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JA9640944

Supporting Information for:
A Carbene - Phosphorus (V) Adduct

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Table I. Summary of X-ray Diffraction Data for 1,3-dimesitylimidazolin-2-phenyltetrafluorophosphonate (**2**).

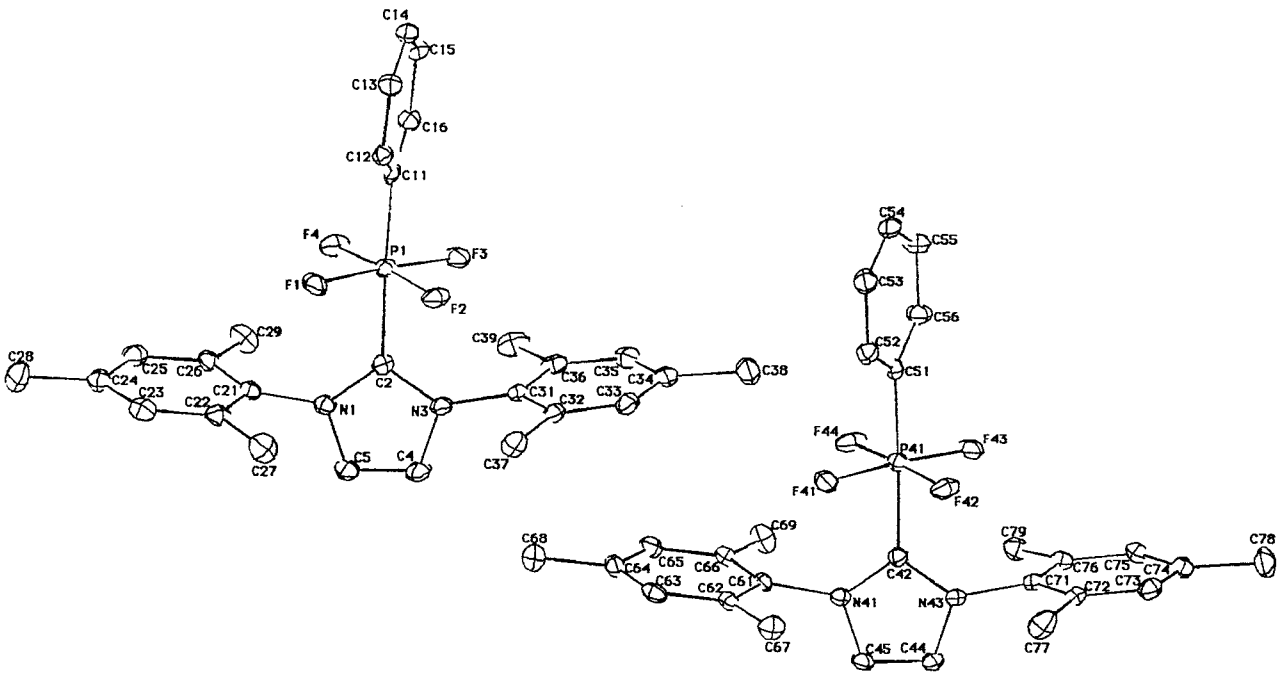
formula	$C_{27}H_{29}F_4N_2P$
crystallization method	from evaporation of thf
color	colorless
shape	irregular block
size, mm	0.44 x 0.34 x 0.47
symmetry	monoclinic
space group	$P2_1/n$ (No. 14)
a, Å	15.022(2)
b, Å	21.290(4)
c, Å	17.280(4)
β, deg	113.21(2)
temperature, °C	-70
volume, $Å^3$	5079.2
Z	8
Fw	488.52
calculated density, g/cc	1.278
μ(Mo), cm^{-1}	1.49
diffractometer	Enraf-Nonius CAD4
radiation (graphite monochromator)	MoKα
scan method	ω
data octants	+++,-++
2θ	$1.9° \leq 2\theta \leq 48.0°$
maximum HKL	17 24 19
scan width	1.20-2.40° ω
scan speed	1.70-5.00°/min
typical peak-with @ half height	0.17°
data collected	8477
2 standards collected 39x	2% fluctuation
variation in azimuthal scan	7.2%
no. of unique data ($I \geq 3.0\ \sigma(I)$)	3970
absorption correction	none
solution method	direct methods (MULTAN)
refinement method	full-matrix least squares on F

Table I (cont'd).

anomalous dispersion	P
weighting scheme	weights $\propto [\sigma^2(I)+0.0009I^2]^{-1/2}$
excluded	2
atoms refined	aniso: all non-hydrogen atoms isotropic: H
parameters varied	845
data/parameter ratio	4.70
R, Rw	0.043. 0.036
error of fit	1.22
max shift Δ/σ	1.36
max residual density, e/Å^3	0.23 (near H69)

Symmetry Operation Codes

a $^1/_2$-X, $-^1/_2$+Y, $^1/_2$-Z



ORTEP drawings of the two independent molecules of (**2**)
[not in crystallographic relative orientations].

