C(7)—C(6)—O	128.8 (4)	C(11)—As—C(12)	99.8 (2)
C(10)—C(6)—O	129.0 (4)	C(11)—As—C(13)	99.3 (2)
C(6)—C(7)—C(8)	108.4 (3)	C(12)—As—C(13)	106.9 (2)

Table 4. *Selected geometric parameters* (Å, °) *for* (II)

Ru—C(1)	2.203 (4)	C(11)—C(12)	1.384 (5)
Ru—C(2)	2.218 (5)	C(11)—C(16)	1.391 (6)
Ru—C(3)	2.197 (6)	C(12)—C(13)	1.384 (5)
Ru—C(4)	2.205 (5)	C(13)—C(14)	1.369 (7)
Ru—C(5)	2.193 (5)	C(14)—C(15)	1.363 (6)
Ru···C(6)	2.636 (4)	C(15)—C(16)	1.377 (5)
Ru—C(7)	2.262 (4)	C(17)—C(18)	1.390 (6)
Ru—C(8)	2.163 (4)	C(17)—C(22)	1.385 (5)
Ru—C(9)	2.159 (4)	C(18)—C(19)	1.381 (6)
Ru—C(10)	2.271 (4)	C(19)—C(20)	1.373 (7)
Ru—As	2.5123 (6)	C(20)—C(21)	1.368 (7)
C(1)—C(2)	1.382 (8)	C(21)—C(22)	1.395 (6)
C(1)—C(5)	1.395 (8)	C(23)—C(24)	1.381 (6)
C(2)—C(3)	1.417 (9)	C(23)—C(28)	1.391 (5)
C(3)—C(4)	1.405 (8)	C(24)—C(25)	1.385 (6)
C(4)—C(5)	1.386 (7)	C(25)—C(26)	1.369 (7)
C(6)—C(7)	1.478 (6)	C(26)—C(27)	1.371 (7)
C(6)—C(10)	1.473 (7)	C(27)—C(28)	1.378 (6)
C(6)—O	1.210 (5)	P—F(1)	1.594 (3)
C(7)—C(8)	1.392 (6)	P—F(2)	1.578 (3)
C(8)—C(9)	1.416 (6)	P—F(3)	1.578 (3)
C(9)—C(10)	1.398 (6)	P—F(4)	1.581 (4)
As—C(11)	1.953 (3)	P—F(5)	1.567 (3)
As—C(17)	1.949 (4)	P—F(6)	1.578 (3)
As—C(23)	1.944 (4)		
C(2)—C(1)—C(5)	108.7 (5)	C(7)—C(8)—C(9)	108.3 (4)
C(1)—C(2)—C(3)	107.0 (5)	C(8)—C(9)—C(10)	108.7 (4)
C(2)—C(3)—C(4)	108.4 (5)	C(6)—C(10)—C(9)	107.0 (4)
C(3)—C(4)—C(5)	106.9 (5)	Ru—As—C(11)	113.4 (1)
C(1)—C(5)—C(4)	109.0 (5)	Ru—As—C(17)	121.4 (1)
C(7)—C(6)—C(10)	102.6 (4)	Ru—As—C(23)	113.5 (1)
C(7)—C(6)—O	129.1 (4)	C(11)—As—C(17)	98.5 (2)
C(10)—C(6)—O	128.3 (4)	C(11)—As—C(23)	100.8 (1)
C(6)—C(7)—C(8)	107.3 (4)	C(17)—As—C(23)	106.5 (2)

For both compounds, data collection, data reduction and cell refinement were carried out using the programs *SERVER4*, *PW*115 and *LLSQ*6 (Mereiter & Völlenkle, 1990). After applying corrections for absorption, both structures were solved by direct methods and refined by full-matrix least-squares with *SHELX*76 (Sheldrick, 1976). H atoms were generated in idealized positions (C—H = 0.96 Å). CP, CPD and benzene H atoms were refined as riding on their parent atoms, methyl H atoms of (I) were refined as rigid CH_3 groups. The isotropic displacement parameters of the H atoms in (I) were set to 1.30 × U_{eq} of the parent C atoms, and in (II), to 1.11 × U_{eq} of the parent C atoms. Disorder in the octahedral PF_6^- anion of (I) was modelled by allowing split occupancies for four of the F atoms. Site occupation factor for F(3)–F(6) refined to PP = 0.664 (5), and for F(3')–F(6') to $1 - PP$ = 0.336 (5). Molecular graphics and tabular matter were produced with *Xtal*3.2 (Hall, Flack & Stewart, 1992).

