	- P3		93.6(1)
P2	- W	- P3		96.1(1)
P1	- W	- HW		68.5(2)
P2	- W	- HW		68.6(2)
P3	- W	- HW		133.1(2)
W	- F2	... HF		127.4(3)
W	- P1	- C11		116.4(2)
W	- P1	- C12		118.8(1)
C11	- P1	- C12		100.5(2)
W	- P2	- C21		117.4(2)
W	- P2	- C22		117.3(2)
C21	- P2	- C22		101.8(2)
W	- P3	- C31		121.0(2)
W	- P3	- C32		114.9(1)
W	- P3	- C33		114.2(2)
C31	- P3	- C32		101.0(2)
C31	- P3	- C33		103.5(2)
C32	- P3	- C33		99.2(2)
P1	- C11	- H11a		109.6(6)
P1	- C11	- H11b		109.2(3)
H11a	- C11	- H11b		110.1(4)
P1	- C12	- H12a		108.7(3)
P1	- C12	- H12b		110.7(4)
P1	- C12	- H12c		110.4(4)
H12a	- C12	- H12b		108.0(5)
H12a	- C12	- H12c		110.5(5)

H12b	- C12	- H12c	108.5(5)
P2	- C21	- H21a	110.5(5)
P2	- C21	- H21b	108.5(4)
H21a	- C21	- H21b	109.7(5)
P2	- C22	- H22a	108.1(4)
P2	- C22	- H22b	111.3(4)
P2	- C22	- H22c	110.6(4)
H22a	- C22	- H22b	108.6(5)
H22a	- C22	- H22c	107.7(5)
H22b	- C22	- H22c	110.4(5)
P3	- C31	- H31a	109.9(4)
P3	- C31	- H31b	109.4(4)
P3	- C31	- H31c	112.0(4)
H31a	- C31	- H31b	107.5(6)
H31a	- C31	- H31c	109.8(5)
H31b	- C31	- H31c	108.1(5)
P3	- C32	- H32a	111.3(3)
P3	- C32	- H32b	110.1(4)
P3	- C32	- H32c	109.2(3)
H32a	- C32	- H32b	108.6(5)
H32a	- C32	- H32c	109.3(6)
H32b	- C32	- H32c	108.2(5)
P3	- C33	- H33a	110.5(4)
P3	- C33	- H33b	110.7(4)
P3	- C33	- H33c	107.9(3)
H33a	- C33	- H33b	110.3(5)
H33a	- C33	- H33c	106.7(5)
H33b	- C33	- H33c	110.6(6)
F2	... HF	- F	170.6(7)