Table II. Fractional Coordinates ($x10^4$) and Isotropic Thermal Parameters

Atom	X	Y	Z	B_{ISO}
P(1)	3908.7(7)	3991.4(5)	3069.2(7)	2.7(0)'
P(41)	-3481.1(7)	779.3(5)	2712.5(6)	2.6(0)'
F(1)	3257(1)	4181(1)	2109(1)	4.3(1)'
F(2)	4186(1)	3339(1)	2738(1)	4.0(1)'
F(3)	4625(1)	3821(1)	4020(1)	4.3(1)'
F(4)	3699(2)	4669(1)	3377(2)	4.6(1)'
F(41)	-3209(2)	993(1)	3671(1)	4.3(1)'
F(42)	-2827(2)	157(1)	3048(2)	4.5(1)'
F(43)	-3813(2)	528(1)	1761(1)	4.7(1)'
F(44)	-4208(1)	1370(1)	2381(2)	4.6(1)'
N(1)	5051(2)	4879(1)	2518(2)	3.2(1)'
N(3)	5934(2)	4153(1)	3316(2)	2.9(1)'
N(41)	-5094(2)	504(1)	3211(2)	2.8(1)'
N(43)	-4951(2)	-209(1)	2387(2)	2.9(1)'
C(2)	5007(3)	4359(2)	2950(2)	2.8(1)'
C(4)	6540(3)	4549(2)	3107(3)	4.0(2)'
C(5)	5991(3)	4992(2)	2618(3)	4.3(2)'
C(11)	2889(2)	3625(2)	3238(2)	2.4(1)'
C(12)	2231(3)	3236(2)	2649(3)	2.8(1)'
C(13)	1489(3)	2949(2)	2798(3)	3.4(2)'
C(14)	1394(3)	3047(2)	3544(3)	3.6(2)'
C(15)	2033(3)	3427(2)	4140(3)	3.7(2)'
C(16)	2777(3)	3717(2)	3988(3)	3.2(2)'
C(21)	4277(3)	5272(2)	1954(3)	2.9(1)'
C(22)	3918(3)	5139(2)	1102(3)	3.4(2)'
C(23)	3274(3)	5559(2)	559(3)	3.9(2)'
C(24)	2978(3)	6097(2)	848(3)	3.7(2)'
C(25)	3351(3)	6202(2)	1704(3)	3.8(2)'
C(26)	4013(3)	5805(2)	2273(3)	3.1(1)'
C(27)	4227(5)	4560(3)	764(4)	5.1(2)'
C(28)	2292(4)	6554(3)	238(4)	5.7(2)'
C(29)	4454(5)	5968(3)	3194(3)	4.7(2)'
C(31)	6349(2)	3618(2)	3852(2)	2.8(1)'
C(32)	6452(3)	3060(2)	3482(3)	3.0(1)'

Table II. Fractional Coordinates ($x10^4$) and Isotropic Thermal Parameters (cont'd.)

C(33)	6909(3)	2571(2)	4019(3)	3.5(2)'
C(34)	7258(3)	2622(2)	4879(3)	3.8(2)'
C(35)	7140(3)	3193(3)	5212(3)	4.0(2)'
C(36)	6690(3)	3702(2)	4724(3)	3.3(2)'
C(37)	6104(4)	2988(3)	2552(3)	4.2(2)'
C(38)	7798(5)	2087(3)	5441(5)	5.5(2)'
C(39)	6577(4)	4319(3)	5096(4)	4.9(2)'
C(42)	-4551(3)	332(2)	2779(2)	2.5(1)'
C(44)	-5743(3)	-361(2)	2565(3)	3.7(2)'
C(45)	-5827(3)	71(2)	3070(3)	3.5(2)'
C(51)	-2466(3)	1231(2)	2650(3)	2.6(1)'
C(52)	-1609(3)	1318(2)	3347(3)	3.5(2)'
C(53)	-847(3)	1664(2)	3296(4)	4.4(2)'
C(54)	-943(4)	1927(2)	2549(4)	4.7(2)'
C(55)	-1783(4)	1856(2)	1858(4)	4.5(2)'
C(56)	-2537(3)	1511(2)	1908(3)	3.8(2)'
C(61)	-5007(2)	1035(2)	3762(2)	2.4(1)'
C(62)	-4455(3)	957(2)	4613(2)	2.7(1)'
C(63)	-4461(3)	1449(2)	5133(3)	3.3(2)'
C(64)	-4977(3)	1996(2)	4832(3)	3.2(2)'
C(65)	-5509(3)	2047(2)	3977(3)	3.4(2)'
C(66)	-5548(3)	1565(2)	3425(2)	2.9(1)'
C(67)	-3855(4)	382(2)	4954(4)	3.9(2)'
C(68)	-4979(5)	2522(3)	5419(4)	5.0(2)'
C(69)	-6188(4)	1629(3)	2501(3)	4.3(2)'
C(71)	-4749(3)	-583(2)	1770(2)	2.6(1)'
C(72)	-4115(3)	-1084(2)	2034(3)	3.0(1)'
C(73)	-4039(3)	-1467(2)	1412(3)	3.4(2)'
C(74)	-4580(3)	-1368(2)	566(3)	3.4(2)'
C(75)	-5202(3)	-863(2)	340(3)	3.3(2)'
C(76)	-5306(3)	-462(2)	927(3)	2.8(1)'
C(77)	-3565(5)	-1228(3)	2949(4)	5.0(2)'
C(78)	-4524(5)	-1813(3)	-95(5)	5.3(2)'
C(79)	-6033(4)	56(2)	666(4)	3.7(2)'
H(4)	7209(30)	4475(18)	3322(24)	4.9(11)

Table II. Fractional Coordinates ($x10^4$) and Isotropic Thermal Parameters (cont'd.)