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[CpMoCl(PMe₃)₃][BF₄] and [Cp*MoCl(PMe₃)₃][PF₆]

JAMES C. FETTINGER, HEINZ-BERNHARD KRAATZ AND RINALDO POLI*

Department of Chemistry and Biochemistry, University of Maryland, College Park, Maryland 20742, USA

ARNOLD L. RHEINGOLD

*Department of Chemistry, University of Delaware, Newark, DE 19719, USA*

Abstract

Chloro(η^5-cyclopentadienyl)tris(trimethylphosphine)-molybdenum(III) tetrafluoroborate, [MoCl(C₅H₅)-(C₃H₉P)₃][BF₄], was obtained from the oxidation of [MoH(C₅H₅)(PMe₃)₃] by AgBF₄, followed by crystallization from dichloromethane. Chloro(η^5-pentamethyl-cyclopentadienyl)tris(trimethylphosphine)molybdenum-(III) hexafluorophosphate, [MoCl(C₁₀H₁₅)(C₃H₉P)₃]-[PF₆], was obtained from the reaction of [MoCl₂-(C₁₀H₁₅)(C₃H₉P)₂] with TlPF₆ and PMe₃ in dichloromethane. Both cations adopt a four-legged piano-stool arrangement.

Comment

Odd-electron complexes having the general formula $[(\text{ring})MX_{2-n}L_{2+n}]^{n+}$ (ring = cyclopentadienide or substituted analogue; X = Cl, Br, I; L = PR$_3$; n = 0 or 1) and possessing a four-legged piano-stool configuration are now well established (Poli, 1992). As part of our ongoing investigation of CpMo^{III} complexes, we now report the crystal structures of [CpMoCl(PMe$_3$)$_3$][BF$_4$] (1) and [Cp*MoCl(PMe$_3$)$_3$][PF$_6$] (2), where Cp and Cp* are η^5-cyclopentadienyl and η^5-pentamethylcyclopentadienyl ligands, respectively.

(1)

(2)
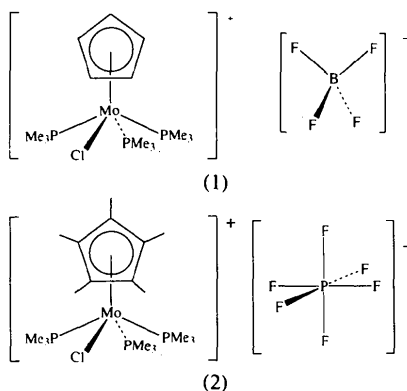
A different salt of the [CpMoCl(PMe$_3$)$_3$]$^+$ cation [with the PF$_6^-$ anion, compound (3)] was prepared previously by one-electron oxidation of [CpMoCl(PMe$_3$)$_3$] and characterized crystallographically (Abugideiri, Kelland, Poli & Rheingold, 1992). However, while compound (3) crystallizes in the orthorhombic space group $P2_12_12_1$, compounds (1) and (2) crystallize under the same conditions in the monoclinic space group $P2_1/c$.

A comparison of selected bond distances and angles for the cations of compounds (1) and (2) is given in Table 3. In both structures, the ions are well separated from each other. The average B—F bond length in (1) is 1.317 (13) Å. The F—B—F angles are very close to the expected tetrahedral value, being in the range 106–114° with an average value of 109.1 (10)°. The PF$_6$ anion in compound (2) is either highly thermally active or disordered among different orientations too close to each other to be distinguished in the E map. Therefore, it was restrained to adopt O_h symmetry with P—F bond lengths of 1.52 (1) Å.

