JOURNAL OF THE AMERICAN CHEMICAL SOCIETY
J. Am. Chem. Soc., 1996, 118(50), 12866-12867, DOI:10.1021/ja9621408

Spectral Data of Compounds 2-5.

(*TBPY*-5-15)-3,3-Bis(trifluoromethyl)-1-butyl-1-[2-(2,2,2-trifluoro-1-hydroxy-1-(trifluoromethyl)ethyl]phenyl-3*H*-2,1λ^5-benzoxaphosphole (2): colorless crystal; mp 119 °C; ^{1}H NMR ($CDCl_3$) δ 9.13 (br s, 1H), 8.07–8.02 (m, 1H), 7.89–7.85 (m, 1H), 7.80–7.72 (m, 3H), 7.55–7.48 (m, 1H), 7.45–7.41 (m, 1H), 7.36–7.32 (m, 1H), 6.16 (dd, $^1J_{H\text{-}P}$ = 273 Hz, $^3J_{H\text{-}H}$ = 5.9 Hz, 1H), 3.21–3.06 (m, 1H), 2.69–2.52 (m, 1H), 1.65–1.46 (m, 1H), 1.45–1.36 (m, 2H), 1.35–1.22 (m, 1H), 0.88 (t, $^3J_{H\text{-}H}$ = 7.3 Hz, 3H); ^{13}C NMR ($CDCl_3$) δ 136.6 (d, $^2J_{C\text{-}P}$ = 12.8 Hz), 136.1 (d, $^1J_{C\text{-}P}$ = 139.7 Hz), 134.7, 134.3 (d, $^3J_{C\text{-}P}$ = 14.7 Hz), 134.1 (d, $^3J_{C\text{-}P}$ = 14.7 Hz), 130.8 (d, $^2J_{C\text{-}P}$ = 16.5 Hz), 130.2, 129.8 (d, $^1J_{C\text{-}P}$ = 139.7 Hz), 129.7, 129.1 (d, $^2J_{C\text{-}P}$ = 16.6 Hz), 127.0 (d, $^3J_{C\text{-}P}$ = 12.9 Hz), 123.4 (q, $^1J_{C\text{-}F}$ = 290.4 Hz), 122.7 (q, $^1J_{C\text{-}F}$ = 286.8 Hz), 122.5 (q, $^1J_{C\text{-}F}$ = 286.8 Hz), 122.3 (q, $^1J_{C\text{-}F}$ = 288.6 Hz), 78.9 (sept, $^2J_{C\text{-}F}$ = 31.2 Hz), 78.6 (sept, $^2J_{C\text{-}F}$ = 31.2 Hz), 34.7 (d, $^1J_{C\text{-}P}$ = 90.1 Hz), 27.7, 23.5 (d, $^2J_{C\text{-}P}$ = 23.9 Hz), 13.6; ^{19}F NMR ($CDCl_3$) δ –72.9 (br s, 3F), –76.3 (q, $^4J_{F\text{-}F}$ = 9.2 Hz, 3F), –76.8 (q, $^4J_{F\text{-}F}$ = 8.2 Hz, 3F), –77.0 (qq, $^4J_{F\text{-}F}$ = 9.2 Hz, $^9J_{F\text{-}F}$ = 4.9 Hz, 3F); ^{31}P NMR ($CDCl_3$) δ –34.4; Anal. Calcd for $C_{22}H_{19}F_{12}O_2P$: C, 46.01; H, 3.33. Found: C, 46.09; H, 3.24.

(*TBPY*-5-11)-1-Butyl-3,3,3',3'-tetrakis(trifluoromethyl)-1,1'-spirobi[3*H*,2,1λ^5-benzoxaphosphole] (3): colorless crystal; mp 109 °C; ^{1}H NMR ($CDCl_3$) δ 8.43–8.38 (m, 2H), 7.72–7.58 (m, 6H), 2.34 (ddt, $^2J_{H\text{-}P}$ = 28.3 Hz, $^2J_{H\text{-}H}$ = 12.2 Hz, $^3J_{H\text{-}H}$ = 4.9 Hz, 1H), 2.20 (ddt, $^2J_{H\text{-}P}$ = 12.2 Hz, $^2J_{H\text{-}H}$ = 12.2 Hz, $^3J_{H\text{-}H}$ = 4.4 Hz, 1H), 1.86–1.70 (m, 1H), 1.32–1.20 (m, 3H), 0.81 (t, $^3J_{H\text{-}H}$ = 7.3 Hz, 3H); ^{13}C NMR ($CDCl_3$) δ 137.1 (d, $^3J_{C\text{-}P}$ = 9.2 Hz), 136.2 (d, $^2J_{C\text{-}P}$ = 18.4 Hz), 133.6 (d, $^4J_{C\text{-}P}$ = 3.6 Hz), 131.3(d, $^2J_{C\text{-}P}$ = 14.7 Hz), 130.3 (d, $^1J_{C\text{-}P}$ = 160.0 Hz), 124.8 (d, $^3J_{C\text{-}P}$ = 14.7 Hz), 122.7 (q, $^1J_{C\text{-}F}$ = 286.8 Hz), 122.5 (q, $^1J_{C\text{-}F}$ = 290.5 Hz), 81.3 (sept, $^2J_{C\text{-}F}$ = 31.2 Hz), 39.2 (d, $^1J_{C\text{-}P}$ = 115.8 Hz), 25.3 (d, $^3J_{C\text{-}P}$ = 7.4 Hz), 23.6 (d, $^2J_{C\text{-}P}$ = 23.9 Hz), 13.2; ^{19}F NMR ($CDCl_3$) δ –75.1 (q, $^4J_{F\text{-}F}$ = 9.3 Hz, 6F), –75.4 (q, $^4J_{F\text{-}F}$ = 9.3 Hz, 6F); ^{31}P NMR ($CDCl_3$) δ –18.8; Anal. Calcd for $C_{22}H_{17}F_{12}O_2P$: C, 46.17; H, 2.99. Found: C, 46.19; H, 2.84.

(*TBPY*-5-12)-1-Butyl-3,3,3',3'-tetrakis(trifluoromethyl)-1,1'-spirobi[3*H*,2,1λ^5-benzoxaphosphole] (4): colorless crystal; mp 115 °C; ^{1}H NMR ($CDCl_3$, 20 °C) δ 7.75–7.69 (m, 2H), 7.65–7.61 (m, 2H), 7.59–7.56 (m, 4H), 2.48 (dt, $^2J_{H\text{-}P}$ = 17.1 Hz, $^3J_{H\text{-}H}$ = 6.8 Hz, 2H), 1.67–1.54 (m, 2H), 1.39–1.29 (m, 2H), 0.83 (t, $^3J_{H\text{-}H}$ = 7.3 Hz, 3H); ^{1}H NMR (toluene-*d*$_8$, -54 °C) δ 7.69 (br s, 1H), 7.52 (br s, 1H), 7.43–7.00 (m, 4H), 6.94 (br s, 1H), 6.85 (br s, 1H), 2.61 (br s, 1H), 2.17 (br s, 1H), 2.08 (br s, 1H) 1.22 (br s, 3H) 0.85 (br s, 3H); ^{13}C NMR ($CDCl_3$, 20 °C) δ 135.9 (br d, $^1J_{C\text{-}P}$ = 88.3 Hz), 134.2 (d, $^2J_{C\text{-}P}$ = 16.5 Hz), 132.2, 132.0 (d, $^3J_{C\text{-}P}$ = 11.1 Hz), 130.3 (d, $^2J_{C\text{-}P}$ = 11.1 Hz), 125.5 (d, $^3J_{C\text{-}P}$ = 11.0 Hz), 122.5 (dq, $^3J_{C\text{-}P}$ = 7.4 Hz, $^1J_{C\text{-}F}$ = 286.8 Hz), 122.0 (q, $^1J_{C\text{-}F}$ = 288.8 Hz), 79.9 (sept, $^2J_{C\text{-}F}$ = 31.3 Hz), 40.2 (d, $^1J_{C\text{-}P}$ = 114.0 Hz), 24.7 (d, $^3J_{C\text{-}P}$ = 7.4 Hz), 24.0 (d, $^2J_{C\text{-}P}$ = 20.2 Hz), 13.3; ^{19}F NMR ($CDCl_3$, 20 °C) δ –74.9 (q, $^4J_{F\text{-}F}$ = 8.5 Hz, 6F), –76.2 (q, $^4J_{F\text{-}F}$ = 8.5 Hz, 6F); ^{19}F NMR (toluene-*d*$_8$, -54 °C) δ –74.5 (br s, 6F), –75.5 (br s, 3F), –76.1 (br s, 3F); ^{9}F NMR (toluene-*d*$_8$, -70 °C) δ –74.3 (br s, 3F), –74.5 (br s, 3F), –75.5 (br s, 3F), –76.0 (br s, 3F); ^{31}P NMR ($CDCl_3$, 20 °C) δ –3.5; ^{31}P NMR (toluene-*d*$_8$, -54 °C) δ –3.6. Anal. Calcd for $C_{22}H_{17}F_{12}O_2P$: C, 46.17; H, 2.99. Found: C, 46.17; H, 2.72.

(*TBPY*-5-11)-(*R,*S**)-1-Butyl-3-methyl-3,3,3'-tris(trifluoromethyl)-1,1'-spirobi[3*H*,2,1λ^5-benzoxaphosphole] (5-*exo*):** colorless oil; ^{1}H NMR ($CDCl_3$) δ 8.43–8.38 (m, 2H), 7.72–7.51 (m, 6H), 2.21 (dt, $^2J_{H\text{-}P}$ = 14.7 Hz, $^3J_{H\text{-}H}$ = 7.3 Hz, 2H), 1.76 (s, 3H), 1.83–1.56 (m, 2H), 1.35–1.15 (m, 3H), 0.82 (t, $^3J_{H\text{-}H}$ = 7.3 Hz, 3H); ^{19}F NMR ($CDCl_3$) δ –75.4 (m, 6F), –79.7 (s, 3F); ^{31}P NMR ($CDCl_3$) δ –22.2.

(*TBPY*-5-11)-(*R,*R**)-1-Butyl-3-methyl-3,3,3'-tris(trifluoromethyl)-1,1'-spirobi[3*H*,2,1λ^5-benzoxaphosphole] (5-*endo*):** colorless crystal; mp 72-73 °C; ^{1}H NMR ($CDCl_3$) δ 8.45–8.36 (m, 1H), 8.35–8.26 (m, 1H), 7.80–7.44 (m, 6H), 2.41 (dddd, $^2J_{H\text{-}P}$ = 17.1 Hz, $^2J_{H\text{-}H}$ = 12.3 Hz, $^3J_{H\text{-}H}$ = 12.3 Hz, $^3J_{H\text{-}H}$ = 4.8 Hz, 1H), 2.22 (dddd, $^2J_{H\text{-}P}$ = 12.3 Hz, $^2J_{H\text{-}H}$ = 12.3 Hz, $^3J_{H\text{-}H}$ = 12.3 Hz, $^3J_{H\text{-}H}$ = 3.8 Hz, 1H), 1.73 (s, 3H), 1.84–1.68 (m, 2H), 1.35–1.15 (m, 3H), 0.81 (t, $^3J_{H\text{-}H}$ = 7.3 Hz, 3H); ^{19}F NMR ($CDCl_3$) δ –74.9 (q, $^4J_{F\text{-}F}$ = 9.3 Hz, 3F), –75.4 (q, $^4J_{F\text{-}F}$ = 9.3 Hz, 3F), –80.1 (s, 3F); ^{31}P NMR ($CDCl_3$) δ –22.7.

Table 1. Rates of Pseudorotation between **4-*R*** and **4-*S*** in Toluene-d_8

temp (K)	k (sec^{-1})
223	1.50×10^2
228	2.43×10^2
231	3.41×10^2
233	4.15×10^2
235	5.05×10^2
237	6.00×10^2
239	7.05×10^2
241	8.70×10^2
243	1.03×10^3

Table 2. Rates of Pseudorotation of **3** to **4** in Toluene-d_8

temp (K)	k (sec^{-1})	$\Delta G^{\neq}$ (kcal mol^{-1})
302	$(1.18 \pm 0.01) \times 10^{-5}$	24.5
308	$(2.45 \pm 0.04) \times 10^{-5}$	24.5
313	$(4.03 \pm 0.07) \times 10^{-5}$	24.6
318	$(7.61 \pm 0.12) \times 10^{-5}$	24.6
323	$(1.29 \pm 0.01) \times 10^{-4}$	24.6
328	$(2.31 \pm 0.01) \times 10^{-4}$	24.6

Table 3. Rates of Pseudorotation between **5-*exo*** and **5-*endo*** in Toluene-d_8

temp (K)	exo:endo	exo to endo (sec^{-1})	endo to exo (sec^{-1})
442	56.3:43.7	$(2.34 \pm 0.03) \times 10^{-6}$	$(3.02 \pm 0.03) \times 10^{-6}$
448	56.2:43.8	$(3.68 \pm 0.06) \times 10^{-6}$	$(4.74 \pm 0.07) \times 10^{-6}$
453	56.2:43.8	$(5.83 \pm 0.12) \times 10^{-6}$	$(7.52 \pm 0.16) \times 10^{-6}$
458	56.1:43.9	$(9.18 \pm 0.09) \times 10^{-6}$	$(1.18 \pm 0.01) \times 10^{-5}$
463	56.0: 44.0	$(1.35 \pm 0.02) \times 10^{-5}$	$(1.74 \pm 0.02) \times 10^{-5}$

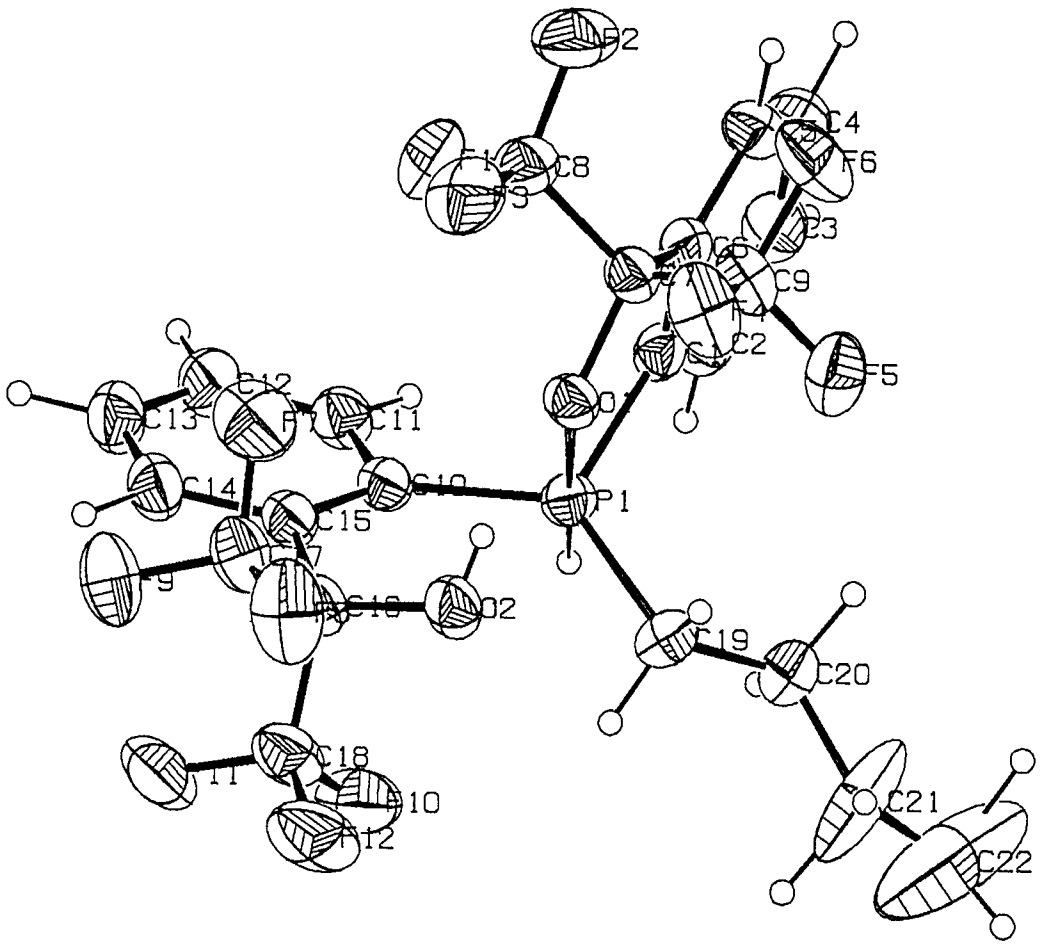
Table 4. Crystallographic Data for **2**-**4**.

compound	**2**	**3**	**4**
formula	$C_{22}H_{19}F_{12}O_2P_1$	$C_{22}H_{17}F_{12}O_2P_1$	$C_{22}H_{17}F_{12}O_2P_1$
mol wt	574.4	572.3	572.3
cryst syst	monoclinic	monoclinic	monoclinic
space group	*P*21/*n*	*P*21/*a*	*P*21/*n*
cryst dimens, mm	0.60*0.50*0.40	0.70*0.60*0.50	0.50*0.50*0.25
color	colorless	colorless	colorless
habit	prism	prism	prism
a, Å	16.653(4)	19.522(4)	12.041(2)
b, Å	12.570(3)	11.819(2)	16.936(3)
c, Å	11.523(3)	10.596(2)	11.401(2)
α, deg	90	90	90
β, deg	92.72(2)	103.50(2)	96.05(1)
γ, deg	90	90	90
V, Å^3	2409(1)	2377.4(8)	2311.9(6)
Z	4	4	4
D_{obs}, D_{calc}, g cm^{-3}	-, 1.58	-, 1.60	-, 1.66
abs coeff, cm^{-1}	19.25	19.51	20.06
F(000)	1160	1152	1152
radiation; λ, Å	Cu *K*α, 1.54178	Cu *K*α, 1.54178	Cu *K*α, 1.54178
temp, °C	23±1	23±1	23±1
2θ max, deg	130	130	130
scan rate, deg/min	6	4	3
linear decay,%	-	-	-
data collected	±*h*, -*k*, ±*l*	±*h*, +*k*, ±*l*	±*h*, +*k*, ±*l*
total data collcd, unique, obsd	4518, 4029, 3594(*F*>3σ(*F*))	4508, 3993, 3767(*F*>3σ(*F*))	4264, 3861, 3016(*F*>5σ(*F*))
R int	0.01	0.02	0.03
no of params refined	350	395	344
R, R_w, *S*	0.057, 0.091, 3.40	0.045, 0.081, 2.70	0.066, 0.093, 2.67
max shift in final cycle	0.43	0.37	0.47
final diff map, max, e/Å^3	0.91	0.41	0.92