H(5)	6122(27)	5316(18)	2334(23)	4.3(11)
H(12)	2284(22)	3162(14)	2096(20)	2.6(8)
H(13)	1015(24)	2698(15)	2358(21)	3.2(9)
H(14)	922(23)	2841(15)	3669(20)	2.5(8)
H(15)	2032(23)	3511(16)	4681(21)	3.2(9)
H(16)	3194(24)	3994(16)	4390(22)	3.3(9)
H(23)	3012(25)	5470(17)	-42(23)	3.8(10)
H(25)	3151(24)	6548(16)	1908(21)	3.3(9)
H(27)	4946(38)	4554(23)	940(31)	9.7(18)
H(27')	3909(36)	4537(22)	177(33)	8.7(17)
H(27")	4144(33)	4176(23)	1043(29)	7.9(15)
H(28)	2533(31)	6668(21)	-214(28)	6.3(14)
H(28')	2269(38)	6904(25)	506(33)	9.6(19)
H(28")	1651(34)	6350(22)	22(29)	7.4(15)
H(29)	4466(37)	5593(25)	3515(31)	10.4(17)
H(29')	4146(36)	6261(25)	3358(32)	9.2(18)
H(29")	5072(38)	6097(25)	3364(32)	10.6(19)
H(33)	6962(19)	2177(14)	3761(17)	1.3(7)
H(35)	7390(23)	3229(14)	5772(21)	2.3(9)
H(37)	5488(36)	2993(22)	2238(31)	7.5(16)
H(37')	6283(33)	2639(22)	2384(28)	6.6(14)
H(37")	6403(38)	3306(25)	2334(33)	11.4(19)
H(38)	7736(39)	2125(26)	5912(35)	10.4(22)
H(38')	8398(40)	2118(26)	5540(34)	9.8(19)
H(38")	7602(35)	1677(25)	5189(30)	8.2(17)
H(39)	6778(29)	4652(18)	4835(24)	4.3(12)
H(39')	6958(29)	4304(19)	5635(25)	4.1(12)
H(39")	5927(33)	4341(20)	5044(25)	6.2(13)
H(44)	-6106(22)	-707(15)	2347(19)	2.0(8)
H(45)	-6282(22)	145(14)	3303(19)	2.0(7)
H(52)	-1541(25)	1136(16)	3898(22)	3.9(10)
H(53)	-254(30)	1694(18)	3840(27)	5.7(12)
H(54)	-456(31)	2134(19)	2485(26)	5.9(12)
H(55)	-1815(28)	2033(19)	1295(27)	6.0(12)
H(56)	-3105(25)	1458(16)	1402(22)	3.6(10)

Table II. Fractional Coordinates ($x10^4$) and Isotropic Thermal Parameters (cont'd.)

H(63)	-4101(22)	1392(15)	5687(21)	2.6(9)
H(65)	-5871(23)	2402(15)	3766(20)	2.1(8)
H(67)	-4218(31)	2(22)	4859(26)	6.1(13)
H(67')	-3494(32)	398(19)	5490(29)	5.7(14)
H(67")	-3408(39)	288(24)	4653(32)	11.9(17)
H(68)	-5284(38)	2413(24)	5763(33)	9.6(19)
H(68')	-5219(31)	2896(21)	5124(27)	6.2(14)
H(68")	-4348(38)	2630(24)	5765(33)	9.7(18)
H(69)	-5892(33)	1578(21)	2139(28)	6.6(14)
H(69')	-6418(32)	2030(22)	2396(27)	7.1(14)
H(69")	-6731(39)	1337(27)	2345(34)	12.4(20)
H(73)	-3611(23)	-1812(15)	1603(19)	2.5(8)
H(75)	-5589(21)	-789(13)	-261(20)	2.0(7)
H(77)	-3177(38)	-923(24)	3239(34)	10.4(19)
H(77')	-3256(32)	-1581(23)	3032(28)	6.6(15)
H(77")	-3961(34)	-1307(23)	3199(29)	7.1(18)
H(78)	-4072(41)	-1648(25)	-315(34)	10.9(19)
H(78')	-5073(41)	-1925(27)	-435(36)	12.7(23)
H(78")	-4289(40)	-2204(28)	165(35)	11.6(21)
H(79)	-6541(27)	-25(17)	853(22)	4.2(10)
H(79')	-6301(26)	111(16)	77(25)	3.9(11)
H(79")	-5761(27)	452(19)	874(23)	4.0(11)

Table III. Anisotropic Thermal Parameters (Å x 10^3) exp[-19.739(U_{11}hha*a*...+2(U_{12}hka*b*...))]

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
P(1)	29.5(6)	30.0(6)	42.5(7)	-2.4(5)	14.5(5)	-1.8(5)
P(41)	31.7(6)	31.8(6)	39.5(7)	-2.3(5)	17.2(5)	-1.7(5)
F(1)	40(1)	69(2)	48(2)	-14(1)	11(1)	18(1)
F(2)	48(1)	33(1)	85(2)	-7(1)	43(1)	-11(1)
F(3)	32(1)	82(2)	45(2)	-13(1)	12(1)	10(1)
F(4)	63(2)	31(1)	103(2)	-9(1)	55(2)	-16(1)
F(41)	53(1)	70(2)	48(2)	-27(1)	29(1)	-22(1)

Table III. Anisotropic Thermal Parameters (cont'd).