Views of the cations of (1) and (2) are shown in Figs. 1 and 2, respectively. Both ions exhibit a typical four-legged piano-stool geometry. The metric parameters and angular distortions of the cation in compound (1) are *significantly different* from those of the same cation in the previously reported structure of (3). In particular, the cation in (3) has a shorter Mo—Cl distance [2.427 (9) *versus* 2.509 (3) Å in (1)] and longer Mo—P distances [2.504 (7) Å for the PMe$_3$ ligand *trans* to Cl and an average of 2.545 (12) Å for the other two PMe$_3$ ligands,

versus 2.455 (2) and 2.505 (2) Å, respectively, for (1)]. The Mo—*Cnt* distance in (1), where *Cnt* is the centroid of the cyclopentadienyl moiety, however, is statistically equivalent to that in compound (3) [1.986 (18) Å]. The *Cnt*—Mo—*L* angles are more homogeneous in (1) (within the range 107–112°) than in (3) {larger for the Cl ligand [123.9 (8)°] and the PMe$_3$ ligand *trans* to Cl [113.3 (8)°], and smaller for the other two PMe$_3$ ligands [104.5 (8) and 104.0 (8)°]}. The angular changes of the four monodentate ligands on going from compound (1) to compound (3) can be viewed collectively as being analogous to a Berry pseudo-rotation for the interconversion of trigonal-bipyramidal and square-pyramidal structures (Huheey, 1983) (see scheme below). The fact that the nature of the anion (and therefore consequent minor differences in packing forces) causes such significant changes in the angular distorsions for the [CpMoCl(PMe$_3$)$_3$]$^+$ cation, suggests that the pseudo-rotation illustrated below has a smooth potential-energy surface for this ion. The phenomenon of the correlation between the *Cnt*—Mo—*L* angles for two ligands in relative *trans* positions in a four-legged piano-stool geometry has been termed 'angular *trans* influence' (Poli, 1990) and has been the subject of a recent theoretical analysis (Lin & Hall, 1993).

(I)   (II)   (III)
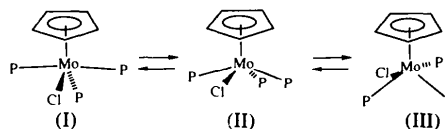
For the [Cp*MoCl(PMe$_3$)$_3$]$^+$ cation of compound (2), the angular distortions are in the opposite direction compared with those of the cation in (3). The *Cnt*—Mo—*L* angles are smaller for the Cl and the PMe$_3$ ligand *trans* to Cl [110.0 (3) and 109.3 (3)°], and larger for the other two PMe$_3$ ligands [120.2 (3) and 120.5 (3)°]. In other words, whereas the cation in (1) is the most symmetrical structure [like structure (II) in the scheme above] and the cation in (3) distorts towards structure (I), the cation in (2) distorts in the other direction, towards structure (III). The average *Cnt*—Mo—*L* angle for the four ligands increases on going from compound (1) (109.7°) and (3) (111.4°) to compound (2) (115°); no doubt an effect of the greater steric bulk of the Cp* ligand in (2). Compound (2) has Mo—P distances similar to those in (3) and an Mo—Cl distance intermediate between those of compounds (1) and (3). The Mo—*Cnt* distance in (2) is significantly longer than those of compounds (1) and (3); perhaps another result of the greater steric interactions in the Cp* complex.

One effect that is identical in both structures examined here [and also in the previously reported structure of (3)] is the shorter Mo—P bond *trans* to the Cl$^-$ ligand relative to the other two Mo—P distances (by *ca*

0.050 Å in all cases). This can be rationalized in terms of the weaker *trans* influence of the Cl^- ligand relative to the PMe_3 ligand.
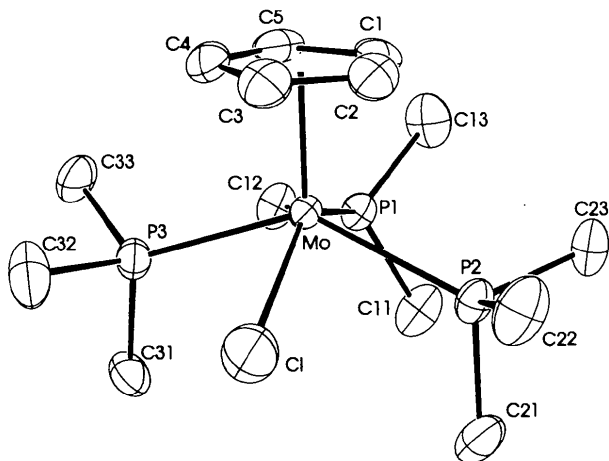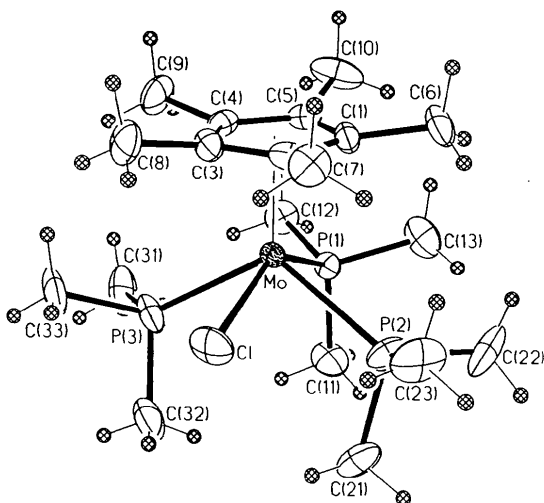

