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**[Ru(η^5 -C₅H₅)(η^4 -C₅H₄O){As(CH₃)₃}]PF₆
and [Ru(η^5 -C₅H₅)(η^4 -C₅H₄O)-
{As(C₆H₅)₃}]PF₆**

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Abstract

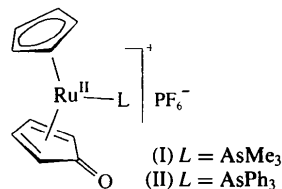
As part of studies on the syntheses and chemical reactions of ruthenium η^5 -cyclopentadienyl- η^4 -cyclopentadienone complexes, the crystal structures of the two title compounds, (η^4 -cyclopentadienone)(η^5 -cyclopentadienyl)(trimethylarsine)ruthenium hexafluorophosphate and (η^4 -cyclopentadienone)(η^5 -cyclopentadienyl)(triphenylarsine)ruthenium hexafluorophosphate, have been determined from single-crystal X-ray diffraction data. The metal complexes of the two title compounds are both of a bent-sandwich type, but differ somewhat in conformation. The cyclopentadienone moieties of both compounds are distinctly puckered at the C(2) and C(4) atoms, and the C=O groups are bent away from the Ru atom. Ru—C bond lengths vary from 2.137 (4) to 2.248 (4) Å in (I), and from 2.159 (4) to 2.271 (4) Å in (II). Ru—As bond lengths are 2.491 (1) Å in (I) and 2.512 (1) Å in (II).

Comment

Cyclopentadienone in the free state is a highly unstable molecule which dimerizes rapidly but can be stabilized by coordination with transition metals. The accessibility of such complexes is limited, however,

since they can be obtained only *via* reactions on certain precursor complexes. The syntheses and reactions of two Ru complexes containing unsubstituted cyclopentadienyl (CP) and cyclopentadienone (CPD), [Ru(η^5 -C₅H₅)(η^4 -C₅H₄O)]₂(PF₆)₂ (Kirchner & Taube, 1991) and [Ru(η^5 -C₅H₅)(η^4 -C₅H₄O)(CH₃CN)]PF₆ (Kirchner, Taube, Scott & Willett, 1993), have been described recently. It was shown that these complexes react with various nucleophiles by substitution on either the metal centre, the CP or the CPD ligand, thus yielding a range of new complexes. While the nucleophiles P(CH₃)₃ and P(C₆H₅)₃ were found to attack the two complexes by substitution on the CP or CPD ligands (Kirchner, Mereiter, Schmid & Taube, 1993), the corresponding arsines displayed ligand substitution on the metal centre.

A view of the metal complex (I) is shown in Fig. 1. The two C₅ rings adopt a staggered conformation in which the cyclopentadienone molecule is oriented so that its C=O group is almost coplanar with the Ru—As bond, as can be seen from the dihedral angle As—Ru—C(6)—O of 0.7 (4)°. This and the specific orientation of the As(CH₃)₃ ligand cause complex (I) to have nearly mirror symmetry, where Ru, As, C(3), C(6), O and C(11) are approximately in the same plane (0.037 Å r.m.s. deviation of these atoms from the corresponding least-squares plane), while the remaining atoms of the complex lie on either side. In comparison with (I), the triphenylarsine compound (II) (Tables 3 and 4) is less symmetric. Here, the configuration of the two C₅ rings lies between staggered and eclipsed, and the bulky As(C₆H₅)₃ group is rotated by *ca* 30° about the Ru—As bond in comparison to the As(CH₃)₃ group (Fig. 1).



Bond lengths and angles of the Ru complexes in (I) and (II) are similar and agree with the values observed in the related compounds Ru(CP)(CPD)Br, [Ru(CP)(CPD)(CH₃CN)]PF₆ and [Ru(CP)(CPD){P(OC₆H₅)₃}]PF₆ (Smith, Kwan, Taube, Bino & Cohen, 1984; Kirchner, Mereiter, Schmid & Taube, 1993; Kirchner, Taube, Scott & Willett, 1993). Selected mean bond lengths for (I) and (II), respectively, are: ⟨Ru—C_{CP}⟩ 2.203 (3), 2.203 (5) Å; ⟨Ru—C_{CPD}⟩ 2.194 (4), 2.214 (4) Å; ⟨C—C⟩_{CP} 1.410 (5), 1.397 (8) Å; ⟨C—C⟩_{CPD} = 1.429 (6), 1.431 (6) Å. The CPD molecules of both compounds display typical behaviour: in their butadiene part [C(7)—C(10)] they exhibit a short-long-short pattern of C—C bond lengths with overall mean values of 1.395 (6) Å (short) and 1.415 (7) Å (long); the CPD molecules are distinctly puckered at the atoms

C(7) and C(10), with the C=O group bent away from the metal centre (Fig. 1), and with puckering angles of 21.5(2)° for (I) and 23.1(2)° for (II), defined as the angles between the least-squares planes through C(7)—C(8)—C(9)—C(10) and C(7)—C(6)(=O)—C(10); the Ru—C bond lengths to C(8) and C(9) are shorter than those to C(7) and C(10) by about 0.1 Å. The angle between the least-squares planes through the CP ring and through the butadiene part of the CPD ring is 34.5(2)° in (I) and 36.3(3)° in (II). The corresponding figures for Ru(CP)(CPD)Br, [Ru(CP)(CPD)(CH₃CN)]PF₆ and [Ru(CP)(CPD){P(OC₆H₅)₃}]PF₆ are 36.2, 36.0 and 36.5°, respectively, and the puckering angles of their CPD molecules 20.6, 18.0 and 23.7°, respectively.