F(42)	41(1)	34(1)	103(2)	4(1)	35(1)	14(1)
F(43)	65(2)	79(2)	42(1)	-42(1)	30(1)	-20(1)
F(44)	38(1)	41(1)	104(2)	6(1)	35(1)	23(1)
N(1)	36(2)	34(2)	54(2)	-4(2)	21(2)	3(2)
N(3)	30(2)	36(2)	49(2)	-2(2)	21(2)	1(2)
N(41)	34(2)	39(2)	37(2)	-7(2)	19(2)	-5(2)
N(43)	41(2)	34(2)	38(2)	-9(2)	21(2)	-2(2)
C(2)	35(2)	28(2)	44(3)	-3(2)	18(2)	-5(2)
C(4)	33(3)	47(3)	74(4)	-5(3)	25(3)	5(3)
C(5)	45(3)	44(3)	84(4)	-6(3)	33(3)	11(3)
C(11)	24(2)	24(2)	43(3)	7(2)	12(2)	5(2)
C(12)	33(2)	29(2)	43(3)	1(2)	14(2)	2(2)
C(13)	34(3)	39(3)	53(3)	-10(2)	13(3)	1(2)
C(14)	34(3)	44(3)	63(4)	-1(2)	22(3)	12(3)
C(15)	41(3)	55(3)	52(3)	5(2)	26(3)	5(3)
C(16)	36(3)	36(3)	48(3)	-3(2)	16(2)	-2(2)
C(21)	34(2)	31(2)	49(3)	-5(2)	19(2)	4(2)
C(22)	47(3)	34(3)	53(3)	-10(2)	26(2)	-5(2)
C(23)	49(3)	54(3)	43(3)	-14(3)	16(3)	-4(3)
C(24)	40(3)	46(3)	56(3)	-4(2)	19(3)	4(3)
C(25)	48(3)	38(3)	67(4)	-2(2)	31(3)	-4(3)
C(26)	46(3)	30(2)	44(3)	-5(2)	22(2)	1(2)
C(27)	92(5)	44(3)	67(5)	0(3)	40(4)	-11(3)
C(28)	50(4)	80(5)	73(5)	16(3)	10(3)	15(4)
C(29)	83(4)	47(3)	50(4)	-13(3)	28(3)	-8(3)
C(31)	24(2)	39(3)	43(3)	-1(2)	15(2)	5(2)
C(32)	29(2)	42(3)	45(3)	0(2)	16(2)	-1(2)
C(33)	35(3)	39(3)	63(4)	0(2)	21(3)	-1(3)
C(34)	30(2)	56(3)	56(3)	-4(2)	15(2)	10(3)
C(35)	31(3)	82(4)	33(3)	-11(3)	6(2)	4(3)
C(36)	26(2)	53(3)	46(3)	-11(2)	12(2)	-11(3)
C(37)	52(4)	59(4)	46(4)	9(3)	16(3)	-9(3)
C(38)	49(4)	75(5)	77(5)	1(3)	16(4)	33(4)
C(39)	44(3)	80(4)	62(4)	-16(3)	20(3)	-27(4)
C(42)	31(2)	32(2)	32(2)	-2(2)	12(2)	0(2)
C(44)	51(3)	46(3)	52(3)	-26(2)	30(3)	-16(2)

Table III. Anisotropic Thermal Parameters (cont'd).

C(45)	39(3)	55(3)	49(3)	-18(2)	29(2)	-9(2)
C(51)	36(2)	27(2)	41(3)	2(2)	20(2)	-5(2)
C(52)	42(3)	44(3)	51(3)	-7(2)	21(3)	-10(2)
C(53)	42(3)	61(3)	67(4)	-18(3)	25(3)	-19(3)
C(54)	55(4)	49(3)	92(5)	-23(3)	48(4)	-22(3)
C(55)	53(3)	58(3)	70(4)	-18(3)	36(3)	1(3)
C(56)	43(3)	53(3)	52(3)	-13(2)	21(3)	-1(3)
C(61)	29(2)	38(2)	29(3)	-3(2)	15(2)	-4(2)
C(62)	29(2)	42(3)	34(3)	-3(2)	15(2)	0(2)
C(63)	36(3)	62(3)	25(3)	-8(2)	11(2)	2(3)
C(64)	41(3)	46(3)	35(3)	-3(2)	18(2)	-6(2)
C(65)	49(3)	39(3)	52(3)	10(2)	30(3)	10(3)
C(66)	33(2)	44(3)	37(3)	1(2)	19(2)	3(2)
C(67)	50(3)	47(3)	46(4)	8(3)	14(3)	12(3)
C(68)	77(4)	55(4)	64(4)	-6(3)	34(4)	-17(3)
C(69)	51(3)	71(4)	38(3)	18(3)	12(3)	5(3)
C(71)	32(2)	31(2)	41(3)	-8(2)	19(2)	-5(2)
C(72)	37(2)	30(2)	46(3)	-5(2)	13(2)	1(2)
C(73)	36(3)	31(3)	61(4)	4(2)	20(3)	2(2)
C(74)	36(2)	44(3)	55(3)	-5(2)	26(2)	-7(2)
C(75)	35(2)	58(3)	37(3)	-3(2)	17(2)	1(2)
C(76)	29(2)	40(3)	39(3)	-4(2)	16(2)	2(2)
C(77)	74(4)	45(4)	52(4)	3(3)	6(4)	10(3)
C(78)	67(4)	69(4)	79(5)	4(4)	43(4)	-26(4)
C(79)	40(3)	53(3)	50(4)	3(3)	19(3)	5(3)

Table IV. Interatomic Distances (Å)

P(1)-F(1)	1.611 (2)	N(41)-C(42)	1.355 (4)
P(1)-F(2)	1.618 (2)	N(41)-C(45)	1.383 (4)
P(1)-F(3)	1.611 (2)	N(41)-C(61)	1.450 (4)
P(1)-F(4)	1.611 (2)	N(43)-C(42)	1.351 (4)
P(41)-F(41)	1.608 (2)	N(43)-C(44)	1.379 (5)
P(41)-F(42)	1.614 (2)	N(43)-C(71)	1.457 (4)
P(41)-F(43)	1.610 (2)	C(4)-C(5)	1.317 (6)

Table IV. Interatomic Distances (Å) (cont'd).