Fig. 1. The molecular configuration and atom-labelling scheme for the $[CpMoCl(PMe_3)_3]^+$ cation. Ellipsoids are drawn at the 40% probability level.

Fig. 2. The molecular configuration and atom-labelling scheme for the $[Cp^*MoCl(PMe_3)_3]^+$ cation. Ellipsoids are drawn at the 40% probability level.

Experimental

Compound (1) was obtained by recrystallizing the mixture of products that results from the oxidation of $[CpMoH(PMe_3)_3]$ by $AgBF_4$ in tetrahydrofuran from an n-heptane-layered CH_2Cl_2 solution. Dark red crystals of (2) were obtained by exchanging a Cl^- ligand in $[Cp^*MoCl_2(PMe_3)_2]$ with PMe_3, a reaction that is assisted by $TlPF_6$ which precipitates Cl^- as insoluble $TlCl$, followed by diffusion of n-heptane into a CH_2Cl_2 solution.

Compound (1)

Crystal data

$[MoCl(C_5H_5)(C_3H_9P)_3][BF_4]$	Mo $K\alpha$ radiation
$M_r = 511.52$	$\lambda = 0.7107$ Å
Monoclinic	Cell parameters from 25
$P2_1/c$	reflections
$a = 13.364$ (2) Å	$\theta = 10.0-16.9°$
$b = 12.991$ (2) Å	$\mu = 0.93$ mm^{-1}
$c = 13.548$ (2) Å	$T = 293$ K
$\beta = 108.350$ (12)°	Block
$V = 2232.4$ (6) Å^3	$0.5 \times 0.5 \times 0.2$ mm
$Z = 4$	Orange–red
$D_x = 1.522$ Mg m^{-3}	

Data collection

Enraf–Nonius CAD-4	2196 observed reflections
diffractometer	$[I > 1.5\sigma(I)]$
$\theta/2\theta$ scans	$R_{int} = 0.040$
Absorption correction:	$\theta_{max} = 22.43°$
empirical (ψ scans,	$h = -14 \rightarrow 13$
4 reflections)	$k = 0 \rightarrow 13$
$T_{min} = 0.672$, $T_{max} =$	$l = 0 \rightarrow 14$
0.997	3 standard reflections
3044 measured reflections	frequency: 60 min
2901 independent reflections	intensity decay: none

Refinement

Refinement on F	$(\Delta/\sigma)_{max} = 0.004$
$R = 0.052$	$\Delta\rho_{max} = 0.76$ e Å^{-3}
$wR = 0.056$	$\Delta\rho_{min} = -0.75$ e Å^{-3}
$S = 1.051$	Atomic scattering factors
2196 reflections	from *International Tables*
217 parameters	*for X-ray Crystallography*
$w = 1/[\sigma^2(F) + 0.0005F^2]$	(1974, Vol. IV)

Compound (2)

Crystal data

$[MoCl(C_{10}H_{15})(C_3H_9P)_3]-$	Mo $K\alpha$ radiation
$[PF_6]$	$\lambda = 0.7107$ Å
$M_r = 639.8$	Cell parameters from 25
Monoclinic	reflections
$P2_1/c$	$\theta = 20-25°$
$a = 12.369$ (6) Å	$\mu = 0.821$ mm^{-1}
$b = 14.664$ (5) Å	$T = 299$ K
$c = 15.769$ (5) Å	Block
$\beta = 90.96$ (3)°	$0.40 \times 0.32 \times 0.22$ mm
$V = 2859.8$ (20) Å^3	Dark red
$Z = 4$	
$D_x = 1.486$ Mg m^{-3}	