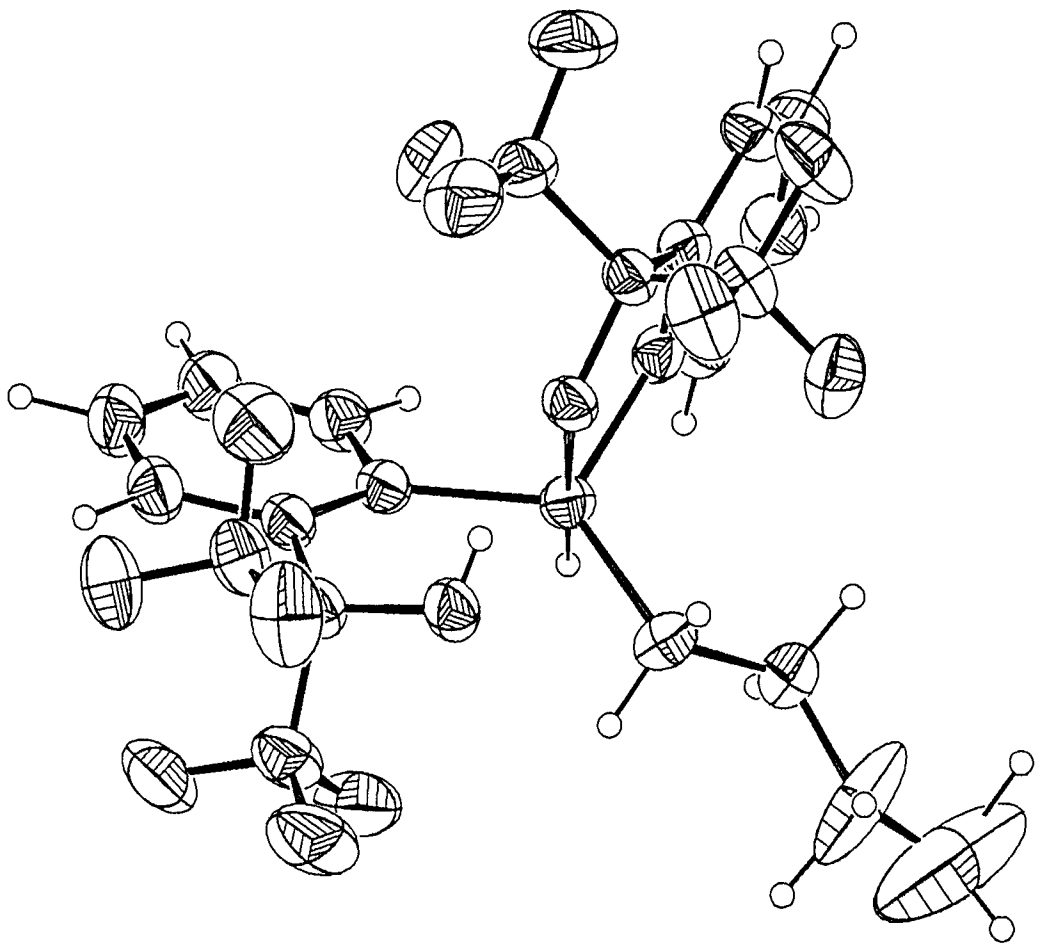
Function mimimized was sum [w($|F_o|^2$-$|F_c|^2$)^2] which w=1.0/[(sigma$|F_o|^2$+0.0007$|F_o|^2$]. R=sum[||F_o|-|F_c||)/sum|F_o|. R_w=[sumw(|F_o|-|F_c|)^2/sum$|F_o|^2$]$^{1/2}$.

Chemical Formula	C22 H19 F12 O2 P1
Formula Weight	574.40
Crystal Size	0.60 * 0.50 * 0.40 mm**3
Unit-cell Dimensions :	a = 16.653 (4) A b = 12.570 (3) A c = 11.523 (3) A alpha = beta = 92.72 (2) degrees gamma =
Volume of unit cell	2409 (1) A**3
Crystal System	Monoclinic
Space Group	P21/n (# 14)
Z value	4
Densities: Dobs ;Dcalc	; 1.58 g/cm**3
F(000)	1160
Linear Absorption Coefficient	19.25 /cm (Cu K-alpha)
Diffractometer used	Mac Science MXC3
Radiation	Cu K-alpha (lambda= 1.54178)
Maximum sine(theta)/lambda	0.584
Total Reflections Measured	4518
Unique Reflections	4029
Internal Consistency : Rint	0.01
Function Minimized was sum[w(|Fo|**2-|Fo|**2)**2] which w = 1.0/[(sigma|Fo|)**2+ 0.0004|Fo|**2]	
Reflections used (F>3.00(sig(F)))	3594
No. of Variables	350
Residuals: R; Rw	0.057; 0.091
Goodness of Fit : S	3.40
Maximum Shift/e.s.d. in final cycle	0.43
Maximum Negative Peak in Final Diff. Map	-0.89 e/A**3 (0.750 0.348 0.601)
Maximum Positive Peak in Final Diff. Map	0.91 e/A**3 (0.201-0.371-0.635)

Compound 2



Apical Carbon-Equatorial Oxyg
Phosphorane
K.-y. Akiba et al.



Apical Carbon-Equatorial Oxyg
Phosphorane
K.-y. Akiba et al. 17

***** fileio *****

...coordination no. 1 56 atoms

	cm	nb	aw	x	y	z	b					
1	P 1	0	1.00000	0.21788	-0.38258	-0.17388	0.00361	0.00763	0.00732	-0.00083	-0.00072	0.00093
2	F 1	0	1.00000	0.14418	-0.28320	0.10923	0.00891	0.01530	0.00835	-0.00066	0.00132	-0.00094
3	F 2	0	1.00000	0.05117	-0.16811	0.08659	0.00682	0.02165	0.01397	0.00198	-0.01187	0.00711
4	F 3	0	1.00000	0.17420	-0.12071	0.08124	0.00777	0.01467	0.01256	-0.00456	-0.01203	0.00033
5	F 4	0	1.00000	0.13760	-0.03833	-0.13211	0.00668	0.00848	0.02155	-0.00173	0.00260	-0.00510
6	F 5	0	1.00000	0.09170	-0.14373	-0.26379	0.00770	0.01322	0.01143	0.00062	0.00544	-0.00348
7	F 6	0	1.00000	0.01642	-0.09385	-0.13155	0.00483	0.01320	0.02339	0.00572	0.00312	0.00000
8	F 7	0	1.00000	0.35783	-0.14509	0.10076	0.00746	0.01312	0.01811	0.00102	-0.01212	-0.00013
9	F 8	0	1.00000	0.43894	-0.08240	-0.01829	0.00883	0.00963	0.02080	-0.00687	0.00335	-0.00851
10	F 9	0	1.00000	0.48020	-0.19512	0.10740	0.00622	0.01239	0.01739	-0.00247	-0.00151	-0.00863
11	F 10	0	1.00000	0.44151	-0.37227	-0.19375	0.00621	0.01559	0.01630	-0.00144	-0.00866	0.00611
12	F 11	0	1.00000	0.51840	-0.34688	-0.04249	0.00424	0.01622	0.02073	0.00448	0.00330	0.00149
13	F 12	0	1.00000	0.50211	-0.22412	-0.16905	0.00531	0.01649	0.02404	-0.00320	0.00944	0.00909
14	O 1	0	1.00000	0.19797	-0.24169	-0.11011	0.00308	0.00768	0.00861	-0.00067	-0.00199	0.00025
15	O 2	0	1.00000	0.34494	-0.20668	-0.13829	0.00358	0.00958	0.01055	-0.00179	0.00402	-0.00025
16	C 1	0	1.00000	0.11154	-0.40025	-0.15684	0.00371	0.00821	0.00678	-0.00186	-0.00022	-0.00044
17	C 2	0	1.00000	0.07219	-0.49422	-0.18996	0.00477	0.00916	0.00911	-0.00332	-0.00067	-0.00050
18	C 3	0	1.00000	-0.00963	-0.50262	-0.17626	0.00497	0.01153	0.01121	-0.00557	0.00055	-0.00027
19	C 4	0	1.00000	-0.05063	-0.41969	-0.12829	0.00393	0.01432	0.01199	-0.00437	0.00183	0.00159
20	C 5	0	1.00000	-0.01225	-0.32756	-0.09583	0.00351	0.01251	0.01053	-0.00098	-0.00110	0.00163
21	C 6	0	1.00000	0.06877	-0.31725	-0.11052	0.00352	0.00912	0.00733	-0.00133	0.00024	0.00006
22	C 7	0	1.00000	0.12087	-0.21994	-0.08074	0.00327	0.00809	0.00855	-0.00008	-0.00140	0.00002
23	C 8	0	1.00000	0.12195	-0.19689	0.04958	0.00485	0.01187	0.00929	-0.00006	-0.00481	0.00191
24	C 9	0	1.00000	0.09160	-0.12275	-0.15206	0.00390	0.00863	0.01385	0.00058	0.00022	-0.00166
25	C 10	0	1.00000	0.28442	-0.40712	-0.04400	0.00337	0.00706	0.00815	0.00027	0.00108	0.00097
26	C 11	0	1.00000	0.25779	-0.49810	0.01248	0.00412	0.00823	0.01090	-0.00125	0.00209	0.00098
27	C 12	0	1.00000	0.29214	-0.53247	0.11678	0.00528	0.00939	0.01168	-0.00035	0.00659	0.00093
28	C 13	0	1.00000	0.35658	-0.47844	0.16577	0.00522	0.01151	0.01136	0.00065	0.00679	-0.00137
29	C 14	0	1.00000	0.38609	-0.39059	0.11010	0.00402	0.01087	0.01070	-0.00067	0.00299	-0.00143
30	C 15	0	1.00000	0.35002	-0.35219	0.00637	0.00333	0.00769	0.00909	0.00008	0.00072	0.00048
31	C 16	0	1.00000	0.39170	-0.25794	-0.05191	0.00328	0.00822	0.01007	-0.00106	0.00052	-0.00068
32	C 17	0	1.00000	0.41831	-0.16997	0.03590	0.00470	0.00907	0.01393	-0.00156	-0.00067	-0.00331
33	C 18	0	1.00000	0.46386	-0.30100	-0.11527	0.00378	0.01106	0.01533	-0.00127	0.00260	0.00298
34	C 19	0	1.00000	0.24797	-0.32465	-0.30912	0.00543	0.00929	0.00758	-0.00081	-0.00009	0.00262
35	C 20	0	1.00000	0.20320	-0.37374	-0.41355	0.00586	0.01324	0.00810	0.00191	-0.00075	-0.00030
36	C 21	0	1.00000	0.23694	-0.32931	-0.52623	0.02619	0.01224	0.00675	-0.00013	0.00051	-0.00351
37	C 22	0	1.00000	0.21942	-0.36156	-0.62182	0.04476	0.02731	0.02114	0.03453	0.01654	0.03453
38	H 2	0	1.00000	0.10375	-0.55393	-0.22460	5.31080	0.00000	0.00000	0.00000	0.00000	0.00000
39	H 3	0	1.00000	-0.03931	-0.56880	-0.19936	6.25343	0.00000	0.00000	0.00000	0.00000	0.00000
40	H 4	0	1.00000	-0.10992	-0.42831	-0.11526	6.57238	0.00000	0.00000	0.00000	0.00000	0.00000
41	H 5	0	1.00000	-0.04325	-0.26665	-0.06062	5.77634	0.00000	0.00000	0.00000	0.00000	0.00000
42	H 11	0	1.00000	0.21219	-0.53928	-0.02486	5.17587	0.00000	0.00000	0.00000	0.00000	0.00000
43	H 12	0	1.00000	0.27246	-0.59490	0.16028	5.98531	0.00000	0.00000	0.00000	0.00000	0.00000
44	H 13	0	1.00000	0.38284	-0.50222	0.24174	6.38375	0.00000	0.00000	0.00000	0.00000	0.00000
45	H 14	0	1.00000	0.43482	-0.35454	0.14656	5.69008	0.00000	0.00000	0.00000	0.00000	0.00000
46	H 19A	0	1.00000	0.30687	-0.33540	-0.31748	5.27510	0.00000	0.00000	0.00000	0.00000	0.00000
47	H 19B	0	1.00000	0.23588	-0.24641	-0.30995	5.27510	0.00000	0.00000	0.00000	0.00000	0.00000
48	H 20A	0	1.00000	0.14472	-0.35482	-0.41263	6.39207	0.00000	0.00000	0.00000	0.00000	0.00000
49	H 20B	0	1.00000	0.20708	-0.45511	-0.40558	6.39207	0.00000	0.00000	0.00000	0.00000	0.00000
50	H 21A	0	1.00000	0.30541	-0.35574	-0.52532	13.50136	0.00000	0.00000	0.00000	0.00000	0.00000
51	H 21B	0	1.00000	0.25000	-0.24867	-0.52288	13.50136	0.00000	0.00000	0.00000	0.00000	0.00000
52	H 22A	0	1.00000	0.23069	-0.33685	-0.68976	25.62547	0.00000	0.00000	0.00000	0.00000	0.00000
53	H 22B	0	1.00000	0.20553	-0.44212	-0.61681	25.62547	0.00000	0.00000	0.00000	0.00000	0.00000
54	H 22C	0	1.00000	0.15011	-0.33503	-0.61437	25.62547	0.00000	0.00000	0.00000	0.00000	0.00000
55	H 1	0	1.00000	0.22699	-0.48588	-0.21651	4.30591	0.00000	0.00000	0.00000	0.00000	0.00000
56	H 2	0	1.00000	0.30243	-0.20077	-0.11861	5.31080	0.00000	0.00000	0.00000	0.00000	0.00000

***** crycar *****

a, b, c, alph, beta, gamm

16.653 12.570 11.523 90.00 92.72 90.00

...matrix no. 1

```
 16.6529999    0.0000000   -0.5465131        0.0000000
  0.0004380   12.5699997    0.0003031        0.0000000
  0.0000000    0.0000000   11.5100327        0.0000000

...matrix no.  2

  0.0600492    0.0000000    0.0028512        0.0000000
 -0.0000021    0.0795545   -0.0000022        0.0000000
  0.0000000    0.0000000    0.0868807        0.0000000

***** cartesian system *****

  1 P  1          3.72338   -4.80899   -2.00136
  2 F  1          2.34133   -3.55973    1.25724
  3 F  2          0.80481   -2.11309    0.99665
  4 F  3          2.85655   -1.51722    0.93508
  5 F  4          2.36365   -0.48179   -1.52059
  6 F  5          1.67124   -1.80673   -3.03623
  7 F  6          0.34534   -1.17973   -1.51414
  8 F  7          5.90388   -1.82359    1.15975
  9 F  8          7.31966   -1.03558   -0.21052
 10 F  9          7.93808   -2.45242    1.23618
 11 F  10         7.45835   -4.67930   -2.23007
 12 F  11         8.65614   -4.36007   -0.48906
 13 F  12         8.45403   -2.81702   -1.94577
 14 O  1          3.35697   -3.03799   -1.26737
 15 O  2          5.81986   -2.59786   -1.59172
 16 C  1          1.94319   -5.03114   -1.80523
 17 C  2          1.30600   -6.21237   -2.18645
 18 C  3         -0.06404   -6.31799   -2.02876
 19 C  4         -0.77303   -5.27556   -1.47662
 20 C  5         -0.15163   -4.11746   -1.10301
 21 C  6          1.20563   -3.98784   -1.27209
 22 C  7          2.05697   -2.76462   -0.92932
 23 C  8          2.00374   -2.47484    0.57067
 24 C  9          1.60852   -1.54297   -1.75022
 25 C  10         4.76049   -5.11739   -0.50644
 26 C  11         4.28616   -6.26100    0.14365
 27 C  12         4.80119   -6.69298    1.34414
 28 C  13         5.84753   -6.01378    1.90802
 29 C  14         6.36939   -4.90951    1.26725
 30 C  15         5.82540   -4.42687    0.07332
 31 C  16         6.55135   -3.24215   -0.59749
 32 C  17         6.94650   -2.13633    0.41321
 33 C  18         7.78766   -3.78340   -1.32676
 34 C  19         4.29838   -4.08083   -3.55798
 35 C  20         3.60990   -4.69795   -4.75997
 36 C  21         4.23335   -4.13948   -6.05692
 37 C  22         3.99383   -4.54490   -7.15717
 38 H  2          1.85050   -6.96292   -2.58515
 39 H  3         -0.54568   -7.14989   -2.29464
 40 H  4         -1.76751   -5.38394   -1.32665
 41 H  5         -0.68711   -3.35183   -0.69774
 42 H  11         3.54719   -6.77866   -0.28614
 43 H  12         4.44968   -7.47773    1.84483
 44 H  13         6.24332   -6.31266    2.78244
 45 H  14         7.16096   -4.45633    1.68691
 46 H  19A        5.28381   -4.21594   -3.65421
 47 H  19B        4.09750   -3.09736   -3.56753
 48 H  20A        2.63553   -4.46015   -4.74938
 49 H  20B        3.67016   -5.72077   -4.66824
 50 H  21A        5.37309   -4.47168   -6.04645
 51 H  21B        4.44901   -3.12583   -6.01837
 52 H  22A        4.21864   -4.23431   -7.93916
 53 H  22B        3.75979   -5.55754   -7.09950
 54 H  22C        2.83554   -4.21145   -7.07142
 55 H  1          3.89839   -6.10748   -2.49204
 56 H  2          5.10119   -2.52358   -1.36521
```