P(41)-F(44)	1.615 (2)	C(11)-C(12)	1.380 (5)
P(1)-C(2)	1.910 (4)	C(11)-C(16)	1.385 (5)
P(1)-C(11)	1.842 (4)	C(12)-C(13)	1.383 (5)
P(41)-C(42)	1.910 (4)	C(13)-C(14)	1.368 (5)
P(41)-C(51)	1.843 (4)	C(14)-C(15)	1.362 (6)
N(1)-C(2)	1.351 (4)	C(15)-C(16)	1.389 (5)
N(1)-C(5)	1.375 (5)	C(21)-C(22)	1.384 (5)
N(1)-C(21)	1.451 (4)	C(21)-C(26)	1.386 (5)
N(3)-C(2)	1.355 (4)	C(22)-C(23)	1.378 (6)
N(3)-C(4)	1.388 (5)	C(22)-C(27)	1.514 (6)
N(3)-C(31)	1.446 (4)	C(23)-C(24)	1.390 (6)
C(24)-C(25)	1.378 (6)	C(27)-H(27')	0.936 (50)
C(24)-C(28)	1.504 (6)	C(27)-H(27")	0.983 (47)
C(25)-C(26)	1.380 (5)	C(28)-H(28)	1.012 (43)
C(26)-C(29)	1.504 (6)	C(28)-H(28')	0.886 (50)
C(31)-C(32)	1.387 (5)	C(28)-H(28")	0.985 (45)
C(31)-C(36)	1.398 (5)	C(29)-H(29)	0.969 (51)
C(32)-C(33)	1.383 (5)	C(29)-H(29')	0.887 (51)
C(32)-C(37)	1.489 (6)	C(29)-H(29")	0.899 (51)
C(33)-C(34)	1.371 (6)	C(33)-H(33)	0.967 (27)
C(34)-C(35)	1.386 (6)	C(35)-H(35)	0.893 (31)
C(34)-C(38)	1.509 (7)	C(37)-H(37)	0.870 (47)
C(35)-C(36)	1.377 (6)	C(37)-H(37')	0.879 (45)
C(36)-C(39)	1.501 (6)	C(37)-H(37")	0.968 (53)
C(44)-C(45)	1.308 (6)	C(38)-H(38)	0.858 (52)
C(51)-C(52)	1.385 (5)	C(38)-H(38')	0.852 (52)
C(51)-C(56)	1.378 (5)	C(38)-H(38")	0.968 (49)
C(52)-C(53)	1.394 (5)	C(39)-H(39)	0.951 (37)
C(53)-C(54)	1.361 (6)	C(39)-H(39')	0.880 (37)
C(54)-C(55)	1.361 (6)	C(39)-H(39")	0.944 (44)
C(55)-C(56)	1.381 (5)	C(44)-H(44)	0.905 (31)
C(61)-C(62)	1.386 (5)	C(45)-H(45)	0.933 (29)
C(61)-C(66)	1.379 (5)	C(52)-H(52)	0.994 (34)
C(62)-C(63)	1.380 (5)	C(53)-H(53)	1.011 (41)
C(62)-C(67)	1.497 (6)	C(54)-H(54)	0.898 (43)

Table IV. Interatomic Distances (Å) (cont'd).

C(63)-C(64)	1.383 (5)	C(55)-H(55)	1.026 (41)
C(64)-C(65)	1.380 (5)	C(56)-H(56)	0.958 (33)
C(64)-C(68)	1.511 (6)	C(63)-H(63)	0.904 (31)
C(65)-C(66)	1.385 (5)	C(65)-H(65)	0.919 (31)
C(66)-C(69)	1.512 (6)	C(67)-H(67)	0.952 (44)
C(71)-C(72)	1.381 (5)	C(67)-H(67')	0.869 (44)
C(71)-C(76)	1.388 (5)	C(67)-H(67")	1.019 (54)
C(72)-C(73)	1.389 (5)	C(68)-H(68)	0.912 (53)
C(72)-C(77)	1.499 (6)	C(68)-H(68')	0.939 (43)
C(73)-C(74)	1.381 (5)	C(68)-H(68")	0.930 (50)
C(74)-C(75)	1.376 (5)	C(69)-H(69)	0.905 (45)
C(74)-C(78)	1.513 (6)	C(69)-H(69')	0.911 (44)
C(75)-C(76)	1.380 (5)	C(69)-H(69")	0.975 (54)
C(76)-C(79)	1.493 (6)	C(73)-H(73)	0.945 (31)
C(4)-H(4)	0.937 (39)	C(75)-H(75)	0.982 (29)
C(5)-H(5)	0.912 (36)	C(77)-H(77)	0.884 (51)
C(12)-H(12)	1.002 (31)	C(77)-H(77')	0.866 (45)
C(13)-H(13)	0.972 (33)	C(77)-H(77")	0.878 (45)
C(14)-H(14)	0.927 (32)	C(78)-H(78)	0.965 (56)
C(15)-H(15)	0.952 (32)	C(78)-H(78')	0.837 (55)
C(16)-H(16)	0.938 (33)	C(78)-H(78")	0.946 (56)
C(23)-H(23)	0.973 (35)	C(79)-H(79)	0.955 (38)
C(25)-H(25)	0.915 (33)	C(79)-H(79')	0.943 (36)
C(27)-H(27)	1.000 (50)	C(79)-H(79")	0.944 (38)