Data collection

Siemens $P4$ diffractometer	$R_{int} = 0.012$
$\theta/2\theta$ scans	$\theta_{max} = 27.50°$
Absorption correction:	$h = -14 \rightarrow 13$
empirical (ψ scan)	$k = 0 \rightarrow 16$
$T_{min} = 0.992$, $T_{max} =$	$l = 0 \rightarrow 18$
1.000	3 standard reflections
4749 measured reflections	frequency: 120 min
4349 independent reflections	intensity decay: none
3516 observed reflections	
$[F > 4\sigma(F)]$	

Refinement

Refinement on F		$(\Delta/\sigma)_{max} = 0.079$	
$R = 0.0694$		$\Delta\rho_{max} = 1.01$ e Å^{-3}	
$wR = 0.1193$		$\Delta\rho_{min} = -0.75$ e Å^{-3}	
$S = 1.89$		Atomic scattering factors	
3516 reflections		from *SHELXTL-Plus*	
281 parameters		(Sheldrick, 1987)	
$w = 1/[\sigma^2(F) + 0.003F^2]$			

Table 1. *Fractional atomic coordinates and equivalent isotropic displacement parameters* (Å^2) *for* (1)

$$B_{eq} = (4/3)\Sigma_i\Sigma_j\beta_{ij}\mathbf{a}_i.\mathbf{a}_j.$$

	x	y	z	B_{eq}
Mo	0.25760 (5)	0.50387 (5)	0.24010 (5)	2.62 (3)
Cl	0.41551 (23)	0.60739 (23)	0.33992 (24)	6.86 (16)
P1	0.19591 (18)	0.32497 (17)	0.22955 (18)	3.46 (11)
P2	0.40076 (18)	0.44848 (18)	0.16863 (18)	3.65 (11)
P3	0.22845 (21)	0.53116 (19)	0.41194 (17)	3.97 (11)
B	0.8129 (8)	0.4387 (7)	0.2055 (8)	3.2 (5)
F1	0.8750 (6)	0.3650 (5)	0.1891 (6)	9.0 (5)
F2	0.8495 (8)	0.5270 (6)	0.1815 (9)	13.6 (9)
F3	0.7156 (6)	0.4257 (8)	0.1376 (7)	11.7 (6)
F4	0.8051 (9)	0.4393 (9)	0.2961 (6)	14.2 (8)
C1	0.1428 (8)	0.5172 (7)	0.0798 (6)	4.7 (5)
C2	0.2114 (8)	0.5997 (8)	0.0882 (7)	4.8 (5)
C3	0.2009 (9)	0.6644 (7)	0.1636 (8)	5.3 (6)
C4	0.1233 (9)	0.6269 (8)	0.2023 (7)	4.9 (5)
C5	0.0867 (7)	0.5350 (9)	0.1516 (8)	4.9 (5)
C11	0.2959 (8)	0.2267 (7)	0.2615 (9)	5.8 (6)
C12	0.1194 (8)	0.2837 (7)	0.3129 (8)	4.8 (5)
C13	0.1080 (9)	0.2787 (8)	0.1074 (8)	6.3 (6)
C21	0.5112 (8)	0.3819 (8)	0.2620 (9)	5.8 (6)
C22	0.4682 (9)	0.5522 (9)	0.1249 (9)	6.3 (6)
C23	0.3694 (8)	0.3669 (7)	0.0553 (7)	5.0 (5)
C31	0.3087 (9)	0.4504 (8)	0.5170 (7)	5.2 (5)
C32	0.2595 (11)	0.6572 (9)	0.4669 (8)	6.8 (7)
C33	0.0968 (9)	0.5146 (9)	0.4233 (8)	6.6 (8)

Table 2. *Fractional atomic coordinates and equivalent isotropic displacement parameters* (Å^2) *for* (2)