***** symrel *****

name, s11, 12, 13, tr1, s21, 22, 23, tr2, s31, 32, 33, tr3

1	no 1	1.	0.	0.	0.0000
		0.	1.	0.	0.0000
		0.	0.	1.	0.0000
2	no 2	-1.	0.	0.	0.5000
		0.	1.	0.	0.5000
		0.	0.	-1.	0.5000
3	no 3	-1.	0.	0.	0.0000
		0.	-1.	0.	0.0000
		0.	0.	-1.	0.0000
4	no 4	1.	0.	0.	0.5000
		0.	-1.	0.	0.5000
		0.	0.	1.	0.5000

***** sdista *****

#intramolecular geometries dmax= 2.00 dmin= 1.00

Intramolecular Distances (A) with e.s.d. in parentheses

atom	atom	distance	atom	atom	distance
P 1	--H 1	1.40 (4)	C 10	--C 11	1.398 (4)
P 1	--C 1	1.805 (3)	C 11	--C 12	1.376 (5)
P 1	--C 19	1.812 (3)	C 12	--C 13	1.369 (5)
P 1	--C 10	1.845 (3)	C 13	--H 13	1.005 (4)
P 1	--O 1	1.952 (2)	C 13	--C 14	1.379 (5)
F 1	--C 8	1.328 (5)	C 14	--H 14	1.004 (3)
F 2	--C 8	1.323 (5)	C 14	--C 15	1.398 (4)
F 3	--C 8	1.333 (5)	C 15	--C 16	1.543 (4)
F 4	--C 9	1.322 (4)	C 16	--C 18	1.534 (5)
F 5	--C 9	1.314 (5)	C 16	--C 17	1.549 (5)
F 6	--C 9	1.335 (4)	C 16	--H 2	1.79 (5)
F 7	--C 17	1.320 (5)	C 19	--H 19B	1.004 (3)
F 8	--C 17	1.319 (5)	C 19	--C 20	1.516 (5)
F 9	--C 17	1.327 (5)	C 20	--H 20A	1.003 (4)
F 10	--C 18	1.314 (5)	C 20	--H 20B	1.029 (4)
F 11	--C 18	1.337 (5)	C 20	--C 21	1.544 (7)
F 12	--C 18	1.327 (5)	C 21	--H 21B	1.037 (6)
O 1	--C 7	1.371 (3)	C 21	--H 21A	1.19 (1)
O 1	--H 2	1.82 (5)	C 21	--C 22	1.20 (1)
O 2	--C 16	1.392 (4)	C 21	--H 22C	1.729 (9)
C 1	--C 6	1.384 (4)	C 21	--H 22B	1.823 (6)
C 1	--C 2	1.395 (4)	C 21	--H 22A	1.885 (5)
C 2	--H 2	1.009 (3)	C 22	--H 22B	1.04 (1)
C 2	--C 3	1.383 (5)	C 22	--H 22C	1.21 (2)
C 3	--C 4	1.376 (6)	C 22	--H 21A	1.77 (2)
C 4	--H 4	1.012 (4)	C 22	--H 21B	1.88 (1)
C 4	--C 5	1.366 (6)	H 19A	--H 19B	1.6328071 (
C 5	--H 5	1.018 (4)	H 20A	--H 20B	1.6328483 (
C 5	--C 6	1.374 (4)	H 21A	--H 21B	1.6327914 (
C 6	--C 7	1.529 (4)	H 22A	--H 22C	1.6329311 (
C 7	--C 8	1.529 (5)	H 22A	--H 22B	1.6329477 (
C 7	--C 9	1.539 (5)	H 22B	--H 22C	1.6330926 (
C 10	--C 15	1.395 (4)			

***** sangle *****

#intramolecular geometries dmax= 2.00 dmin= 1.00

Apical Carbon-Equatorial Oxy

Phosphorane

K.-y. Akiba et al.

10

Intramolecular Angles (degrees) with e.s.d. in parentheses

atom	atom	atom	angle
H 1	--P 1	--C 1	93 (2)
H 1	--P 1	--C 19	92 (2)
H 1	--P 1	--C 10	93 (1)
H 1	--P 1	--O 1	176 (1)
C 1	--P 1	--C 19	117.1 (1)
C 1	--P 1	--C 10	116.5 (1)
C 1	--P 1	--O 1	83.4 (1)
C 19	--P 1	--C 10	125.8 (1)
C 19	--P 1	--O 1	91.0 (1)
C 10	--P 1	--O 1	87.3 (1)
C 7	--O 1	--H 2	150 (2)
C 7	--O 1	--P 1	116.8 (2)
H 2	--O 1	--P 1	93 (2)
C 6	--C 1	--C 2	120.0 (3)
C 6	--C 1	--P 1	118.3 (2)
C 2	--C 1	--P 1	121.7 (2)
H 2	--C 2	--C 3	121.5 (3)
H 2	--C 2	--C 1	119.4 (3)
C 3	--C 2	--C 1	119.1 (3)
C 4	--C 3	--C 2	119.9 (4)
H 4	--C 4	--C 5	119.8 (4)
H 4	--C 4	--C 3	119.0 (4)
C 5	--C 4	--C 3	121.2 (3)
H 5	--C 5	--C 4	120.4 (3)
H 5	--C 5	--C 6	119.8 (3)
C 4	--C 5	--C 6	119.7 (3)
C 5	--C 6	--C 1	120.2 (3)
C 5	--C 6	--C 7	126.7 (3)
C 1	--C 6	--C 7	113.1 (2)
O 1	--C 7	--C 8	108.2 (2)
O 1	--C 7	--C 6	108.2 (2)
O 1	--C 7	--C 9	107.6 (2)
C 8	--C 7	--C 6	110.6 (3)
C 8	--C 7	--C 9	111.3 (3)
C 6	--C 7	--C 9	110.7 (2)
F 2	--C 8	--F 1	106.7 (3)
F 2	--C 8	--F 3	107.2 (3)
F 2	--C 8	--C 7	113.5 (3)
F 1	--C 8	--F 3	106.4 (3)
F 1	--C 8	--C 7	110.1 (3)
F 3	--C 8	--C 7	112.5 (3)
F 5	--C 9	--F 4	107.7 (3)
F 5	--C 9	--F 6	105.8 (3)
F 5	--C 9	--C 7	110.4 (3)
F 4	--C 9	--F 6	106.9 (3)
F 4	--C 9	--C 7	112.2 (3)
F 6	--C 9	--C 7	113.4 (3)
C 15	--C 10	--C 11	118.1 (3)
C 15	--C 10	--P 1	133.1 (2)
C 11	--C 10	--P 1	108.8 (2)
C 12	--C 11	--C 10	122.4 (3)
C 13	--C 12	--C 11	119.3 (3)
H 13	--C 13	--C 12	120.8 (4)
H 13	--C 13	--C 14	119.5 (4)
C 12	--C 13	--C 14	119.7 (3)
H 14	--C 14	--C 13	117.7 (3)
H 14	--C 14	--C 15	120.5 (3)
C 13	--C 14	--C 15	121.7 (3)
C 10	--C 15	--C 14	118.7 (3)
C 10	--C 15	--C 16	123.9 (3)
C 14	--C 15	--C 16	117.0 (3)
O 2	--C 16	--C 18	104.3 (3)
O 2	--C 16	--C 15	114.7 (2)
O 2	--C 16	--C 17	105.6 (2)
F 7	--C 17	--F 9	107.2 (3)
F 7	--C 17	--C 16	109.7 (3)
F 9	--C 17	--C 16	115.2 (3)
F 10	--C 18	--F 12	107.6 (4)
F 10	--C 18	--F 11	107.4 (3)
F 10	--C 18	--C 16	111.4 (3)
F 12	--C 18	--F 11	106.3 (3)
F 12	--C 18	--C 16	111.7 (3)
F 11	--C 18	--C 16	112.2 (3)
H 19B	--C 19	--C 20	107.5 (3)
H 19B	--C 19	--P 1	109.8 (2)
C 20	--C 19	--P 1	111.9 (2)
H 20A	--C 20	--H 20B	107.0 (4)
H 20A	--C 20	--C 19	109.6 (3)
H 20A	--C 20	--C 21	108.4 (5)
H 20B	--C 20	--C 19	107.9 (3)
H 20B	--C 20	--C 21	114.3 (4)
C 19	--C 20	--C 21	109.6 (4)
H 21B	--C 21	--H 21A	94.2 (7)
H 21B	--C 21	--C 22	114.0 (7)
H 21B	--C 21	--C 20	114.0 (4)
H 21B	--C 21	--H 22C	103.3 (5)
H 21B	--C 21	--H 22B	146.7 (4)
H 21B	--C 21	--H 22A	95.0 (3)
H 21A	--C 21	--C 22	96 (1)
H 21A	--C 21	--C 20	106.2 (4)
H 21A	--C 21	--H 22C	140.3 (4)
H 21A	--C 21	--H 22B	92.1 (4)
H 21A	--C 21	--H 22A	90.1 (4)
C 22	--C 21	--C 20	124.7 (9)
C 22	--C 21	--H 22C	44.3 (9)
C 22	--C 21	--H 22B	32.7 (6)
C 22	--C 21	--H 22A	20.5 (6)
C 20	--C 21	--H 22C	98.7 (6)
C 20	--C 21	--H 22B	95.4 (4)
C 20	--C 21	--H 22A	144.9 (6)
H 22C	--C 21	--H 22B	54.7 (2)
H 22C	--C 21	--H 22A	53.5 (2)
H 22B	--C 21	--H 22A	52.2 (1)
H 22B	--C 22	--C 21	108.9 (9)
H 22B	--C 22	--H 22C	93 (1)
H 22B	--C 22	--H 21A	100.4 (9)
H 22B	--C 22	--H 21B	139.2 (8)
C 21	--C 22	--H 22C	92 (1)
C 21	--C 22	--H 21A	41.8 (7)
C 21	--C 22	--H 21B	30.3 (4)
H 22C	--C 22	--H 21A	133.6 (8)
H 22C	--C 22	--H 21B	88.9 (7)
H 21A	--C 22	--H 21B	53.1 (4)
C 19	--H 19B	--H 19A	35.3 (2)
C 20	--H 20A	--H 20B	37.0 (2)
C 20	--H 20B	--H 20A	36.0 (2)
C 21	--H 21A	--H 21B	39.3 (3)
C 21	--H 21A	--C 22	42.2 (5)
H 21B	--H 21A	--C 22	66.7 (4)
C 21	--H 21B	--H 21A	46.5 (6)
C 21	--H 21B	--C 22	35.6 (4)
H 21A	--H 21B	--C 22	60.2 (5)
H 22C	--H 22A	--H 22B	60.0062336 (
H 22C	--H 22A	--C 21	58.3 (3)
H 22B	--H 22A	--C 21	61.9 (2)
C 22	--H 22B	--H 22A	28.4 (6)
C 22	--H 22B	--H 22C	48 (1)
C 22	--H 22B	--C 21	38.4 (6)

```
O 2   --C 16 --H 2       24  (2)
C 18  --C 16 --C 15     108.4  (3)
C 18  --C 16 --C 17     110.9  (3)
C 18  --C 16 --H 2      126  (2)
C 15  --C 16 --C 17     112.6  (3)
C 15  --C 16 --H 2       96  (2)
C 17  --C 16 --H 2      102  (2)
F 8   --C 17 --F 7      107.0  (3)
F 8   --C 17 --F 9      106.3  (3)
F 8   --C 17 --C 16     111.0  (3)
```

```
H 22A--H 22B--H 22C     59.9964096 (
H 22A--H 22B--C 21      65.8  (2)
H 22C--H 22B--C 21      59.7  (3)
C 22  --H 22C--H 22A    31.4  (5)
C 22  --H 22C--H 22B    39.5  (6)
C 22  --H 22C--C 21     43.8  (5)
H 22A--H 22C--H 22B     59.9974208 (
H 22A--H 22C--C 21      68.1  (2)
H 22B--H 22C--C 21      65.6  (2)
C 16  --H 2   --O 1     130  (3)
```

***** torsan *****

```
# ns1, atm1, ns2, atm2, ns3, atm3
no.  1    ( 1 O 1  )    ( 1 P 1  )    ( 1 C 10 )
# ns1, atm1, ns2, atm2, ns3, atm3
no.  2    ( 1 H 1  )    ( 1 P 1  )    ( 1 C 10 )
# ns1, atm1, ns2, atm2, ns3, atm3
no.  3    ( 1 C 1  )    ( 1 P 1  )    ( 1 C 10 )
# ns1, atm1, ns2, atm2, ns3, atm3
no.  4    ( 1 C 19 )    ( 1 P 1  )    ( 1 C 10 )
# ns1, atm1, ns2, atm2, ns3, atm3
no.  5    ( 1 P 1  )    ( 1 C 10 )    ( 1 C 15 )
# ns1, atm1, ns2, atm2, ns3, atm3
no.  6    ( 1 P 1  )    ( 1 C 10 )    ( 1 C 11 )
# ns1, atm1, ns2, atm2, ns3, atm3
no.  7    ( 1 C 10 )    ( 1 C 15 )    ( 1 C 16 )
# ns1, atm1, ns2, atm2, ns3, atm3
no.  8    ( 1 C 15 )    ( 1 C 16 )    ( 1 O 2  )
# ns1, atm1, ns2, atm2, ns3, atm3
no.  9    ( 1 O 1  )    ( 1 P 1  )    ( 1 C 19 )
# ns1, atm1, ns2, atm2, ns3, atm3
no. 10    ( 1 H 1  )    ( 1 P 1  )    ( 1 C 19 )
# ns1, atm1, ns2, atm2, ns3, atm3
no. 11    ( 1 C 1  )    ( 1 P 1  )    ( 1 C 19 )
# ns1, atm1, ns2, atm2, ns3, atm3
no. 12    ( 1 P 1  )    ( 1 C 19 )    ( 1 C 20 )
# ns1, atm1, ns2, atm2, ns3, atm3
no. 13    ( 1 C 19 )    ( 1 C 20 )    ( 1 C 21 )
# ns1, atm1, ns2, atm2, ns3, atm3
no. 14    ( 1 C 20 )    ( 1 C 21 )    ( 1 C 22 )
# ns1, atm1, ns2, atm2, ns3, atm3
```

angle between plane no. a and no. b

a	b	angle	a	b	angle	a	b	angle	a	b	angle	a	b	angle
1	2	4.01	1	3	98.72	1	4	89.31	1	5	53.94	1	6	56.71
1	7	60.85	1	8	65.99	1	9	54.23	1	10	54.33	1	11	94.83
1	12	69.44	1	13	74.81	1	14	71.13	2	3	94.71	2	4	85.30
2	5	49.93	2	6	52.71	2	7	56.89	2	8	62.13	2	9	54.14
2	10	53.99	2	11	90.86	2	12	66.00	2	13	71.39	2	14	68.04
3	4	9.41	3	5	44.78	3	6	42.00	3	7	38.67	3	8	35.83
3	9	92.90	3	10	90.06	3	11	8.57	3	12	41.83	3	13	39.07
3	14	47.29	4	5	35.37	4	6	32.60	4	7	29.49	4	8	27.44
4	9	87.39	4	10	84.52	4	11	9.46	4	12	35.73	4	13	34.03
4	14	42.30	5	6	2.77	5	7	9.71	5	8	17.63	5	9	67.96
5	10	65.50	5	11	41.52	5	12	30.73	5	13	34.74	5	14	38.26
6	7	8.07	6	8	16.03	6	9	69.33	6	10	66.80	6	11	38.81
6	12	29.79	6	13	33.49	6	14	37.57	7	8	21.20	7	9	65.30
7	10	62.61	7	11	37.22	7	12	21.92	7	13	25.43	7	14	29.88
8	9	85.35	8	10	82.81	8	11	29.69	8	12	41.91	8	13	44.13
8	14	50.13	9	10	2.87	9	11	96.85	9	12	51.66	9	13	53.85
9	14	45.61	10	11	93.99	10	12	48.80	10	13	51.00	10	14	42.77
11	12	45.19	11	13	43.40	11	14	51.68	12	13	5.42	12	14	8.24
13	14	8.29												

atom x y z b(equiv.)