Table V. Intramolecular Angles (°)

F(1)-P(1)-F(2)	89.2 (1)	N(1)-C(21)-C(26)	118.9 (4)
F(1)-P(1)-F(3)	176.0 (1)	N(3)-C(31)-C(32)	118.5 (4)
F(1)-P(1)-F(4)	89.9 (1)	N(3)-C(31)-C(36)	118.2 (4)
F(2)-P(1)-F(3)	90.3 (1)	N(43)-C(44)-C(45)	107.6 (4)
F(2)-P(1)-F(4)	175.3 (1)	N(41)-C(45)-C(44)	107.8 (4)
F(3)-P(1)-F(4)	90.2 (1)	N(41)-C(61)-C(62)	117.8 (3)
F(41)-P(41)-F(42)	89.5 (1)	N(41)-C(61)-C(66)	118.5 (3)

Table V. Intramolecular Angles (°) (cont'd).

F(41)-P(41)-F(43)	175.6 (1)	N(43)-C(71)-C(72)	119.7 (4)
F(41)-P(41)-F(44)	90.4 (1)	N(43)-C(71)-C(76)	117.0 (3)
F(42)-P(41)-F(43)	89.6 (1)	N(3)-C(4)-H(4)	120 (2)
F(42)-P(41)-F(44)	175.4 (2)	N(1)-C(5)-H(5)	119 (3)
F(43)-P(41)-F(44)	90.2 (1)	N(43)-C(44)-H(44)	122 (2)
F(1)-P(1)-C(2)	89.2 (1)	N(41)-C(45)-H(45)	119 (2)
F(1)-P(1)-C(11)	93.6 (1)	C(12)-C(11)-C(16)	117.3 (4)
F(2)-P(1)-C(2)	87.7 (1)	C(11)-C(12)-C(13)	121.5 (4)
F(2)-P(1)-C(11)	92.2 (1)	C(12)-C(13)-C(14)	120.0 (4)
F(3)-P(1)-C(2)	86.8 (1)	C(13)-C(14)-C(15)	119.9 (4)
F(3)-P(1)-C(11)	90.4 (1)	C(14)-C(15)-C(16)	120.1 (5)
F(4)-P(1)-C(2)	87.6 (1)	C(11)-C(16)-C(15)	121.2 (4)
F(4)-P(1)-C(11)	92.5 (1)	C(22)-C(21)-C(26)	122.5 (4)
F(41)-P(41)-C(42)	87.5 (1)	C(21)-C(22)-C(23)	117.8 (4)
F(41)-P(41)-C(51)	91.9 (1)	C(21)-C(22)-C(27)	121.8 (5)
F(42)-P(41)-C(42)	88.7 (1)	C(23)-C(22)-C(27)	120.4 (5)
F(42)-P(41)-C(51)	92.8 (1)	C(22)-C(23)-C(24)	121.9 (4)
F(43)-P(41)-C(42)	88.1 (1)	C(23)-C(24)-C(25)	117.8 (4)
F(43)-P(41)-C(51)	92.5 (1)	C(23)-C(24)-C(28)	120.6 (5)
F(44)-P(41)-C(42)	86.7 (1)	C(25)-C(24)-C(28)	121.5 (5)
F(44)-P(41)-C(51)	91.8 (1)	C(24)-C(25)-C(26)	122.6 (4)
C(2)-P(1)-C(11)	177.2 (2)	C(21)-C(26)-C(25)	117.2 (4)
C(42)-P(41)-C(51)	178.4 (3)	C(21)-C(26)-C(29)	122.3 (4)
C(2)-N(1)-C(5)	110.1 (4)	C(25)-C(26)-C(29)	120.4 (4)
C(2)-N(1)-C(21)	130.0 (3)	C(32)-C(31)-C(36)	123.1 (4)
C(5)-N(1)-C(21)	119.7 (3)	C(31)-C(32)-C(33)	116.8 (4)
C(2)-N(3)-C(4)	109.9 (3)	C(31)-C(32)-C(37)	122.0 (4)
C(2)-N(3)-C(31)	131.2 (3)	C(33)-C(32)-C(37)	121.1 (4)
C(4)-N(3)-C(31)	118.9 (3)	C(32)-C(33)-C(34)	123.0 (4)
C(42)-N(41)-C(45)	109.5 (3)	C(33)-C(34)-C(35)	117.6 (4)
C(42)-N(41)-C(61)	130.9 (3)	C(33)-C(34)-C(38)	121.1 (5)
C(45)-N(41)-C(61)	119.7 (3)	C(35)-C(34)-C(38)	121.2 (5)
C(42)-N(43)-C(44)	110.0 (3)	C(34)-C(35)-C(36)	123.2 (4)
C(42)-N(43)-C(71)	130.9 (3)	C(31)-C(36)-C(35)	116.3 (4)
C(44)-N(43)-C(71)	118.8 (3)	C(31)-C(36)-C(39)	121.3 (5)

Table V. Intramolecular Angles (°) (cont'd).