$$U_{eq} = (1/3)\Sigma_i\Sigma_j U_{ij}a_i^*a_j^*\mathbf{a}_i.\mathbf{a}_j.$$

	x	y	z	U_{eq}
Mo	0.7384 (1)	0.1594 (1)	0.8207 (1)	0.028 (1)
Cl	0.7094 (3)	0.2766 (2)	0.7084 (2)	0.068 (1)
P1	0.7524 (2)	−0.0091 (2)	0.8386 (2)	0.036 (1)
P2	0.5514 (3)	0.1270 (2)	0.7557 (2)	0.058 (1)
P3	0.9024 (3)	0.1439 (2)	0.7258 (2)	0.057 (1)
P4	0.2437 (2)	0.3464 (2)	0.0145 (2)	0.057 (1)
F1	0.1767 (7)	0.2784 (6)	0.0637 (6)	0.163 (6)
F2	0.3101 (8)	0.4157 (8)	−0.0336 (7)	0.232 (10)
F3	0.3471 (6)	0.2980 (6)	0.0421 (6)	0.148 (6)
F4	0.2535 (9)	0.4065 (7)	0.0938 (6)	0.176 (7)
F5	0.1410 (6)	0.3960 (7)	−0.0119 (8)	0.255 (12)
F6	0.2340 (10)	0.2864 (8)	−0.0627 (6)	0.247 (12)
C1	0.6646 (8)	0.1934 (7)	0.9539 (6)	0.041 (3)
C2	0.6874 (9)	0.2748 (7)	0.9098 (6)	0.045 (3)
C3	0.8010 (8)	0.2811 (7)	0.9015 (7)	0.044 (3)
C4	0.8463 (7)	0.2015 (7)	0.9379 (6)	0.042 (3)
C5	0.7625 (9)	0.1496 (6)	0.9726 (6)	0.041 (3)
C6	0.5556 (10)	0.1675 (8)	0.9910 (8)	0.064 (4)
C7	0.6070 (10)	0.3540 (8)	0.8950 (9)	0.063 (4)
C8	0.8590 (11)	0.3644 (8)	0.8736 (9)	0.070 (5)
C9	0.9684 (8)	0.1897 (9)	0.9537 (9)	0.068 (5)
C10	0.7803 (13)	0.0746 (9)	1.0396 (7)	0.082 (6)
C11	0.7414 (11)	−0.0763 (8)	0.7408 (8)	0.070 (5)
C12	0.8769 (9)	−0.0556 (8)	0.8833 (8)	0.057 (4)
C13	0.6526 (11)	−0.0679 (8)	0.9023 (9)	0.071 (5)
C21	0.5590 (11)	0.1009 (11)	0.6446 (9)	0.080 (5)
C22	0.4599 (10)	0.0381 (10)	0.7910 (12)	0.096 (7)
C23	0.4600 (10)	0.2241 (10)	0.7534 (9)	0.089 (6)

C31	1.0165 (10)	0.0616 (10)	0.7443 (11)	0.089 (6)
C32	0.8692 (12)	0.1203 (11)	0.6174 (8)	0.086 (6)
C33	0.9836 (13)	0.2474 (10)	0.7160 (10)	0.097 (6)

Table 3. *Selected geometric parameters* (Å, °)

Cnt is the centroid of the cyclopentadienyl moiety.

	(1)	(2)
Mo—Cl	2.509 (3)	2.489 (3)
Mo—P1	2.455 (2)	2.493 (2)
Mo—P2	2.506 (2)	2.559 (3)
Mo—P3	2.504 (2)	2.551 (3)
Mo—Cnt	1.971 (9)	2.017 (10)
Cl—Mo—P1	138.5 (1)	140.7 (1)
Cl—Mo—P2	75.36 (9)	74.0 (1)
Cl—Mo—P3	76.9 (1)	75.6 (1)
P1—Mo—P2	89.4 (1)	85.5 (1)
P1—Mo—P3	92.3 (1)	85.6 (1)
P2—Mo—P3	139.5 (1)	118.1 (1)
Cl—Mo—Cnt	111.9 (3)	110.0 (3)
P1—Mo—Cnt	109.7 (3)	109.3 (3)
P2—Mo—Cnt	110.1 (3)	120.2 (3)
P3—Mo—Cnt	107.2 (3)	120.5 (3)

The title structures (1) and (2) were solved by direct methods using *NRCVAX* (Gabe, Le Page, Charland, Lee & White, 1989) and the *SHELXTL-Plus* program library (Sheldrick, 1987), respectively, to locate the Mo atoms. The remaining non-H atoms were located in the subsequent difference Fourier syntheses. All H atoms were included in calculated positions [C—H = 0.950 for (1) and 0.960 Å for (2)] with idealized U [U(H) = 1.2(U of the attached C atom)]. All non-H atoms were refined with anisotropic displacement parameters. Due to disorder and/or high thermal motion within the PF$_6$ counterion in compound (2), the anion was restrained to adopt O_h symmetry by the use of *DFIX* instructions (Sheldrick, 1987) with P—F distances of 1.52 (1) Å. Molecular graphics were obtained using *ORTEP*II (Johnson, 1976).

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