Positional parameters and equivalent isotropic thermal parameters with e.s.d. in parentheses

atom	x	y	z	B(eq)
P 1	0.21788 (4)	-0.38258 (6)	-0.17388 (6)	4.23 (9)
F 1	0.1442 (2)	-0.2832 (2)	0.1092 (2)	8.0 (1)
F 2	0.0512 (2)	-0.1681 (3)	0.0866 (2)	9.5 (1)
F 3	0.1742 (2)	-0.1207 (2)	0.0812 (2)	8.2 (1)
F 4	0.1376 (2)	-0.0383 (2)	-0.1321 (2)	8.1 (1)
F 5	0.0917 (2)	-0.1437 (2)	-0.2638 (2)	7.7 (1)
F 6	0.0164 (1)	-0.0938 (2)	-0.1316 (3)	8.7 (1)
F 7	0.3578 (2)	-0.1451 (2)	0.1008 (3)	8.7 (1)
F 8	0.4389 (2)	-0.0824 (2)	-0.0183 (3)	9.0 (1)
F 9	0.4802 (2)	-0.1951 (2)	0.1074 (2)	8.0 (1)
F 10	0.4415 (2)	-0.3723 (2)	-0.1938 (2)	8.4 (1)
F 11	0.5184 (1)	-0.3469 (2)	-0.0425 (3)	8.6 (1)
F 12	0.5021 (2)	-0.2241 (2)	-0.1690 (3)	9.6 (1)
O 1	0.1980 (1)	-0.2417 (2)	-0.1101 (2)	4.3 (1)
O 2	0.3449 (1)	-0.2067 (2)	-0.1383 (2)	5.2 (1)
C 1	0.1115 (2)	-0.4002 (2)	-0.1568 (2)	4.3 (1)
C 2	0.0722 (2)	-0.4942 (3)	-0.1900 (3)	5.3 (1)
C 3	-0.0096 (2)	-0.5026 (3)	-0.1763 (3)	6.2 (1)
C 4	-0.0506 (2)	-0.4197 (4)	-0.1283 (3)	6.6 (1)
C 5	-0.0122 (2)	-0.3276 (3)	-0.0958 (3)	5.8 (1)
C 6	0.0688 (2)	-0.3172 (2)	-0.1105 (2)	4.5 (1)
C 7	0.1209 (2)	-0.2199 (2)	-0.0807 (3)	4.4 (1)
C 8	0.1220 (2)	-0.1969 (3)	0.0496 (3)	5.9 (1)
C 9	0.0916 (2)	-0.1228 (3)	-0.1521 (4)	5.7 (1)
C 10	0.2844 (2)	-0.4071 (2)	-0.0440 (2)	4.2 (1)
C 11	0.2578 (2)	-0.4981 (2)	0.0125 (3)	5.2 (1)
C 12	0.2921 (2)	-0.5325 (3)	0.1168 (3)	6.0 (1)
C 13	0.3566 (2)	-0.4784 (3)	0.1658 (3)	6.4 (1)
C 14	0.3861 (2)	-0.3906 (3)	0.1101 (3)	5.7 (1)
C 15	0.3500 (2)	-0.3522 (2)	0.0064 (3)	4.4 (1)
C 16	0.3917 (2)	-0.2579 (2)	-0.0519 (3)	4.7 (1)
C 17	0.4183 (2)	-0.1700 (3)	0.0359 (4)	6.1 (1)
C 18	0.4639 (2)	-0.3010 (3)	-0.1153 (4)	6.4 (1)
C 19	0.2480 (2)	-0.3246 (3)	-0.3091 (3)	5.3 (1)
C 20	0.2032 (2)	-0.3737 (4)	-0.4136 (3)	6.4 (1)
C 21	0.2369 (6)	-0.3293 (4)	-0.5262 (4)	13.5 (3)
C 22	0.219 (1)	-0.3616 (9)	-0.6218 (8)	25.8 (8)
H 2	0.1037500 (	-0.5539300 (	-0.2246000 (	5.31 (0)
H 3	-0.0393100 (	-0.5688000 (	-0.1993600 (	6.25 (0)
H 4	-0.1099200 (	-0.4283100 (	-0.1152600 (	6.57 (0)
H 5	-0.0432499 (	-0.2666500 (	-0.0606200 (	5.78 (0)
H 11	0.2121900 (	-0.5392800 (	-0.0248600 (	5.18 (0)
H 12	0.2724600 (	-0.5949000 (	0.1602800 (	5.98 (0)
H 13	0.3828400 (	-0.5022200 (	0.2417400 (	6.38 (0)
H 14	0.4348200 (	-0.3545400 (	0.1465600 (	5.69 (0)
H 19A	0.3068700 (	-0.3354000 (	-0.3174800 (	5.28 (0)
H 19B	0.2358800 (	-0.2464100 (	-0.3099500 (	5.28 (0)
H 20A	0.1447200 (	-0.3548200 (	-0.4126300 (	6.39 (0)
H 20B	0.2070800 (	-0.4551100 (	-0.4055800 (	6.39 (0)
H 21A	0.3054100 (	-0.3557400 (	-0.5253200 (	13.50 (0)
H 21B	0.2500000 (	-0.2486700 (	-0.5228800 (	13.50 (0)
H 22A	0.2306900 (	-0.3368500 (	-0.6897600 (	25.62 (0)
H 22B	0.2055300 (	-0.4421200 (	-0.6168100 (	25.62 (0)
H 22C	0.1501100 (	-0.3350300 (	-0.6143700 (	25.62 (0)
H 1	0.227 (2)	-0.486 (3)	-0.216 (3)	4.30 (0)
H 2	0.302 (3)	-0.201 (4)	-0.119 (4)	5.31 (0)

atom u11, 22, 33, 12, 13, 23

U values with e.s.d. in parentheses

atom	u11	u22	u33	u12	u13	u23

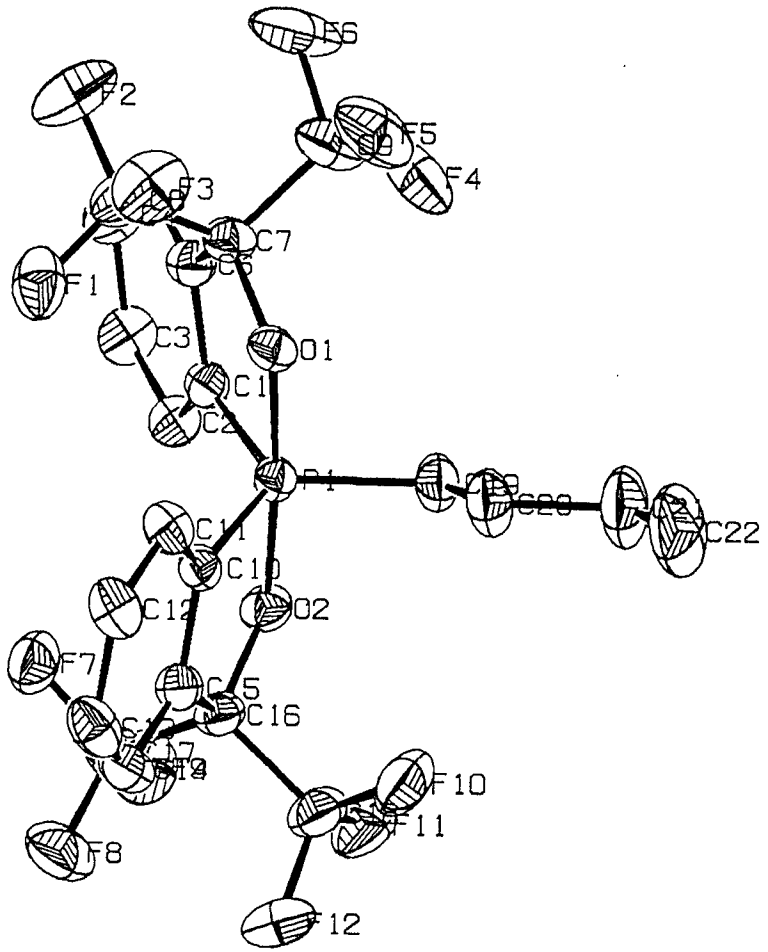
Apical Carbon-Equatorial Oxyg
Phosphorane
K.-y. Akiba et al.

P 1	0.0506 (4)	0.061 (3)	0.0491 (5)	-0.0044 (3)	0.0045 (3)	-0.0026 (3)
F 1	0.125 (2)	0.122 (4)	0.056 (1)	-0.003 (2)	-0.004 (1)	0.005 (1)
F 2	0.096 (2)	0.173 (4)	0.094 (2)	0.010 (2)	0.034 (1)	-0.044 (2)
F 3	0.109 (2)	0.117 (4)	0.084 (1)	-0.024 (1)	0.002 (1)	-0.044 (1)
F 4	0.094 (2)	0.068 (4)	0.145 (2)	-0.009 (1)	-0.025 (2)	0.010 (1)
F 5	0.108 (2)	0.106 (4)	0.077 (1)	0.003 (1)	-0.017 (1)	0.020 (1)
F 6	0.068 (1)	0.106 (4)	0.157 (2)	0.030 (1)	0.000 (1)	0.011 (2)
F 7	0.104 (2)	0.105 (4)	0.122 (2)	0.005 (1)	-0.001 (2)	-0.044 (2)
F 8	0.124 (2)	0.077 (4)	0.140 (2)	-0.036 (1)	-0.041 (2)	0.012 (1)
F 9	0.087 (2)	0.099 (4)	0.117 (2)	-0.013 (1)	-0.042 (1)	-0.006 (1)
F 10	0.087 (2)	0.125 (4)	0.109 (2)	-0.008 (1)	0.030 (1)	-0.032 (2)
F 11	0.059 (1)	0.130 (4)	0.139 (2)	0.024 (1)	0.007 (1)	0.012 (2)
F 12	0.074 (2)	0.132 (4)	0.161 (3)	-0.017 (1)	0.044 (2)	0.034 (2)
O 1	0.043 (1)	0.061 (4)	0.058 (1)	-0.0035 (8)	0.0012 (8)	-0.0073 (9)
O 2	0.050 (1)	0.077 (4)	0.071 (1)	-0.009 (1)	-0.001 (1)	0.015 (1)
C 1	0.052 (2)	0.066 (4)	0.046 (1)	-0.010 (1)	-0.002 (1)	-0.001 (1)
C 2	0.067 (2)	0.073 (4)	0.061 (2)	-0.018 (2)	-0.002 (1)	-0.002 (1)
C 3	0.070 (2)	0.092 (4)	0.075 (2)	-0.030 (2)	-0.001 (2)	0.002 (2)
C 4	0.055 (2)	0.115 (5)	0.080 (2)	-0.023 (2)	0.008 (2)	0.007 (2)
C 5	0.049 (2)	0.100 (4)	0.071 (2)	-0.005 (2)	0.008 (1)	-0.004 (2)
C 6	0.049 (2)	0.073 (4)	0.049 (2)	-0.007 (1)	0.000 (1)	0.001 (1)
C 7	0.046 (2)	0.065 (4)	0.057 (2)	-0.000 (1)	0.000 (1)	-0.005 (1)
C 8	0.068 (2)	0.095 (4)	0.062 (2)	-0.000 (2)	0.009 (2)	-0.018 (2)
C 9	0.055 (2)	0.069 (4)	0.093 (3)	0.003 (1)	-0.008 (2)	0.001 (2)
C 10	0.047 (1)	0.056 (4)	0.055 (2)	0.001 (1)	0.005 (1)	0.004 (1)
C 11	0.058 (2)	0.066 (4)	0.073 (2)	-0.007 (1)	0.005 (2)	0.008 (2)
C 12	0.074 (2)	0.075 (4)	0.078 (2)	-0.002 (2)	0.004 (2)	0.024 (2)
C 13	0.073 (2)	0.092 (4)	0.076 (2)	0.003 (2)	-0.007 (2)	0.025 (2)
C 14	0.056 (2)	0.087 (4)	0.072 (2)	-0.004 (2)	-0.007 (2)	0.011 (2)
C 15	0.047 (2)	0.062 (4)	0.061 (2)	0.000 (1)	0.002 (1)	0.003 (1)
C 16	0.046 (2)	0.066 (4)	0.068 (2)	-0.006 (1)	-0.003 (1)	0.002 (1)
C 17	0.066 (2)	0.073 (4)	0.093 (3)	-0.008 (2)	-0.016 (2)	-0.002 (2)
C 18	0.053 (2)	0.088 (4)	0.103 (3)	-0.007 (2)	0.014 (2)	0.010 (2)
C 19	0.076 (2)	0.074 (4)	0.051 (2)	-0.004 (2)	0.013 (1)	-0.000 (1)
C 20	0.082 (2)	0.106 (4)	0.054 (2)	0.010 (2)	-0.001 (2)	-0.003 (2)
C 21	0.37 (1)	0.098 (5)	0.045 (2)	-0.001 (5)	-0.017 (4)	0.002 (2)
C 22	0.63 (3)	0.22 (1)	0.142 (7)	0.18 (1)	0.17 (1)	0.061 (7)

Chemical Formula	C22 H17 F12 O2 P1
Formula Weight	572.30
Crystal Size	0.70 * 0.60 * 0.50 mm**3
Unit-cell Dimensions :	a = 19.522 (4) A b = 11.819 (2) A c = 10.596 (2) A alpha = beta = 103.50 (2) degrees gamma =
Volume of unit cell	2377.4 (8) A**3
Crystal System	Monoclinic
Space Group	P21/a (# 14)
Z value	4
Densities: Dobs ;Dcalc	: 1.60 g/cm**3
F(000)	1152
Linear Absorption Coefficient	19.51 /cm (Cu K-alpha)
Diffractometer used	Mac Science MXC3
Radiation	Cu K-alpha (lambda= 1.54178)
Maximum sine(theta)/lambda	0.585
Total Reflections Measured	4508
Unique Reflections	3993
Internal Consistency : Rint	0.02
Function Minimized was sum[w(|Fo|**2-|Fc|**2)**2] which w = 1.0/[(sigma|Fo|)**2+ 0.0007|Fo|**2]	
Reflections used (F>3.00(sig(F)))	3767
No. of Variables	395
Residuals: R; Rw	0.045; 0.081
Goodness of Fit : S	2.70
Maximum Shift/e.s.d. in final cycle	0.37
Maximum Negative Peak in Final Diff. Map	-0.34 e/A**3 (0.384 0.645 0.869)
Maximum Positive Peak in Final Diff. Map	0.41 e/A**3 (-0.136-0.229 0.217)

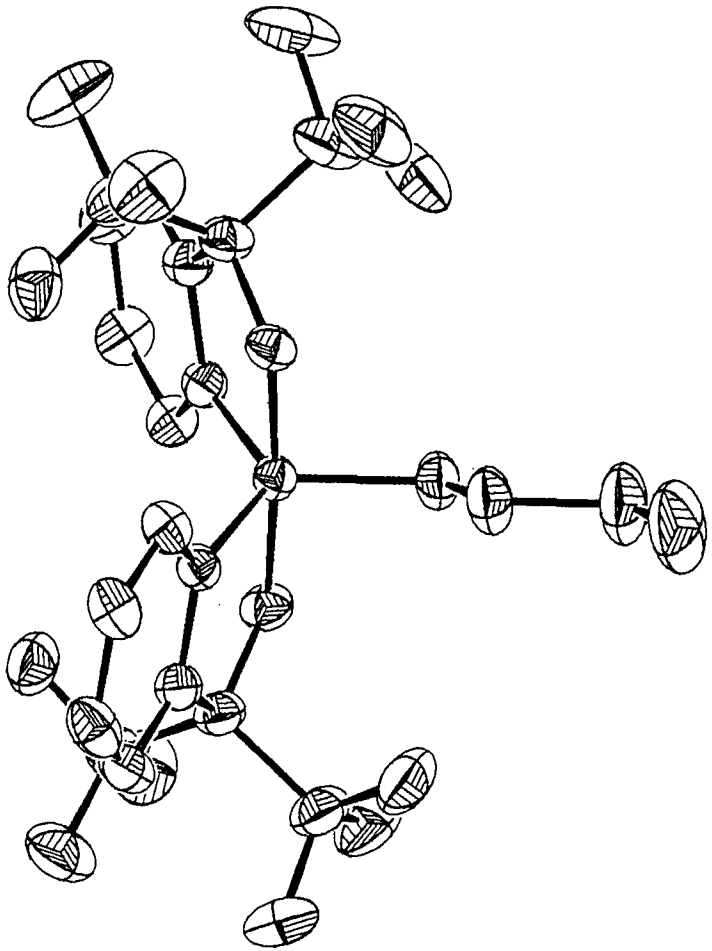
Compound 3

Apical Carbon-Equatorial Oxyg
Phosphorane
K.-y. Akiba et al.



Apical Carbon-Equatorial Oxyg
Phosphorane
K.-y. Akiba et al.

16



Apical Carbon-Equatorial Oxyg
Phosphorane
K.-y. Akiba et al.