P(1)-C(2)-N(1)	128.9 (3)	C(35)-C(36)-C(39)	122.5 (5)
P(1)-C(2)-N(3)	126.1 (3)	C(52)-C(51)-C(56)	117.2 (4)
P(41)-C(42)-N(41)	127.0 (3)	C(51)-C(52)-C(53)	121.3 (4)
P(41)-C(42)-N(43)	127.8 (3)	C(52)-C(53)-C(54)	119.7 (5)
P(1)-C(11)-C(12)	122.4 (3)	C(53)-C(54)-C(55)	120.0 (5)
P(1)-C(11)-C(16)	120.2 (3)	C(54)-C(55)-C(56)	120.3 (5)
P(41)-C(51)-C(52)	121.6 (3)	C(51)-C(56)-C(55)	121.5 (5)
P(41)-C(51)-C(56)	121.2 (3)	C(62)-C(61)-C(66)	123.5 (4)
N(1)-C(2)-N(3)	105.0 (3)	C(61)-C(62)-C(63)	116.5 (4)
N(41)-C(42)-N(43)	105.1 (3)	C(61)-C(62)-C(67)	122.0 (4)
N(3)-C(4)-C(5)	107.0 (4)	C(63)-C(62)-C(67)	121.4 (4)
N(1)-C(5)-C(4)	108.0 (4)	C(62)-C(63)-C(64)	122.7 (4)
N(1)-C(21)-C(22)	118.1 (4)	C(63)-C(64)-C(65)	118.1 (4)
C(63)-C(64)-C(68)	121.4 (5)	C(45)-C(44)-H(44)	130 (2)
C(65)-C(64)-C(68)	120.5 (5)	C(44)-C(45)-H(45)	133 (2)
C(64)-C(65)-C(66)	121.9 (4)	C(51)-C(52)-H(52)	119 (2)
C(61)-C(66)-C(65)	117.3 (4)	C(53)-C(52)-H(52)	119 (2)
C(61)-C(66)-C(69)	122.9 (4)	C(52)-C(53)-H(53)	115 (2)
C(65)-C(66)-C(69)	119.8 (4)	C(54)-C(53)-H(53)	126 (2)
C(72)-C(71)-C(76)	122.8 (4)	C(53)-C(54)-H(54)	122 (3)
C(71)-C(72)-C(73)	117.0 (4)	C(55)-C(54)-H(54)	118 (3)
C(71)-C(72)-C(77)	121.9 (4)	C(54)-C(55)-H(55)	118 (2)
C(73)-C(72)-C(77)	121.1 (4)	C(56)-C(55)-H(55)	121 (2)
C(72)-C(73)-C(74)	122.3 (4)	C(51)-C(56)-H(56)	121 (2)
C(73)-C(74)-C(75)	118.1 (4)	C(55)-C(56)-H(56)	118 (2)
C(73)-C(74)-C(78)	121.3 (5)	C(62)-C(63)-H(63)	116 (2)
C(75)-C(74)-C(78)	120.6 (5)	C(64)-C(63)-H(63)	122 (2)
C(74)-C(75)-C(76)	122.3 (4)	C(64)-C(65)-H(65)	119 (2)
C(71)-C(76)-C(75)	117.4 (4)	C(66)-C(65)-H(65)	119 (2)
C(71)-C(76)-C(79)	121.4 (4)	C(62)-C(67)-H(67)	114 (3)
C(75)-C(76)-C(79)	121.1 (4)	C(62)-C(67)-H(67')	114 (3)
C(5)-C(4)-H(4)	133 (3)	C(62)-C(67)-H(67")	112 (3)
C(4)-C(5)-H(5)	132 (3)	C(64)-C(68)-H(68)	113 (3)
C(11)-C(12)-H(12)	120 (2)	C(64)-C(68)-H(68')	112 (3)
C(13)-C(12)-H(12)	119 (2)	C(64)-C(68)-H(68")	110 (3)

Table V. Intramolecular Angles (°) (cont'd).