***** file10 *****

...coordination no. 1 54 atoms

	cm	nb	aw	x	y	z	b					
1	P 1	0	1.00000	-0.11399	-0.14888	0.27027	0.00219	0.00681	0.00770	-0.00022	-0.00023	0.00177
2	F 1	0	1.00000	-0.30577	-0.13635	0.21667	0.00334	0.01542	0.01549	-0.00306	0.00325	0.00122
3	F 2	0	1.00000	-0.33698	-0.02139	0.34718	0.00415	0.01498	0.03611	0.00347	0.00487	0.01431
4	F 3	0	1.00000	-0.30654	-0.19005	0.40715	0.00508	0.01483	0.02241	-0.00283	0.00933	0.01150
5	F 4	0	1.00000	-0.13046	0.00703	0.56095	0.00811	0.01861	0.01219	-0.00537	-0.01246	0.00323
6	F 5	0	1.00000	-0.20224	-0.11281	0.60605	0.01033	0.01603	0.01021	0.00042	0.00344	0.00968
7	F 6	0	1.00000	-0.23626	0.05433	0.55005	0.01141	0.01569	0.01800	0.00707	-0.00647	0.01737
8	F 7	0	1.00000	-0.14673	-0.12939	-0.08501	0.00359	0.01293	0.01321	0.00257	0.00591	0.00197
9	F 8	0	1.00000	-0.08777	-0.25323	-0.15965	0.00774	0.01468	0.01046	0.00298	-0.00006	0.00788
10	F 9	0	1.00000	-0.04060	-0.09549	-0.08694	0.00477	0.01611	0.01709	-0.00254	0.01122	0.00679
11	F 10	0	1.00000	0.02815	-0.32592	0.21253	0.00368	0.01818	0.01841	0.00681	0.01090	0.00397
12	F 11	0	1.00000	0.06110	-0.19920	0.09761	0.00276	0.01815	0.02469	0.00171	0.00568	0.00782
13	F 12	0	1.00000	0.01922	-0.35447	0.01124	0.00522	0.01809	0.02249	0.00836	-0.00635	0.00893
14	O 1	0	1.00000	-0.17287	-0.15896	0.37335	0.00317	0.00739	0.00789	0.00002	0.00021	0.00370
15	O 2	0	1.00000	-0.06090	-0.13844	0.15823	0.00242	0.00837	0.01165	-0.00058	-0.00091	0.00427
16	C 1	0	1.00000	-0.14844	-0.00737	0.22897	0.00233	0.00687	0.00856	-0.00061	-0.00066	0.00220
17	C 2	0	1.00000	-0.12814	0.06804	0.14327	0.00284	0.00762	0.01095	-0.00081	0.00104	0.00352
18	C 3	0	1.00000	-0.15798	0.17451	0.12724	0.00383	0.00749	0.01406	-0.00045	0.00379	0.00456
19	C 4	0	1.00000	-0.20661	0.20701	0.19555	0.00386	0.00717	0.01706	0.00106	0.00233	0.00472
20	C 5	0	1.00000	-0.22700	0.13359	0.28082	0.00364	0.00803	0.01440	0.00121	-0.00019	0.00580
21	C 6	0	1.00000	-0.19793	0.02636	0.29612	0.00278	0.00745	0.00950	-0.00010	-0.00125	0.00336
22	C 7	0	1.00000	-0.21419	-0.06614	0.38363	0.00340	0.00819	0.00952	0.00078	0.00024	0.00540
23	C 8	0	1.00000	-0.29207	-0.10351	0.33943	0.00334	0.01039	0.01717	0.00056	0.00413	0.00813
24	C 9	0	1.00000	-0.19567	-0.02928	0.52714	0.00655	0.01090	0.01120	0.00103	-0.00273	0.00842
25	C 10	0	1.00000	-0.14794	-0.28038	0.19020	0.00250	0.00681	0.00732	-0.00004	0.00012	0.00179
26	C 11	0	1.00000	-0.19832	-0.35011	0.22223	0.00334	0.00776	0.00908	-0.00154	0.00032	0.00290
27	C 12	0	1.00000	-0.21624	-0.45026	0.15560	0.00422	0.00828	0.01090	-0.00260	0.00024	0.00232
28	C 13	0	1.00000	-0.18459	-0.48090	0.05744	0.00526	0.00739	0.01002	-0.00116	-0.00124	0.00145
29	C 14	0	1.00000	-0.13371	-0.41312	0.02538	0.00465	0.00828	0.00900	0.00165	-0.00127	0.00366
30	C 15	0	1.00000	-0.11599	-0.31225	0.09212	0.00288	0.00743	0.00857	0.00126	0.00103	0.00260
31	C 16	0	1.00000	-0.06215	-0.22594	0.07116	0.00267	0.00864	0.01014	0.00147	0.00028	0.00426
32	C 17	0	1.00000	-0.08369	-0.17604	-0.06747	0.00360	0.01019	0.01102	0.00085	0.00229	0.00508
33	C 18	0	1.00000	0.01246	-0.27646	0.09722	0.00319	0.01262	0.01438	0.00379	0.00242	0.00584
34	C 19	0	1.00000	-0.03862	-0.16048	0.40779	0.00280	0.00996	0.01031	-0.00035	-0.00065	-0.00049
35	C 20	0	1.00000	-0.03507	-0.27172	0.48042	0.00436	0.01085	0.01108	0.00083	0.00171	-0.00264
36	C 21	0	1.00000	0.02809	-0.27963	0.59254	0.00555	0.01605	0.01515	0.00250	0.00426	-0.00585
37	C 22	0	1.00000	0.03348	-0.39075	0.66352	0.00932	0.01741	0.01746	0.00623	0.00748	-0.00786
38	H 19A	0	1.00000	-0.00052	-0.14027	0.38693	4.85286	0.00000	0.00000	0.00000	0.00000	0.00000
39	H 19B	0	1.00000	-0.04093	-0.09383	0.47072	4.85286	0.00000	0.00000	0.00000	0.00000	0.00000
40	H 3	0	1.00000	-0.14403	0.22473	0.06673	5.15270	0.00000	0.00000	0.00000	0.00000	0.00000
41	H 5	0	1.00000	-0.25788	0.15651	0.31654	5.13040	0.00000	0.00000	0.00000	0.00000	0.00000
42	H 13	0	1.00000	-0.20363	-0.55114	0.00857	5.45664	0.00000	0.00000	0.00000	0.00000	0.00000
43	H 20A	0	1.00000	-0.07919	-0.29080	0.52018	6.06334	0.00000	0.00000	0.00000	0.00000	0.00000
44	H 2	0	1.00000	-0.09445	0.04699	0.09846	4.27202	0.00000	0.00000	0.00000	0.00000	0.00000
45	H 4	0	1.00000	-0.22954	0.28309	0.18879	5.54882	0.00000	0.00000	0.00000	0.00000	0.00000
46	H 22A	0	1.00000	0.06125	-0.42400	0.61770	11.09858	0.00000	0.00000	0.00000	0.00000	0.00000
47	H 12	0	1.00000	-0.25610	-0.49319	0.17589	5.17023	0.00000	0.00000	0.00000	0.00000	0.00000
48	H 20B	0	1.00000	-0.03780	-0.34341	0.42662	6.06334	0.00000	0.00000	0.00000	0.00000	0.00000
49	H 11	0	1.00000	-0.22208	-0.33177	0.29168	4.31371	0.00000	0.00000	0.00000	0.00000	0.00000
50	H 14	0	1.00000	-0.11228	-0.42912	-0.03378	5.01496	0.00000	0.00000	0.00000	0.00000	0.00000
51	H 21A	0	1.00000	0.06436	-0.27391	0.56109	8.45401	0.00000	0.00000	0.00000	0.00000	0.00000
52	H 21B	0	1.00000	0.00828	-0.20616	0.64843	8.45401	0.00000	0.00000	0.00000	0.00000	0.00000
53	H 22B	0	1.00000	0.06784	-0.39672	0.73784	11.09858	0.00000	0.00000	0.00000	0.00000	0.00000
54	H 22C	0	1.00000	-0.00927	-0.39349	0.67645	11.09858	0.00000	0.00000	0.00000	0.00000	0.00000

***** crycar *****

a, b, c, alph, beta, gamm

19.522 11.819 10.596 90.00 103.50 90.00

...matrix no. 1

19.5219994 0.0000000 -2.4732752 0.0000000

```
 0.0005135   11.8190002    0.0002787        0.0000000
 0.0000000    0.0000000   10.3033066        0.0000000

...matrix no.  2

 0.0512243    0.0000000    0.0122962        0.0000000
-0.0000022    0.0846095   -0.0000028        0.0000000
 0.0000000    0.0000000    0.0970562        0.0000000

***** cartesian system *****

 1 P  1        -2.89376   -1.75960    2.78467
 2 F  1        -6.50513   -1.61162    2.23242
 3 F  2        -7.43719   -0.25288    3.57710
 4 F  3        -6.99127   -2.24624    4.19499
 5 F  4        -3.93422    0.08318    5.77964
 6 F  5        -5.44706   -1.33324    6.24432
 7 F  6        -5.97269    0.64216    5.66733
 8 F  7        -2.65421   -1.52936   -0.87588
 9 F  8        -1.31859   -2.99302   -1.64492
10 F  9        -0.57757   -1.12864   -0.89577
11 F  10        0.02390   -3.85197    2.18976
12 F  11        0.95138   -2.35429    1.00571
13 F  12        0.34741   -4.18947    0.11581
14 O  1        -4.29817   -1.87873    3.84674
15 O  2        -1.58024   -1.63621    1.63029
16 C  1        -3.46415   -0.08712    2.35915
17 C  2        -2.85590    0.80414    1.47615
18 C  3        -3.39879    2.06249    1.31099
19 C  4        -4.51709    2.44660    2.01481
20 C  5        -5.12604    1.57886    2.89337
21 C  6        -4.59638    0.31153    3.05102
22 C  7        -5.13024   -0.78171    3.95266
23 C  8        -6.54129   -1.22344    3.49725
24 C  9        -5.12363   -0.34601    5.43129
25 C  10       -3.35850   -3.31383    1.95969
26 C  11       -4.42124   -4.13799    2.28970
27 C  12       -4.60628   -5.32169    1.60319
28 C  13       -3.74563   -5.68384    0.59182
29 C  14       -2.67306   -4.88273    0.26150
30 C  15       -2.49219   -3.69052    0.94914
31 C  16       -1.38929   -2.67040    0.73318
32 C  17       -1.46692   -2.08068   -0.69516
33 C  18        0.00279   -3.26745    1.00169
34 C  19       -1.76252   -1.89662    4.20159
35 C  20       -1.87285   -3.21134    4.94991
36 C  21       -0.91714   -3.30477    6.10512
37 C  22       -0.98747   -4.61807    6.83645
38 H  19A      -0.96714   -1.65774    3.98666
39 H  19B      -1.96326   -1.10887    4.84997
40 H  3        -2.97680    2.65603    0.68754
41 H  5        -5.81722    1.84975    3.26141
42 H  13       -3.99646   -6.51403    0.08830
43 H  20A      -2.83250   -3.43686    5.35957
44 H  2        -2.08737    0.55535    1.01446
45 H  4        -4.94801    3.34578    1.94516
46 H  22A      -0.33202   -5.01105    6.36435
47 H  12       -5.43461   -5.82909    1.81225
48 H  20B      -1.79308   -4.05866    4.39560
49 H  11       -5.05685   -3.92122    3.00527
50 H  14       -2.10838   -5.07184   -0.34805
51 H  21A      -0.13129   -3.23715    5.78108
52 H  21B      -1.44210   -2.43642    6.68097
53 H  22B      -0.50051   -4.68859    7.60219
54 H  22C      -1.85402   -4.65047    6.96967

***** symrel *****

# name, s11, 12, 13, tr1,  s21, 22, 23, tr2, s31, 32, 33, tr3
```

1	no 1	1.	0.	0.	0.0000
		0.	1.	0.	0.0000
		0.	0.	1.	0.0000
2	no 2	-1.	0.	0.	0.5000
		0.	1.	0.	0.5000
		0.	0.	-1.	0.0000
3	no 3	-1.	0.	0.	0.0000
		0.	-1.	0.	0.0000
		0.	0.	-1.	0.0000
4	no 4	1.	0.	0.	0.5000
		0.	-1.	0.	0.5000
		0.	0.	1.	0.0000

***** sdista *****

#intramolecular geometries dmax= 2.00 dmin= 1.00

Intramolecular Distances (A) with e.s.d. in parentheses

atom	atom	distance	atom	atom	distance
P 1	--O 2	1.753 (2)	C 1	--C 2	1.394 (3)
P 1	--O 1	1.765 (2)	C 2	--C 3	1.380 (3)
P 1	--C 1	1.818 (2)	C 3	--C 4	1.376 (4)
P 1	--C 19	1.818 (2)	C 4	--C 5	1.377 (4)
P 1	--C 10	1.820 (2)	C 5	--C 6	1.382 (3)
F 1	--C 8	1.324 (4)	C 6	--C 7	1.514 (3)
F 2	--C 8	1.323 (3)	C 7	--C 9	1.541 (4)
F 3	--C 8	1.317 (4)	C 7	--C 8	1.547 (3)
F 4	--C 9	1.312 (4)	C 10	--C 15	1.383 (3)
F 5	--C 9	1.319 (4)	C 10	--C 11	1.385 (3)
F 6	--C 9	1.324 (4)	C 11	--C 12	1.381 (3)
F 7	--C 17	1.321 (3)	C 12	--C 13	1.376 (4)
F 8	--C 17	1.325 (3)	C 13	--C 14	1.379 (4)
F 9	--C 17	1.318 (3)	C 14	--C 15	1.388 (3)
F 10	--C 18	1.324 (3)	C 15	--C 16	1.518 (3)
F 11	--C 18	1.317 (3)	C 16	--C 18	1.538 (3)
F 12	--C 18	1.324 (4)	C 16	--C 17	1.547 (3)
O 1	--C 7	1.381 (3)	C 19	--C 20	1.517 (4)
O 2	--C 16	1.382 (3)	C 20	--C 21	1.502 (4)
C 1	--C 6	1.385 (3)	C 21	--C 22	1.505 (7)

***** sangle *****

#intramolecular geometries dmax= 2.00 dmin= 1.00

Intramolecular Angles (degrees) with e.s.d. in parentheses

atom	atom	atom	angle	atom	atom	atom	angle
O 2	--P 1	--O 1	175.79 (6)	F 4	--C 9	--C 7	110.6 (3)
O 2	--P 1	--C 1	90.93 (8)	F 5	--C 9	--F 6	106.9 (3)
O 2	--P 1	--C 19	93.0 (1)	F 5	--C 9	--C 7	112.2 (2)
O 2	--P 1	--C 10	87.30 (8)	F 6	--C 9	--C 7	112.3 (2)
O 1	--P 1	--C 1	87.32 (8)	C 15	--C 10	--C 11	119.5 (2)
O 1	--P 1	--C 19	91.2 (1)	C 15	--C 10	--P 1	113.8 (2)
O 1	--P 1	--C 10	90.68 (8)	C 11	--C 10	--P 1	126.6 (2)
C 1	--P 1	--C 19	116.6 (1)	C 12	--C 11	--C 10	119.6 (2)
C 1	--P 1	--C 10	126.84 (8)	C 13	--C 12	--C 11	120.5 (2)
C 19	--P 1	--C 10	116.6 (1)	C 12	--C 13	--C 14	120.6 (2)
C 7	--O 1	--P 1	118.2 (1)	C 13	--C 14	--C 15	118.8 (2)
C 16	--O 2	--P 1	118.6 (1)	C 10	--C 15	--C 14	120.9 (2)
C 6	--C 1	--C 2	119.3 (2)	C 10	--C 15	--C 16	112.1 (2)

C 6	--C 1	--P 1	113.8 (1)	C 14	--C 15	--C 16	127.0 (2)
C 2	--C 1	--P 1	126.8 (2)	O 2	--C 16	--C 15	108.1 (2)
C 3	--C 2	--C 1	119.1 (2)	O 2	--C 16	--C 18	107.6 (2)
C 4	--C 3	--C 2	120.8 (2)	O 2	--C 16	--C 17	107.9 (2)
C 3	--C 4	--C 5	120.6 (2)	C 15	--C 16	--C 18	111.8 (2)
C 4	--C 5	--C 6	118.8 (3)	C 15	--C 16	--C 17	110.6 (2)
C 5	--C 6	--C 1	121.3 (2)	C 18	--C 16	--C 17	110.8 (2)
C 5	--C 6	--C 7	126.5 (2)	F 9	--C 17	--F 7	106.5 (2)
C 1	--C 6	--C 7	112.2 (2)	F 9	--C 17	--F 8	108.2 (2)
O 1	--C 7	--C 6	108.4 (2)	F 9	--C 17	--C 16	112.4 (2)
O 1	--C 7	--C 9	107.2 (2)	F 7	--C 17	--F 8	106.8 (2)
O 1	--C 7	--C 8	107.5 (2)	F 7	--C 17	--C 16	109.3 (2)
C 6	--C 7	--C 9	111.4 (2)	F 8	--C 17	--C 16	113.2 (2)
C 6	--C 7	--C 8	110.6 (2)	F 11	--C 18	--F 10	107.0 (2)
C 9	--C 7	--C 8	111.5 (2)	F 11	--C 18	--F 12	107.3 (2)
F 3	--C 8	--F 2	107.8 (3)	F 11	--C 18	--C 16	112.5 (2)
F 3	--C 8	--F 1	106.7 (2)	F 10	--C 18	--F 12	106.8 (2)
F 3	--C 8	--C 7	112.2 (2)	F 10	--C 18	--C 16	110.0 (2)
F 2	--C 8	--F 1	106.9 (2)	F 12	--C 18	--C 16	112.9 (2)
F 2	--C 8	--C 7	113.0 (2)	C 20	--C 19	--P 1	113.9 (2)
F 1	--C 8	--C 7	109.9 (2)	C 21	--C 20	--C 19	112.8 (3)
F 4	--C 9	--F 5	107.7 (2)	C 20	--C 21	--C 22	113.5 (4)
F 4	--C 9	--F 6	106.8 (3)				

***** sdista *****

#intermolecular geometries dmax= 4.00 dmin= 1.00

Intermolecular Distances (A) with e.s.d. in parentheses

atom	atom	adc	distance	atom	atom	adc	distance
F 1	--C 13	(2)	3.405 (3)	F 8	--C 5	(9)	3.788 (3)
F 1	--C 14	(2)	3.677 (3)	F 8	--C 4	(9)	3.971 (3)
F 1	--F 11	(3)	3.255 (2)	F 9	--F 9	(10)	3.105 (4)
F 1	--F 10	(3)	3.263 (2)	F 9	--C 2	(10)	3.497 (3)
F 1	--F 12	(3)	3.599 (2)	F 9	--F 11	(10)	3.505 (3)
F 1	--C 18	(3)	3.628 (3)	F 9	--O 2	(10)	3.583 (2)
F 2	--F 8	(2)	3.846 (3)	F 10	--C 22	(11)	3.889 (6)
F 2	--F 10	(3)	3.236 (3)	F 10	--C 8	(12)	3.552 (3)
F 3	--F 6	(4)	3.139 (3)	F 11	--C 3	(10)	3.383 (4)
F 3	--F 4	(4)	3.826 (3)	F 11	--C 2	(10)	3.491 (3)
F 3	--C 5	(4)	3.833 (3)	F 12	--C 22	(8)	3.784 (6)
F 3	--F 10	(3)	3.405 (2)	F 12	--F 12	(13)	3.517 (4)
F 3	--F 11	(3)	3.898 (3)	F 12	--C 14	(13)	3.619 (4)
F 4	--F 9	(5)	3.926 (3)	F 12	--C 13	(13)	3.979 (4)
F 4	--C 19	(7)	3.713 (4)	F 12	--C 3	(10)	3.984 (4)
F 5	--F 7	(5)	3.205 (2)	C 1	--C 13	(2)	3.913 (3)
F 5	--F 8	(5)	3.365 (3)	C 2	--C 13	(2)	3.820 (3)
F 5	--C 17	(5)	3.761 (3)	C 2	--C 12	(2)	3.849 (3)
F 5	--F 9	(5)	3.974 (3)	C 2	--C 21	(7)	3.918 (4)
F 5	--C 5	(4)	3.620 (4)	C 3	--C 12	(2)	3.708 (3)
F 5	--C 4	(4)	3.724 (4)	C 3	--C 13	(2)	3.720 (4)
F 5	--C 12	(6)	3.805 (4)	C 3	--C 21	(7)	3.644 (4)
F 6	--C 11	(6)	3.189 (4)	C 3	--C 22	(7)	3.852 (6)
F 6	--C 12	(6)	3.456 (4)	C 4	--C 14	(2)	3.716 (3)
F 6	--O 1	(6)	3.995 (3)	C 4	--C 13	(2)	3.738 (3)
F 7	--C 4	(9)	3.427 (3)	C 4	--C 21	(7)	3.778 (4)
F 7	--C 5	(9)	3.980 (3)	C 5	--C 14	(2)	3.756 (3)
F 7	--C 12	(2)	3.356 (3)	C 5	--C 13	(2)	3.843 (4)
F 7	--C 13	(2)	3.802 (3)	C 6	--C 13	(2)	3.910 (3)
F 8	--C 22	(8)	3.718 (7)	C 13	--C 22	(11)	3.959 (6)
F 8	--C 21	(8)	3.858 (5)				

symmetry operater list

no. 2 -1. 0. 0. -0.5000
0. 1. 0. 0.5000

	0.	0.	-1.	0.0000
no. 3	1.	0.	0.	-0.5000
	0.	-1.	0.	-0.5000
	0.	0.	1.	0.0000
no. 4	-1.	0.	0.	-0.5000
	0.	1.	0.	-0.5000
	0.	0.	-1.	1.0000
no. 5	1.	0.	0.	0.0000
	0.	1.	0.	0.0000
	0.	0.	1.	1.0000
no. 6	-1.	0.	0.	-0.5000
	0.	1.	0.	0.5000
	0.	0.	-1.	1.0000
no. 7	-1.	0.	0.	0.0000
	0.	-1.	0.	0.0000
	0.	0.	-1.	1.0000
no. 8	1.	0.	0.	0.0000
	0.	1.	0.	0.0000
	0.	0.	1.	-1.0000
no. 9	-1.	0.	0.	-0.5000
	0.	1.	0.	-0.5000
	0.	0.	-1.	0.0000
no. 10	-1.	0.	0.	0.0000
	0.	-1.	0.	0.0000
	0.	0.	-1.	0.0000
no. 11	-1.	0.	0.	0.0000
	0.	-1.	0.	-1.0000
	0.	0.	-1.	1.0000
no. 12	1.	0.	0.	0.5000
	0.	-1.	0.	-0.5000
	0.	0.	1.	0.0000
no. 13	-1.	0.	0.	0.0000
	0.	-1.	0.	-1.0000
	0.	0.	-1.	0.0000

***** torsan *****

ns1, atm1, ns2, atm2, ns3, atm3
no. 1 (1 O 1) (1 P 1) (1 C 19)
ns1, atm1, ns2, atm2, ns3, atm3
no. 2 (1 O 2) (1 P 1) (1 C 19)
ns1, atm1, ns2, atm2, ns3, atm3
no. 3 (1 C 1) (1 P 1) (1 C 19)
ns1, atm1, ns2, atm2, ns3, atm3
no. 4 (1 C 10) (1 P 1) (1 C 19)
ns1, atm1, ns2, atm2, ns3, atm3
no. 5 (1 P 1) (1 C 19) (1 C 20)
ns1, atm1, ns2, atm2, ns3, atm3
no. 6 (1 C 19) (1 C 20) (1 C 21)
ns1, atm1, ns2, atm2, ns3, atm3
no. 7 (1 C 20) (1 C 21) (1 C 22)
ns1, atm1, ns2, atm2, ns3, atm3

angle between plane no. a and no. b

a	b	angle	a	b	angle	a	b	angle	a	b	angle	a	b	angle
1	2	0.15	1	3	87.61	1	4	88.63	1	5	117.47	1	6	117.74

1	7	116.19	2	3	87.46	2	4	88.48	2	5	117.33	2	6	117.59
2	7	116.05	3	4	1.02	3	5	29.87	3	6	30.14	3	7	28.59
4	5	28.84	4	6	29.12	4	7	27.57	5	6	0.66	5	7	1.43
6	7	1.55												

atom x y z b(equiv.)

Positional parameters and equivalent isotropic thermal parameters with e.s.d. in parentheses

atom	x	y	z	B(eq)
P 1	-0.11399 (2)	-0.14888 (4)	0.27026 (4)	3.48 (4)
F 1	-0.30577 (8)	-0.1364 (2)	0.2167 (2)	6.85 (6)
F 2	-0.3370 (1)	-0.0214 (2)	0.3472 (3)	9.84 (9)
F 3	-0.3065 (1)	-0.1900 (2)	0.4072 (2)	8.33 (7)
F 4	-0.1304 (1)	0.0070 (2)	0.5610 (2)	9.31 (8)
F 5	-0.2022 (2)	-0.1128 (2)	0.6060 (2)	9.45 (9)
F 6	-0.2363 (2)	0.0543 (2)	0.5500 (2)	10.8 (1)
F 7	-0.14673 (8)	-0.1294 (1)	-0.0850 (2)	6.15 (6)
F 8	-0.0878 (1)	-0.2532 (2)	-0.1596 (2)	7.98 (7)
F 9	-0.0406 (1)	-0.0955 (2)	-0.0869 (2)	7.76 (6)
F 10	0.02815 (9)	-0.3259 (2)	0.2125 (2)	7.88 (7)
F 11	0.06110 (8)	-0.1992 (2)	0.0976 (2)	8.23 (7)
F 12	0.0192 (1)	-0.3545 (2)	0.0112 (2)	9.10 (8)
O 1	-0.17287 (8)	-0.1590 (1)	0.3734 (1)	4.05 (5)
O 2	-0.06090 (7)	-0.1384 (1)	0.1582 (2)	4.40 (5)
C 1	-0.1484 (1)	-0.0074 (2)	0.2290 (2)	3.67 (6)
C 2	-0.1281 (1)	0.0680 (2)	0.1433 (2)	4.39 (6)
C 3	-0.1580 (1)	0.1745 (2)	0.1272 (3)	5.30 (7)
C 4	-0.2066 (1)	0.2070 (2)	0.1956 (3)	5.70 (8)
C 5	-0.2270 (2)	0.1336 (2)	0.2808 (3)	5.31 (8)
C 6	-0.1979 (1)	0.0264 (2)	0.2961 (2)	4.11 (6)
C 7	-0.2142 (1)	-0.0661 (2)	0.3836 (2)	4.50 (6)
C 8	-0.2921 (1)	-0.1035 (2)	0.3394 (3)	5.94 (8)
C 9	-0.1957 (2)	-0.0293 (3)	0.5271 (3)	6.8 (1)
C 10	-0.1479 (1)	-0.2804 (2)	0.1902 (2)	3.58 (6)
C 11	-0.1983 (1)	-0.3501 (2)	0.2222 (2)	4.41 (6)
C 12	-0.2162 (2)	-0.4503 (2)	0.1556 (2)	5.24 (7)
C 13	-0.1846 (2)	-0.4809 (2)	0.0574 (2)	5.50 (8)
C 14	-0.1337 (2)	-0.4131 (2)	0.0254 (2)	5.13 (7)
C 15	-0.1160 (1)	-0.3122 (2)	0.0921 (2)	4.05 (6)
C 16	-0.0622 (1)	-0.2259 (2)	0.0712 (2)	4.35 (6)
C 17	-0.0837 (1)	-0.1760 (2)	-0.0675 (2)	5.21 (7)
C 18	0.0125 (1)	-0.2765 (2)	0.0972 (3)	5.94 (8)
C 19	-0.0386 (1)	-0.1605 (2)	0.4078 (2)	4.84 (7)
C 20	-0.0351 (2)	-0.2717 (2)	0.4804 (3)	5.98 (8)
C 21	0.0281 (2)	-0.2796 (4)	0.5925 (4)	8.3 (1)
C 22	0.0335 (4)	-0.3908 (5)	0.6635 (5)	10.8 (2)
H 19A	-0.000 (2)	-0.140 (3)	0.387 (3)	4.85 (0)
H 19B	-0.041 (2)	-0.094 (3)	0.471 (3)	4.85 (0)
H 3	-0.144 (2)	0.225 (3)	0.067 (3)	5.15 (0)
H 5	-0.258 (2)	0.156 (3)	0.316 (4)	5.13 (0)
H 13	-0.204 (2)	-0.551 (3)	0.008 (4)	5.46 (0)
H 20A	-0.079 (2)	-0.291 (3)	0.520 (4)	6.06 (0)
H 2	-0.094 (2)	0.047 (3)	0.098 (3)	4.27 (0)
H 4	-0.230 (2)	0.283 (3)	0.189 (3)	5.55 (0)
H 22A	0.061 (4)	-0.424 (6)	0.618 (7)	11.10 (0)
H 12	-0.256 (2)	-0.493 (3)	0.176 (3)	5.17 (0)
H 20B	-0.038 (2)	-0.343 (3)	0.427 (4)	6.06 (0)
H 11	-0.222 (2)	-0.332 (3)	0.292 (3)	4.31 (0)
H 14	-0.112 (2)	-0.429 (3)	-0.034 (4)	5.01 (0)
H 21A	0.064 (3)	-0.274 (5)	0.561 (5)	8.45 (0)
H 21B	0.008 (2)	-0.206 (4)	0.648 (4)	8.45 (0)
H 22B	0.068 (4)	-0.397 (5)	0.738 (7)	11.10 (0)
H 22C	-0.009 (4)	-0.393 (6)	0.676 (7)	11.10 (0)

atom u11, 22, 33, 12, 13, 23

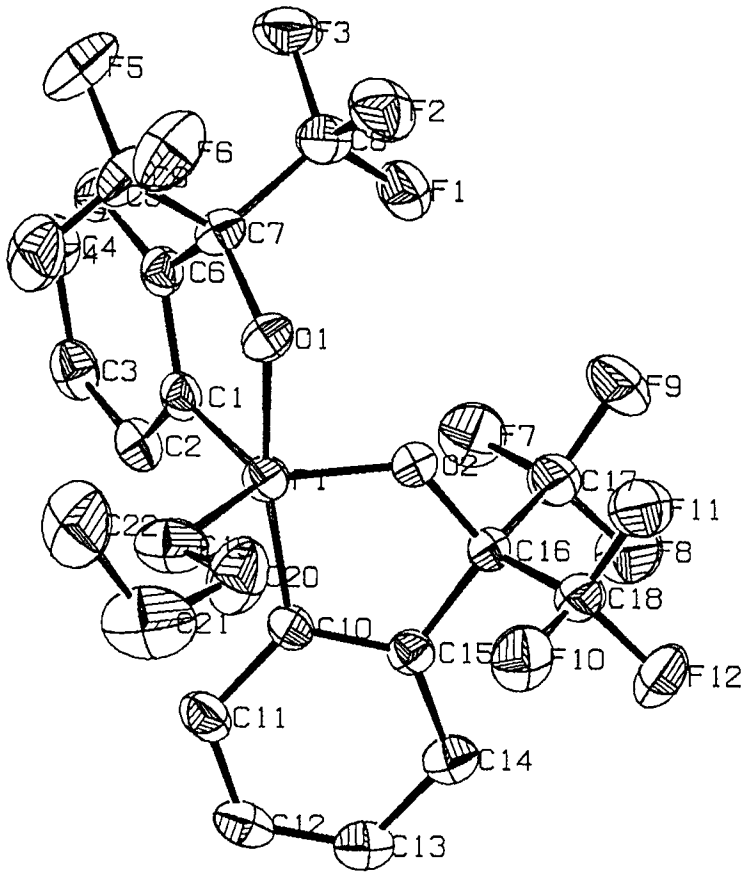
U values with e.s.d. in parentheses

atom	u11	u22	u33	u12	u13	u23
P 1	0.0400 (4)	0.048 (1)	0.0414 (5)	-0.0012 (2)	0.0088 (2)	-0.0007 (2)
F 1	0.0610 (9)	0.109 (2)	0.083 (1)	-0.0174 (8)	0.0060 (7)	0.0100 (9)
F 2	0.076 (1)	0.106 (2)	0.194 (2)	0.020 (1)	0.071 (1)	0.015 (1)
F 3	0.093 (1)	0.105 (2)	0.120 (1)	-0.016 (1)	0.057 (1)	0.029 (1)
F 4	0.148 (2)	0.132 (2)	0.066 (1)	-0.030 (1)	0.016 (1)	-0.038 (1)
F 5	0.188 (2)	0.113 (2)	0.055 (1)	0.002 (1)	0.048 (1)	0.0106 (9)
F 6	0.208 (2)	0.111 (2)	0.097 (1)	0.040 (2)	0.086 (2)	-0.020 (1)
F 7	0.0655 (9)	0.092 (2)	0.071 (1)	0.0146 (7)	0.0098 (7)	0.0182 (7)
F 8	0.141 (2)	0.104 (2)	0.0562 (9)	0.017 (1)	0.0390 (9)	-0.0002 (8)
F 9	0.087 (1)	0.114 (2)	0.092 (1)	-0.0144 (9)	0.0336 (9)	0.035 (1)
F 10	0.0672 (9)	0.129 (2)	0.099 (1)	0.0387 (9)	0.0197 (8)	0.034 (1)
F 11	0.0504 (7)	0.128 (2)	0.133 (2)	0.0097 (8)	0.0387 (9)	0.018 (1)
F 12	0.095 (1)	0.128 (2)	0.121 (2)	0.048 (1)	0.044 (1)	-0.020 (1)
O 1	0.0579 (9)	0.052 (1)	0.0424 (8)	0.0001 (6)	0.0183 (6)	0.0006 (6)
O 2	0.0442 (7)	0.059 (1)	0.063 (1)	-0.0033 (6)	0.0212 (6)	-0.0028 (6)
C 1	0.0425 (9)	0.049 (2)	0.046 (1)	-0.0035 (7)	0.0109 (8)	-0.0020 (8)
C 2	0.052 (1)	0.054 (2)	0.059 (1)	-0.0046 (8)	0.0174 (9)	0.0032 (9)
C 3	0.070 (1)	0.053 (2)	0.076 (2)	-0.002 (1)	0.022 (1)	0.012 (1)
C 4	0.070 (1)	0.051 (2)	0.092 (2)	0.006 (1)	0.023 (1)	0.007 (1)
C 5	0.066 (1)	0.057 (2)	0.077 (2)	0.007 (1)	0.029 (1)	-0.000 (1)
C 6	0.051 (1)	0.053 (2)	0.051 (1)	-0.0006 (8)	0.0166 (9)	-0.0038 (8)
C 7	0.062 (1)	0.058 (2)	0.051 (1)	0.0044 (9)	0.0268 (9)	0.0007 (9)
C 8	0.061 (1)	0.074 (2)	0.092 (2)	0.003 (1)	0.040 (1)	0.013 (1)
C 9	0.120 (2)	0.077 (2)	0.060 (2)	0.006 (2)	0.042 (2)	-0.008 (1)
C 10	0.0456 (9)	0.048 (2)	0.039 (1)	-0.0002 (7)	0.0089 (7)	0.0004 (7)
C 11	0.061 (1)	0.055 (2)	0.049 (1)	-0.0088 (8)	0.014 (1)	0.0010 (9)
C 12	0.077 (1)	0.058 (2)	0.059 (1)	-0.015 (1)	0.011 (1)	0.001 (1)
C 13	0.096 (2)	0.052 (2)	0.054 (1)	-0.006 (1)	0.007 (1)	-0.004 (1)
C 14	0.085 (2)	0.058 (2)	0.048 (1)	0.009 (1)	0.018 (1)	-0.0039 (9)
C 15	0.052 (1)	0.052 (2)	0.046 (1)	0.0072 (8)	0.0129 (8)	0.0032 (8)
C 16	0.049 (1)	0.061 (2)	0.054 (1)	0.0084 (8)	0.0211 (9)	0.0009 (9)
C 17	0.066 (1)	0.072 (2)	0.059 (1)	0.005 (1)	0.025 (1)	0.007 (1)
C 18	0.058 (1)	0.089 (2)	0.077 (2)	0.022 (1)	0.029 (1)	0.007 (1)
C 19	0.051 (1)	0.070 (2)	0.055 (1)	-0.002 (1)	-0.002 (1)	-0.002 (1)
C 20	0.080 (2)	0.077 (2)	0.060 (1)	0.005 (1)	-0.013 (1)	0.005 (1)
C 21	0.101 (2)	0.114 (3)	0.081 (2)	0.014 (2)	-0.029 (2)	0.013 (2)
C 22	0.170 (5)	0.123 (4)	0.094 (3)	0.035 (4)	-0.039 (3)	0.023 (2)

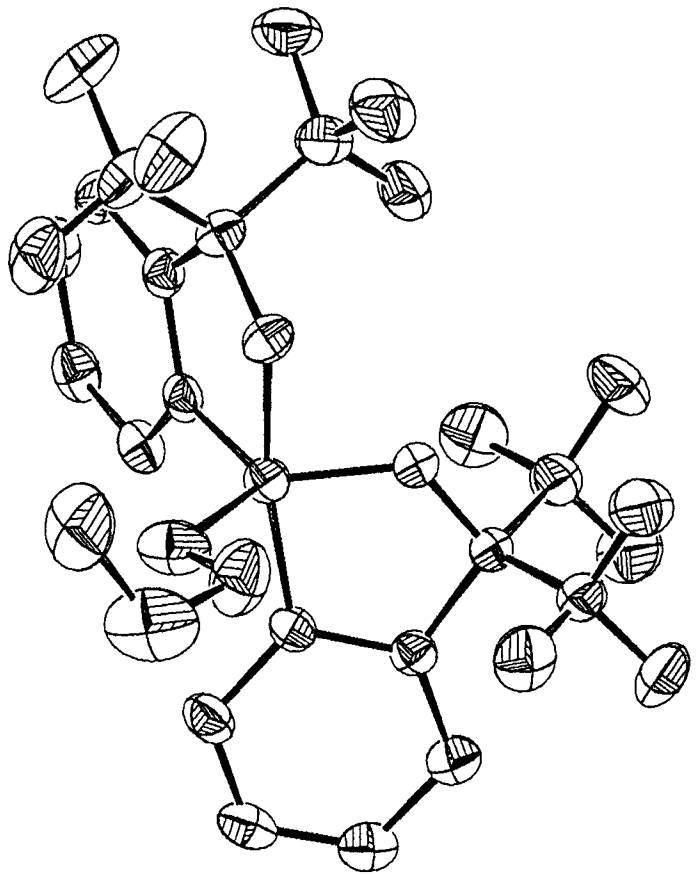
Chemical Formula	C22 H17 F12 O2 P1
Formula Weight	572.32
Crystal Size	0.50 * 0.50 * 0.25 mm**3
Unit-cell Dimensions :	a = 12.041 (2) A b = 16.936 (3) A c = 11.401 (2) A alpha = beta = 96.05 (1) degrees gamma =
Volume of unit cell	2311.9 (6) A**3
Crystal System	Monoclinic
Space Group	P21/n (# 14)
Z value	4
Densities: Dobs :Dcalc	: 1.66 g/cm**3
F(000)	1152
Linear Absorption Coefficient	20.06 /cm (Cu K-alpha)
Diffractometer used	Mac Science MXC3
Radiation	Cu K-alpha (lambda= 1.54178)
Maximum sine(theta)/lambda	0.584
Total Reflections Measured	4264
Unique Reflections	3861
Internal Consistency : Rint	0.03
Function Minimized was sum[w(|Fo|**2-|Fc|**2)**2] which w = 1.0/[(sigma|Fo|)**2+ 0.0007|Fo|**2]	
Reflections used (F>5.00(sig(F)))	3016
No. of Variables	344
Residuals: R; Rw	0.066; 0.093
Goodness of Fit : S	2.67
Maximum Shift/e.s.d. in final cycle	0.18
Maximum Negative Peak in Final Diff. Map	-0.59 e/A**3 (0.916 0.591 0.999)
Maximum Positive Peak in Final Diff. Map	0.92 e/A**3 (0.203 0.346 0.007)

Compound 4

Apical Carbon-Equatorial Oxy
Phosphorane
K.-y. Akiba et al.