C(12)-C(13)-H(13)	120 (2)	C(66)-C(69)-H(69)	116 (3)
C(14)-C(13)-H(13)	120 (2)	C(66)-C(69)-H(69')	109 (3)
C(13)-C(14)-H(14)	121 (2)	C(66)-C(69)-H(69")	110 (3)
C(15)-C(14)-H(14)	119 (2)	C(72)-C(73)-H(73)	116 (2)
C(14)-C(15)-H(15)	125 (2)	C(74)-C(73)-H(73)	122 (2)
C(16)-C(15)-H(15)	115 (2)	C(74)-C(75)-H(75)	119 (2)
C(11)-C(16)-H(16)	119 (2)	C(76)-C(75)-H(75)	119 (2)
C(15)-C(16)-H(16)	120 (2)	C(72)-C(77)-H(77)	114 (4)
C(22)-C(23)-H(23)	119 (2)	C(72)-C(77)-H(77')	113 (3)
C(24)-C(23)-H(23)	119 (2)	C(72)-C(77)-H(77")	111 (3)
C(24)-C(25)-H(25)	119 (2)	C(74)-C(78)-H(78)	109 (3)
C(26)-C(25)-H(25)	118 (2)	C(74)-C(78)-H(78')	112 (4)
C(22)-C(27)-H(27)	111 (3)	C(74)-C(78)-H(78")	108 (4)
C(22)-C(27)-H(27')	111 (3)	C(76)-C(79)-H(79)	111 (2)
C(22)-C(27)-H(27")	112 (3)	C(76)-C(79)-H(79')	112 (2)
C(24)-C(28)-H(28)	110 (3)	C(76)-C(79)-H(79")	113 (2)
C(24)-C(28)-H(28')	110 (4)	H(27)-C(27)-H(27')	111 (4)
C(24)-C(28)-H(28")	106 (3)	H(27)-C(27)-H(27")	100 (4)
C(26)-C(29)-H(29)	108 (3)	H(27')-C(27)-H(27")	112 (4)
C(26)-C(29)-H(29')	116 (3)	H(28)-C(28)-H(28')	107 (5)
C(26)-C(29)-H(29")	113 (3)	H(28)-C(28)-H(28")	114 (4)
C(32)-C(33)-H(33)	117 (2)	H(28')-C(28)-H(28")	110 (4)
C(34)-C(33)-H(33)	120 (2)	H(29)-C(29)-H(29')	107 (4)
C(34)-C(35)-H(35)	117 (2)	H(29)-C(29)-H(29")	106 (5)
C(36)-C(35)-H(35)	119 (2)	H(29')-C(29)-H(29")	107 (5)
C(32)-C(37)-H(37)	121 (3)	H(37)-C(37)-H(37')	101 (4)
C(32)-C(37)-H(37')	115 (3)	H(37)-C(37)-H(37")	107 (4)
C(32)-C(37)-H(37")	109 (3)	H(37')-C(37)-H(37")	102 (4)
C(34)-C(38)-H(38)	108 (4)	H(38)-C(38)-H(38')	108 (5)
C(34)-C(38)-H(38')	109 (4)	H(38)-C(38)-H(38")	113 (5)
C(34)-C(38)-H(38")	114 (3)	H(38')-C(38)-H(38")	106 (5)
C(36)-C(39)-H(39)	110 (2)	H(39)-C(39)-H(39')	109 (4)
C(36)-C(39)-H(39')	107 (3)	H(39)-C(39)-H(39")	115 (4)
C(36)-C(39)-H(39")	107 (3)	H(39')-C(39)-H(39")	109 (4)
H(67)-C(67)-H(67')	107 (4)	H(77)-C(77)-H(77')	111 (4)

Table V. Intramolecular Angles (°) (cont'd).

H(67)-C(67)-H(67")	101 (4)	H(77)-C(77)-H(77")	107 (5)
H(67')-C(67)-H(67")	107 (4)	H(77')-C(77)-H(77")	100 (4)
H(68)-C(68)-H(68')	113 (4)	H(78)-C(78)-H(78')	119 (5)
H(68)-C(68)-H(68")	107 (5)	H(78)-C(78)-H(78")	109 (4)
H(68')-C(68)-H(68")	102 (4)	H(78')-C(78)-H(78")	99 (5)
H(69)-C(69)-H(69')	103 (4)	H(79)-C(79)-H(79')	109 (3)
H(69)-C(69)-H(69")	109 (4)	H(79)-C(79)-H(79")	108 (3)
H(69')-C(69)-H(69")	109 (4)	H(79')-C(79)-H(79")	104 (3)

Table VI. Intramolecular Non-Bonding Distances (Å)

F(1)...C(21)	2.853 (4)	F(43)...C(71)	2.757 (4)
F(1)...C(22)	3.089 (4)	F(43)...C(72)	3.518 (4)
F(1)...C(26)	3.615 (4)	F(43)...C(76)	3.001 (4)
F(1)...C(27)	3.293 (7)	F(43)...C(79)	3.278 (6)
F(2)...C(31)	3.113 (4)	F(44)...C(61)	3.145 (4)
F(2)...C(32)	3.185 (4)	F(44)...C(66)	3.216 (4)
F(2)...C(37)	3.113 (6)	F(44)...C(69)	3.111 (6)
F(3)...C(31)	2.752 (4)	C(2)...C(27)	3.512 (8)
F(3)...C(32)	3.611 (4)	C(2)...C(29)	3.589 (7)
F(3)...C(35)	3.764 (5)	C(2)...C(37)	3.550 (7)
F(3)...C(36)	2.862 (4)	C(2)...C(39)	3.526 (8)
F(3)...C(39)	2.980 (6)	C(4)...C(37)	3.449 (8)
F(4)...C(21)	3.184 (4)	C(4)...C(39)	3.451 (8)
F(4)...C(26)	3.228 (4)	C(5)...C(27)	3.383 (9)
F(4)...C(29)	3.054 (6)	C(5)...C(29)	3.530 (8)
F(41)...C(61)	2.767 (4)	C(42)...C(67)	3.484 (7)
F(41)...C(62)	2.926 (4)	C(42)...C(69)	3.602 (7)
F(41)...C(63)	3.821 (5)	C(42)...C(77)	3.600 (7)
F(41)...C(66)	3.582 (4)	C(42)...C(79)	3.497 (7)
F(41)...C(67)	3.041 (6)	C(44)...C(77)	3.582 (8)
F(42)...C(71)	3.267 (4)	C(44)...C(79)	3.259 (7)
F(42)...C(72)	3.334 (4)	C(45)...C(67)	3.495 (7)
F(42)...C(77)	3.131 (7)	C(45)...C(69)	3.442 (8)
F(42)...C(5)a	3.399 (5)		