Apical Carbon-Equatorial Oxyg
Phosphorane
K.-y. Akiba et al. 26



Apical Carbon-Equatorial Oxyg
Phosphorane
K.-y. Akiba et al.

***** fileio *****

...coordination no. 1 54 atoms

	cm	nb	aw	x	y	z	b					
1	P 1	0	1.00000	0.22201	0.19316	-0.10183	0.00721	0.00238	0.00680	0.00136	-0.00073	0.00137
2	F 1	0	1.00000	0.19286	-0.00764	-0.01978	0.01391	0.00366	0.01151	-0.00295	-0.00180	0.00257
3	F 2	0	1.00000	0.07759	0.01485	0.10696	0.00891	0.00657	0.01673	-0.00293	0.00391	0.00468
4	F 3	0	1.00000	0.24059	-0.02932	0.16246	0.01208	0.00489	0.01477	0.00057	0.00809	-0.00039
5	F 4	0	1.00000	0.26010	0.21088	0.23071	0.01686	0.00693	0.01022	-0.00017	-0.00734	0.00170
6	F 5	0	1.00000	0.27324	0.09523	0.30589	0.01593	0.00993	0.00660	0.00756	0.00181	-0.00133
7	F 6	0	1.00000	0.11547	0.14339	0.24884	0.01081	0.01154	0.00929	0.00442	-0.00289	0.00637
8	F 7	0	1.00000	0.26959	0.03269	-0.27784	0.01355	0.00413	0.01602	0.00606	0.00011	-0.00087
9	F 8	0	1.00000	0.17013	0.03392	-0.44428	0.02194	0.00476	0.00993	0.00223	-0.00389	0.00394
10	F 9	0	1.00000	0.10149	-0.00855	-0.29188	0.01758	0.00308	0.01684	-0.00346	0.00001	0.00322
11	F 10	0	1.00000	-0.01753	0.21956	-0.33127	0.00878	0.00551	0.01483	0.00439	0.00010	-0.00221
12	F 11	0	1.00000	-0.06272	0.10004	-0.31351	0.00865	0.00824	0.01592	-0.00513	0.00853	-0.00319
13	F 12	0	1.00000	-0.00170	0.14030	-0.47172	0.01227	0.00813	0.00846	-0.00247	0.00115	-0.00628
14	O 1	0	1.00000	0.16134	0.15198	0.01888	0.00667	0.00400	0.00651	0.00217	0.00047	0.00137
15	O 2	0	1.00000	0.13025	0.13546	-0.17947	0.00687	0.00314	0.00642	-0.00034	0.00062	0.00020
16	C 1	0	1.00000	0.35380	0.15262	-0.03717	0.00673	0.00229	0.00731	-0.00024	-0.00174	0.00055
17	C 2	0	1.00000	0.45631	0.15932	-0.08145	0.00766	0.00319	0.00930	-0.00106	-0.00133	0.00236
18	C 3	0	1.00000	0.55049	0.12525	-0.02072	0.00651	0.00359	0.01244	-0.00002	-0.00204	0.00107
19	C 4	0	1.00000	0.54173	0.08462	0.08294	0.00745	0.00388	0.01251	0.00131	-0.00163	-0.00209
20	C 5	0	1.00000	0.43983	0.07600	0.12612	0.00814	0.00351	0.00881	0.00127	-0.00003	-0.00143
21	C 6	0	1.00000	0.34601	0.11012	0.06561	0.00665	0.00276	0.00720	0.00013	-0.00127	-0.00020
22	C 7	0	1.00000	0.22771	0.10525	0.09725	0.00702	0.00346	0.00653	0.00173	0.00080	0.00112
23	C 8	0	1.00000	0.18427	0.01998	0.08774	0.00766	0.00434	0.00990	0.00016	0.00303	0.00217
24	C 9	0	1.00000	0.21903	0.13938	0.22145	0.00930	0.00644	0.00674	0.00246	-0.00024	0.00074
25	C 10	0	1.00000	0.26666	0.22859	-0.24428	0.00713	0.00218	0.00790	0.00082	-0.00017	0.00104
26	C 11	0	1.00000	0.34157	0.28949	-0.26458	0.00877	0.00248	0.01084	-0.00069	0.00037	0.00152
27	C 12	0	1.00000	0.36088	0.30841	-0.37905	0.00887	0.00314	0.01203	0.00021	0.00354	0.00420
28	C 13	0	1.00000	0.30681	0.26878	-0.47290	0.00849	0.00444	0.00943	0.00120	0.00295	0.00409
29	C 14	0	1.00000	0.23068	0.20898	-0.45567	0.00853	0.00415	0.00767	0.00114	0.00095	0.00261
30	C 15	0	1.00000	0.21215	0.19070	-0.34075	0.00680	0.00257	0.00695	0.00121	0.00008	0.00123
31	C 16	0	1.00000	0.13217	0.12992	-0.30253	0.00758	0.00280	0.00637	-0.00027	0.00024	-0.00071
32	C 17	0	1.00000	0.16639	0.04638	-0.32977	0.01171	0.00331	0.00898	-0.00009	-0.00034	0.00081
33	C 18	0	1.00000	0.00976	0.14727	-0.35468	0.00745	0.00453	0.00864	-0.00126	0.00278	-0.00147
34	C 19	0	1.00000	0.18917	0.29171	-0.04820	0.01477	0.00417	0.01224	0.00502	0.00174	0.00996
35	C 20	0	1.00000	0.07338	0.31315	-0.07027	0.01441	0.00674	0.01381	0.00368	-0.00523	-0.00275
36	C 21	0	1.00000	0.05155	0.39507	-0.01233	0.02416	0.00591	0.02006	0.01339	0.00040	0.01567
37	C 22	0	1.00000	0.05486	0.39156	0.11447	0.02084	0.00725	0.01598	0.00353	-0.01036	0.00629
38	H 2 A	0	1.00000	0.45992	0.18882	-0.15810	4.26813	0.00000	0.00000	0.00000	0.00000	0.00000
39	H 3 A	0	1.00000	0.62608	0.12823	-0.04934	4.76571	0.00000	0.00000	0.00000	0.00000	0.00000
40	H 4 A	0	1.00000	0.61117	0.06232	0.12821	5.13025	0.00000	0.00000	0.00000	0.00000	0.00000
41	H 5 A	0	1.00000	0.43383	0.04621	0.20204	4.47016	0.00000	0.00000	0.00000	0.00000	0.00000
42	H 11A	0	1.00000	0.38264	0.31899	-0.19620	4.49441	0.00000	0.00000	0.00000	0.00000	0.00000
43	H 12A	0	1.00000	0.41419	0.35241	-0.39285	4.91899	0.00000	0.00000	0.00000	0.00000	0.00000
44	H 13A	0	1.00000	0.32263	0.28289	-0.55529	4.89593	0.00000	0.00000	0.00000	0.00000	0.00000
45	H 14A	0	1.00000	0.18969	0.17994	-0.52432	4.51359	0.00000	0.00000	0.00000	0.00000	0.00000
46	H 19A	0	1.00000	0.23405	0.33323	-0.08665	6.37851	0.00000	0.00000	0.00000	0.00000	0.00000
47	H 19B	0	1.00000	0.20958	0.29527	0.03974	6.37851	0.00000	0.00000	0.00000	0.00000	0.00000
48	H 20A	0	1.00000	0.02622	0.27117	-0.03960	7.80998	0.00000	0.00000	0.00000	0.00000	0.00000
49	H 20B	0	1.00000	0.05300	0.31749	-0.15904	7.80998	0.00000	0.00000	0.00000	0.00000	0.00000
50	H 21A	0	1.00000	-0.02435	0.41531	-0.04102	10.10225	0.00000	0.00000	0.00000	0.00000	0.00000
51	H 21B	0	1.00000	0.10936	0.43410	-0.02991	10.10225	0.00000	0.00000	0.00000	0.00000	0.00000
52	H 22A	0	1.00000	0.04178	0.44409	0.14925	9.44914	0.00000	0.00000	0.00000	0.00000	0.00000
53	H 22B	0	1.00000	-0.00228	0.35292	0.13888	9.44914	0.00000	0.00000	0.00000	0.00000	0.00000
54	H 22C	0	1.00000	0.13144	0.37171	0.14999	9.44914	0.00000	0.00000	0.00000	0.00000	0.00000

***** crycar *****

a, b, c, alph, beta, gamm

12.041 16.937 11.401 90.00 96.05 90.00

...matrix no. 1

12.0410004 0.0000000 -1.2013056 0.0000000

```
 0.0003167  16.9370003   0.0002999          0.0000000
 0.0000000   0.0000000  11.3375340          0.0000000

...matrix no.  2

 0.0830496   0.0000000   0.0087998          0.0000000
-0.0000016   0.0590423  -0.0000017          0.0000000
 0.0000000   0.0000000   0.0882026          0.0000000

***** cartesian system *****

 1 P  1          2.79555   3.27159  -1.15450
 2 F  1          2.34599  -0.12934  -0.22426
 3 F  2          0.80577   0.25157   1.21266
 4 F  3          2.70178  -0.49647   1.84190
 5 F  4          2.85471   3.57183   2.61568
 6 F  5          2.92262   1.61309   3.46804
 7 F  6          1.09144   2.42871   2.82123
 8 F  7          3.57990   0.55367  -3.15002
 9 F  8          2.58225   0.57442  -5.03704
10 F  9          1.57268  -0.14487  -3.30920
11 F  10         0.18688   3.71858  -3.75578
12 F  11        -0.37859   1.69426  -3.55443
13 F  12         0.54621   2.37612  -5.34814
14 O  1          1.92001   2.57414   0.21405
15 O  2          1.78394   2.29427  -2.03475
16 C  1          4.30476   2.58503  -0.42142
17 C  2          5.59228   2.69852  -0.92344
18 C  3          6.65334   2.12153  -0.23491
19 C  4          6.42334   1.43341   0.94034
20 C  5          5.14448   1.28739   1.42989
21 C  6          4.08749   1.86523   0.74386
22 C  7          2.62503   1.78272   1.10258
23 C  8          2.11339   0.33849   0.99476
24 C  9          2.37131   2.36081   2.51070
25 C  10         3.50431   3.87164  -2.76953
26 C  11         4.43069   4.90312  -2.99968
27 C  12         4.80071   5.22354  -4.29749
28 C  13         4.26240   4.55228  -5.36152
29 C  14         3.32502   3.53943  -5.16617
30 C  15         2.96384   3.22985  -3.86326
31 C  16         1.95489   2.20041  -3.42994
32 C  17         2.39966   0.78549  -3.73878
33 C  18         0.54360   2.49421  -4.02120
34 C  19         2.33570   4.94074  -0.54647
35 C  20         0.96798   5.30382  -0.79669
36 C  21         0.63553   6.69131  -0.13979
37 C  22         0.52306   6.63190   1.29781
38 H  2  A       5.72782   3.19814  -1.79246
39 H  3  A       7.59790   2.17202  -0.55939
40 H  4  A       7.20508   1.05575   1.45359
41 H  5  A       4.98104   0.78286   2.29064
42 H  11A        4.84306   5.40280  -2.22442
43 H  12A        5.45919   5.96878  -4.45395
44 H  13A        4.55186   4.79124  -6.29562
45 H  14A        2.91393   3.04755  -5.94450
46 H  19A        2.92229   5.64396  -0.98240
47 H  19B        2.47581   5.00107   0.45055
48 H  20A        0.36329   4.59280  -0.44897
49 H  20B        0.82923   5.37730  -1.80312
50 H  21A       -0.24392   7.03409  -0.46507
51 H  21B        1.35273   7.35238  -0.33911
52 H  22A        0.32378   7.52161   1.69213
53 H  22B       -0.19429   5.97745   1.57456
54 H  22C        1.40249   6.29574   1.70052

***** symrel *****

# name, s11, 12, 13, tr1,  s21, 22, 23, tr2, s31, 32, 33, tr3
```

Apical Carbon-Equatorial Oxygen
Phosphorane
K.-y. Akiba et al.

1	no 1	1.	0.	0.	0.0000
		0.	1.	0.	0.0000
		0.	0.	1.	0.0000
2	no 2	-1.	0.	0.	0.5000
		0.	1.	0.	0.5000
		0.	0.	-1.	0.5000
3	no 3	-1.	0.	0.	0.0000
		0.	-1.	0.	0.0000
		0.	0.	-1.	0.0000
4	no 4	1.	0.	0.	0.5000
		0.	-1.	0.	0.5000
		0.	0.	1.	0.5000

***** sdista *****

#intramolecular geometries dmax= 2.00 dmin= 1.00

Intramolecular Distances (A) with e.s.d. in parentheses

atom	atom	distance	atom	atom	distance
P 1	--O 2	1.659 (2)	C 1	--C 6	1.387 (5)
P 1	--O 1	1.768 (3)	C 2	--C 3	1.390 (6)
P 1	--C 1	1.813 (4)	C 3	--C 4	1.381 (7)
P 1	--C 19	1.835 (5)	C 4	--C 5	1.377 (6)
P 1	--C 10	1.863 (4)	C 5	--C 6	1.386 (5)
F 1	--C 8	1.326 (5)	C 6	--C 7	1.508 (5)
F 2	--C 8	1.328 (5)	C 7	--C 8	1.536 (6)
F 3	--C 8	1.327 (5)	C 7	--C 9	1.543 (6)
F 4	--C 9	1.308 (7)	C 10	--C 15	1.378 (5)
F 5	--C 9	1.334 (6)	C 10	--C 11	1.405 (6)
F 6	--C 9	1.319 (6)	C 11	--C 12	1.387 (7)
F 7	--C 17	1.339 (6)	C 12	--C 13	1.368 (6)
F 8	--C 17	1.328 (5)	C 13	--C 14	1.394 (6)
F 9	--C 17	1.317 (6)	C 14	--C 15	1.387 (6)
F 10	--C 18	1.303 (6)	C 15	--C 16	1.505 (6)
F 11	--C 18	1.307 (6)	C 16	--C 17	1.515 (6)
F 12	--C 18	1.332 (5)	C 16	--C 18	1.558 (6)
O 1	--C 7	1.383 (4)	C 19	--C 20	1.437 (9)
O 2	--C 16	1.409 (4)	C 20	--C 21	1.57 (1)
C 1	--C 2	1.386 (6)	C 21	--C 22	1.44 (1)

***** sangle *****

#intramolecular geometries dmax= 2.00 dmin= 1.00

Intramolecular Angles (degrees) with e.s.d. in parentheses

atom	atom	atom	angle	atom	atom	atom	angle
O 2	--P 1	--O 1	82.9 (1)	F 4	--C 9	--C 7	111.0 (4)
O 2	--P 1	--C 1	119.9 (2)	F 6	--C 9	--F 5	105.1 (4)
O 2	--P 1	--C 19	124.0 (2)	F 6	--C 9	--C 7	113.2 (4)
O 2	--P 1	--C 10	87.8 (1)	F 5	--C 9	--C 7	112.1 (4)
O 1	--P 1	--C 1	87.1 (2)	C 15	--C 10	--C 11	118.0 (4)
O 1	--P 1	--C 19	88.8 (2)	C 15	--C 10	--P 1	112.9 (3)
O 1	--P 1	--C 10	170.6 (1)	C 11	--C 10	--P 1	129.0 (3)
C 1	--P 1	--C 19	114.8 (2)	C 12	--C 11	--C 10	119.9 (4)
C 1	--P 1	--C 10	99.0 (2)	C 13	--C 12	--C 11	120.6 (4)
C 19	--P 1	--C 10	95.1 (2)	C 12	--C 13	--C 14	120.8 (4)
C 7	--O 1	--P 1	118.1 (2)	C 15	--C 14	--C 13	118.0 (4)
C 16	--O 2	--P 1	119.4 (2)	C 10	--C 15	--C 14	122.6 (4)
C 2	--C 1	--C 6	119.5 (3)	C 10	--C 15	--C 16	110.7 (3)

C 2	--C 1	--P 1	126.6 (3)		C 14	--C 15	--C 16	126.7 (3)
C 6	--C 1	--P 1	113.9 (3)		O 2	--C 16	--C 15	108.7 (3)
C 1	--C 2	--C 3	119.7 (4)		O 2	--C 16	--C 17	107.4 (3)
C 4	--C 3	--C 2	120.1 (4)		O 2	--C 16	--C 18	104.7 (3)
C 5	--C 4	--C 3	120.7 (4)		C 15	--C 16	--C 17	112.5 (3)
C 4	--C 5	--C 6	119.2 (4)		C 15	--C 16	--C 18	111.6 (3)
C 5	--C 6	--C 1	120.8 (4)		C 17	--C 16	--C 18	111.4 (3)
C 5	--C 6	--C 7	126.8 (4)		F 9	--C 17	--F 8	107.0 (4)
C 1	--C 6	--C 7	112.3 (3)		F 9	--C 17	--F 7	106.7 (4)
O 1	--C 7	--C 6	108.1 (3)		F 9	--C 17	--C 16	114.1 (4)
O 1	--C 7	--C 8	108.8 (3)		F 8	--C 17	--F 7	106.3 (4)
O 1	--C 7	--C 9	106.7 (3)		F 8	--C 17	--C 16	112.8 (4)
C 6	--C 7	--C 8	111.0 (3)		F 7	--C 17	--C 16	109.3 (4)
C 6	--C 7	--C 9	110.8 (3)		F 10	--C 18	--F 11	108.0 (4)
C 8	--C 7	--C 9	111.2 (4)		F 10	--C 18	--F 12	106.7 (4)
F 1	--C 8	--F 3	106.7 (4)		F 10	--C 18	--C 16	110.4 (3)
F 1	--C 8	--F 2	107.5 (4)		F 11	--C 18	--F 12	107.6 (4)
F 1	--C 8	--C 7	109.7 (4)		F 11	--C 18	--C 16	112.8 (4)
F 3	--C 8	--F 2	106.9 (4)		F 12	--C 18	--C 16	111.1 (4)
F 3	--C 8	--C 7	113.5 (3)		C 20	--C 19	--P 1	114.2 (4)
F 2	--C 8	--C 7	112.2 (4)		C 19	--C 20	--C 21	110.6 (6)
F 4	--C 9	--F 6	107.0 (5)		C 22	--C 21	--C 20	113.4 (6)
F 4	--C 9	--F 5	108.0 (4)					

***** sdista *****

#intermolecular geometries dmax= 4.00 dmin= 1.00

Intermolecular Distances (A) with e.s.d. in parentheses

atom	atom	adc	distance	atom	atom	adc	distance
F 1	--C 12	(2)	3.361 (5)	F 7	--C 22	(9)	3.980 (9)
F 1	--C 13	(2)	3.788 (6)	F 8	--F 12	(11)	3.651 (4)
F 1	--F 2	(3)	3.305 (4)	F 8	--F 11	(11)	3.700 (4)
F 1	--C 4	(4)	3.594 (5)	F 9	--C 11	(2)	3.534 (5)
F 1	--C 3	(4)	3.665 (5)	F 9	--C 12	(2)	3.664 (6)
F 2	--F 2	(3)	2.955 (6)	F 9	--F 12	(11)	3.606 (4)
F 2	--F 11	(3)	3.074 (5)	F 10	--C 1	(12)	3.440 (5)
F 2	--F 9	(3)	3.172 (5)	F 10	--C 6	(12)	3.464 (5)
F 2	--C 8	(3)	3.707 (5)	F 10	--C 2	(12)	3.500 (5)
F 2	--O 2	(3)	3.723 (4)	F 10	--C 5	(12)	3.526 (5)
F 2	--C 12	(5)	3.985 (6)	F 10	--C 4	(12)	3.551 (6)
F 3	--C 22	(6)	3.607 (8)	F 10	--C 3	(12)	3.552 (6)
F 3	--F 11	(3)	3.125 (4)	F 11	--C 8	(3)	3.700 (6)
F 3	--C 3	(4)	3.526 (6)	F 12	--C 2	(12)	3.634 (5)
F 4	--C 13	(7)	3.507 (5)	F 12	--C 11	(12)	3.846 (5)
F 4	--C 14	(7)	3.630 (5)	F 12	--C 19	(12)	3.906 (7)
F 4	--F 10	(8)	3.075 (5)	F 12	--C 1	(12)	3.951 (5)
F 4	--F 11	(8)	3.910 (5)	O 1	--C 12	(5)	3.972 (5)
F 5	--F 8	(7)	3.388 (4)	C 2	--C 22	(9)	3.878 (9)
F 5	--C 14	(7)	3.414 (5)	C 3	--C 5	(4)	3.620 (6)
F 5	--C 13	(7)	3.866 (6)	C 3	--C 4	(4)	3.769 (7)
F 5	--C 21	(8)	3.753 (9)	C 3	--C 13	(8)	3.562 (6)
F 6	--F 12	(7)	3.618 (4)	C 3	--C 14	(8)	3.578 (6)
F 6	--C 14	(7)	3.677 (5)	C 4	--C 4	(4)	3.522 (9)
F 6	--F 8	(7)	3.953 (4)	C 4	--C 5	(4)	3.639 (6)
F 6	--F 9	(3)	3.543 (5)	C 9	--C 14	(7)	3.854 (6)
F 6	--C 12	(5)	3.354 (5)	C 13	--C 20	(9)	3.770 (8)
F 6	--C 11	(5)	3.476 (5)	C 21	--C 21	(14)	3.78 (1)
F 7	--C 4	(4)	3.603 (5)	C 21	--C 22	(14)	3.97 (1)

symmetry operater list

no. 2	-1.	0.	0.	0.5000
	0.	1.	0.	-0.5000
	0.	0.	-1.	-0.5000

Apical Carbon-Equatorial Oxygen Phosphorane

K.-y. Akiba et al.

no. 3	-1.	0.	0.	0.0000
	0.	-1.	0.	0.0000
	0.	0.	-1.	0.0000
no. 4	-1.	0.	0.	1.0000
	0.	-1.	0.	0.0000
	0.	0.	-1.	0.0000
no. 5	1.	0.	0.	-0.5000
	0.	-1.	0.	0.5000
	0.	0.	1.	0.5000
no. 6	-1.	0.	0.	0.5000
	0.	1.	0.	-0.5000
	0.	0.	-1.	0.5000
no. 7	1.	0.	0.	0.0000
	0.	1.	0.	0.0000
	0.	0.	1.	1.0000
no. 8	1.	0.	0.	0.5000
	0.	-1.	0.	0.5000
	0.	0.	1.	0.5000
no. 9	1.	0.	0.	0.5000
	0.	-1.	0.	0.5000
	0.	0.	1.	-0.5000
no. 10	1.	0.	0.	0.0000
	0.	1.	0.	0.0000
	0.	0.	1.	-1.0000
no. 11	-1.	0.	0.	0.0000
	0.	-1.	0.	0.0000
	0.	0.	-1.	-1.0000
no. 12	1.	0.	0.	-0.5000
	0.	-1.	0.	0.5000
	0.	0.	1.	-0.5000
no. 13	-1.	0.	0.	0.5000
	0.	1.	0.	0.5000
	0.	0.	-1.	-0.5000
no. 14	-1.	0.	0.	0.0000
	0.	-1.	0.	1.0000
	0.	0.	-1.	0.0000
no. 15	-1.	0.	0.	0.5000
	0.	1.	0.	0.5000
	0.	0.	-1.	0.5000

atom x y z b(equiv.)

Positional parameters and equivalent isotropic thermal parameters with e.s.d. in parentheses

atom	x	y	z	B(eq)
P 1	0.22201 (8)	0.19316 (6)	-0.10183 (8)	3.5 (3)
F 1	0.1929 (2)	-0.0076 (2)	-0.0198 (2)	6.0 (3)
F 2	0.0776 (2)	0.0148 (2)	0.1070 (3)	7.1 (3)
F 3	0.2406 (2)	-0.0293 (2)	0.1625 (3)	6.8 (3)
F 4	0.2601 (3)	0.2109 (2)	0.2307 (3)	7.7 (3)
F 5	0.2732 (3)	0.0952 (2)	0.3059 (2)	8.0 (3)
F 6	0.1155 (2)	0.1434 (2)	0.2488 (2)	8.0 (3)
F 7	0.2696 (3)	0.0327 (2)	-0.2778 (3)	7.0 (3)
F 8	0.1701 (3)	0.0339 (2)	-0.4443 (2)	7.7 (3)

F 9	0.1015	(3)	-0.0086	(2)	-0.2919	(3)	7.5	(3)			
F 10	-0.0175	(2)	0.2196	(2)	-0.3313	(3)	6.4	(3)			
F 11	-0.0627	(2)	0.1000	(2)	-0.3135	(3)	7.6	(3)			
F 12	-0.0017	(2)	0.1403	(2)	-0.4717	(2)	7.0	(3)			
O 1	0.1613	(2)	0.1520	(2)	0.0189	(2)	3.9	(3)			
O 2	0.1302	(2)	0.1355	(2)	-0.1795	(2)	3.6	(3)			
C 1	0.3538	(3)	0.1526	(2)	-0.0372	(3)	3.4	(3)			
C 2	0.4563	(3)	0.1593	(3)	-0.0814	(4)	4.3	(3)			
C 3	0.5505	(3)	0.1252	(3)	-0.0207	(4)	4.8	(3)			
C 4	0.5417	(4)	0.0846	(3)	0.0829	(4)	5.1	(3)			
C 5	0.4398	(4)	0.0760	(3)	0.1261	(4)	4.4	(3)			
C 6	0.3460	(3)	0.1101	(2)	0.0656	(3)	3.6	(3)			
C 7	0.2277	(3)	0.1052	(2)	0.0972	(3)	3.8	(3)			
C 8	0.1843	(4)	0.0200	(3)	0.0877	(4)	4.8	(3)			
C 9	0.2190	(4)	0.1394	(4)	0.2214	(4)	5.4	(3)			
C 10	0.2667	(3)	0.2286	(2)	-0.2443	(3)	3.6	(3)			
C 11	0.3416	(4)	0.2895	(2)	-0.2646	(4)	4.5	(3)			
C 12	0.3609	(4)	0.3084	(3)	-0.3790	(4)	5.0	(3)			
C 13	0.3068	(4)	0.2688	(3)	-0.4729	(4)	4.9	(3)			
C 14	0.2307	(4)	0.2090	(3)	-0.4557	(4)	4.5	(3)			
C 15	0.2122	(3)	0.1907	(2)	-0.3408	(3)	3.5	(3)			
C 16	0.1322	(3)	0.1299	(2)	-0.3025	(3)	3.6	(3)			
C 17	0.1664	(4)	0.0464	(3)	-0.3298	(4)	5.1	(3)			
C 18	0.0098	(4)	0.1473	(3)	-0.3547	(4)	4.7	(3)			
C 19	0.1892	(5)	0.2917	(3)	-0.0482	(5)	6.5	(3)			
C 20	0.0734	(6)	0.3131	(4)	-0.0703	(6)	7.8	(3)			
C 21	0.0516	(7)	0.3951	(4)	-0.0123	(7)	10.2	(4)			
C 22	0.0549	(7)	0.3916	(4)	0.1145	(6)	9.5	(4)			
H 2 A	0.4599200	(	0.1888200	(	-0.1581000	(	4.27	(0)			
H 3 A	0.6260800	(	0.1282300	(	-0.0493400	(	4.76	(0)			
H 4 A	0.6111700	(	0.0623200	(	0.1282100	(	5.13	(0)			
H 5 A	0.4338300	(	0.0462099	(	0.2020400	(	4.47	(0)			
H 11A	0.3826400	(	0.3189900	(	-0.1962000	(	4.49	(0)			
H 12A	0.4141900	(	0.3524100	(	-0.3928500	(	4.92	(0)			
H 13A	0.3226300	(	0.2828900	(	-0.5552900	(	4.90	(0)			
H 14A	0.1896900	(	0.1799400	(	-0.5243200	(	4.51	(0)			
H 19A	0.2340500	(	0.3332300	(	-0.0866500	(	6.38	(0)			
H 19B	0.2095800	(	0.2952700	(	0.0397400	(	6.38	(0)			
H 20A	0.0262200	(	0.2711700	(	-0.0396000	(	7.81	(0)			
H 20B	0.0530000	(	0.3174900	(	-0.1590400	(	7.81	(0)			
H 21A	-0.0243500	(	0.4153100	(	-0.0410200	(	10.10	(0)			
H 21B	0.1093600	(	0.4341000	(	-0.0299100	(	10.10	(0)			
H 22A	0.0417800	(	0.4440900	(	0.1492500	(	9.45	(0)			
H 22B	-0.0022800	(	0.3529200	(	0.1388800	(	9.45	(0)			
H 22C	0.1314400	(	0.3717100	(	0.1499900	(	9.45	(0)			

atom u11, 22, 33, 12, 13, 23

U values with e.s.d. in parentheses

atom	u11	u22	u33	u12	u13	u23
P 1	0.0524 (6)	0.03 (1)	0.0443 (5)	0.0070 (4)	0.0047 (4)	-0.0036 (4)
F 1	0.101 (2)	0.05 (1)	0.075 (2)	-0.015 (1)	0.009 (1)	-0.009 (1)
F 2	0.065 (2)	0.10 (1)	0.109 (2)	-0.015 (2)	0.016 (2)	0.019 (2)
F 3	0.088 (2)	0.07 (1)	0.096 (2)	0.003 (1)	-0.001 (2)	0.039 (2)
F 4	0.122 (3)	0.10 (1)	0.066 (2)	-0.001 (2)	0.006 (2)	-0.036 (2)
F 5	0.116 (2)	0.14 (1)	0.043 (1)	0.039 (2)	-0.004 (1)	0.009 (2)
F 6	0.078 (2)	0.17 (1)	0.060 (2)	0.023 (2)	0.022 (1)	-0.014 (2)
F 7	0.098 (2)	0.06 (1)	0.104 (2)	0.031 (2)	-0.003 (2)	0.000 (2)
F 8	0.159 (3)	0.07 (1)	0.065 (2)	0.011 (2)	0.014 (2)	-0.019 (2)
F 9	0.128 (3)	0.04 (1)	0.110 (2)	-0.018 (2)	0.011 (2)	0.000 (2)
F 10	0.064 (2)	0.08 (1)	0.096 (2)	0.022 (1)	-0.008 (1)	0.000 (2)
F 11	0.063 (2)	0.12 (1)	0.104 (2)	-0.026 (2)	-0.011 (1)	0.041 (2)
F 12	0.089 (2)	0.12 (1)	0.055 (2)	-0.013 (2)	-0.022 (1)	0.006 (2)
O 1	0.048 (1)	0.06 (1)	0.042 (1)	0.011 (1)	0.005 (1)	0.002 (1)
O 2	0.050 (1)	0.04 (1)	0.042 (1)	-0.002 (1)	0.001 (1)	0.003 (1)
C 1	0.049 (2)	0.03 (1)	0.048 (2)	-0.001 (2)	0.002 (2)	-0.008 (2)

C 2	0.056 (2)	0.05 (1)	0.060 (2)	-0.005 (2)	0.008 (2)	-0.006 (2)
C 3	0.047 (2)	0.05 (1)	0.081 (3)	-0.000 (2)	0.004 (2)	-0.010 (2)
C 4	0.054 (2)	0.06 (1)	0.081 (3)	0.007 (2)	-0.007 (2)	-0.008 (2)
C 5	0.059 (2)	0.05 (1)	0.057 (2)	0.006 (2)	-0.005 (2)	-0.000 (2)
C 6	0.048 (2)	0.04 (1)	0.047 (2)	0.001 (2)	-0.001 (2)	-0.006 (2)
C 7	0.051 (2)	0.05 (1)	0.042 (2)	0.009 (2)	0.004 (2)	0.004 (2)
C 8	0.056 (2)	0.06 (1)	0.064 (3)	0.001 (2)	0.007 (2)	0.015 (2)
C 9	0.068 (3)	0.09 (1)	0.044 (2)	0.013 (3)	0.002 (2)	-0.001 (2)
C 10	0.052 (2)	0.03 (1)	0.051 (2)	0.004 (2)	0.004 (2)	-0.001 (2)
C 11	0.064 (2)	0.04 (1)	0.070 (3)	-0.004 (2)	0.005 (2)	0.002 (2)
C 12	0.064 (3)	0.04 (1)	0.078 (3)	0.001 (2)	0.014 (2)	0.017 (2)
C 13	0.062 (2)	0.06 (1)	0.061 (3)	0.006 (2)	0.014 (2)	0.014 (2)
C 14	0.062 (2)	0.06 (1)	0.050 (2)	0.006 (2)	0.009 (2)	0.005 (2)
C 15	0.049 (2)	0.04 (1)	0.045 (2)	0.006 (2)	0.004 (2)	0.000 (2)
C 16	0.055 (2)	0.04 (1)	0.041 (2)	-0.001 (2)	-0.002 (2)	0.001 (2)
C 17	0.085 (3)	0.05 (1)	0.058 (2)	-0.000 (2)	0.003 (2)	-0.002 (2)
C 18	0.054 (2)	0.06 (1)	0.056 (2)	-0.006 (2)	-0.005 (2)	0.014 (2)
C 19	0.107 (4)	0.06 (1)	0.080 (3)	0.026 (3)	0.034 (3)	0.008 (3)
C 20	0.105 (4)	0.10 (1)	0.090 (4)	0.019 (4)	-0.009 (3)	-0.025 (4)
C 21	0.175 (8)	0.08 (1)	0.131 (6)	0.069 (5)	0.054 (5)	0.002 (4)
C 22	0.151 (6)	0.10 (1)	0.104 (5)	0.018 (5)	0.022 (4)	-0.050 (4)