Bond lengths for the two arsine ligands are in good agreement with literature data. The Ru—As bond lengths of 2.491(1) Å in (I) and 2.512(1) Å in (II) may

be compared with 2.516 and 2.536 Å in [(η -H)₃Ru₃(η ³-CC₆H₅)(CO)₇{As(C₆H₅)₃}₂] (Rahman, Beanan, Bavaro, Modi, Keister & Churchill, 1984), and 2.448–2.468 Å in marcasite-type RuAs₂ (Kjekshus, Rakke & Andresen, 1977).

Experimental

The trimethylarsine compound, (I), was prepared from equimolar amounts of [Ru(η ⁵-C₅H₅)(η ⁴-C₅H₄O)(CH₃CN)]PF₆ and As(CH₃)₃ in nitromethane (Kirchner, Mereiter, Schmid & Taube 1993), and was recrystallized from nitromethane/ether. Compound (II) was obtained in an analogous fashion using As(C₆H₅)₃ (Kirchner, Taube, Scott & Willett, 1993).

Compound (I)

Crystal data

[Ru(C₅H₅)(C₅H₄O)-
{As(CH₃)₃}]PF₆
M_r = 511.24
Monoclinic
*P*2₁/*c*
a = 8.421(2) Å
b = 11.421(2) Å
c = 17.431(4) Å
 β = 93.84(1)°
V = 1672.7(6) Å³
Z = 4
D_x = 2.030 Mg m⁻³

Mo *K* α radiation
 λ = 0.71069 Å
Cell parameters from 25
reflections
 θ = 14–26°
 μ = 3.03 mm⁻¹
T = 294 K
Prism
0.50 × 0.33 × 0.22 mm
Yellow

Data collection

Philips PW1100 diffractometer
 $\theta/2\theta$ scans
Absorption correction:
by Gaussian integration
from crystal shape
*T*_{min} = 0.46, *T*_{max} = 0.52
4087 measured reflections
3657 independent reflections

2888 observed reflections
[*F_o* > 6 σ (*F_o*)]
*R*_{int} = 0.011
 θ _{max} = 27°
h = 0 → 10
k = 0 → 14
l = -22 → 22
3 standard reflections
frequency: 120 min
intensity decay: 1.2%

Refinement

Refinement on *F*
R = 0.026
wR = 0.030
S = 1.31
2888 reflections
232 parameters
H-atom positions refined
with riding model (C—H
0.96 Å)
w = [σ^2 (*F_o*) + 0.0002*F_o*²]
(Δ/σ)_{max} < 0.01

$\Delta\rho$ _{max} = 0.45 e Å⁻³
 $\Delta\rho$ _{min} = -0.59 e Å⁻³
Extinction correction:
SHELX76 (Sheldrick,
1976)
Extinction coefficient:
 χ = 0.00204 (7)
Atomic scattering factors
from *International Tables*
for X-ray Crystallography
(1974, Vol. IV, Table
2.2B)

Compound (II)

Crystal data

[Ru(C₅H₅)(C₅H₄O)-
{As(C₆H₅)₃}]PF₆

Mo *K* α radiation
 λ = 0.71069 Å

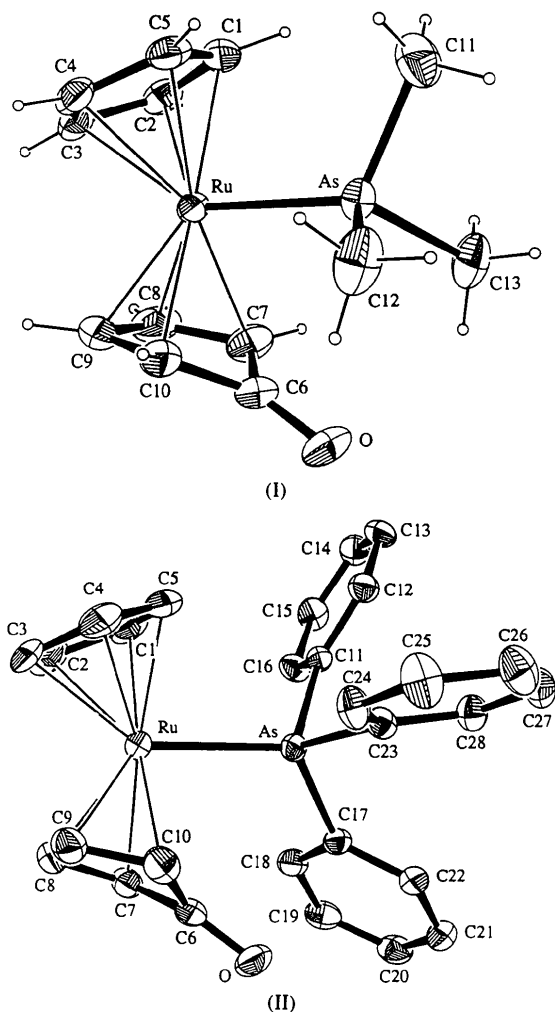


Fig. 1. Perspective ORTEP (Johnson, 1965) plots of the sandwich complexes in (I) and (II) with atom numbering. Displacement ellipsoids are shown at the 30% probability level. H atoms in (II) have been omitted for clarity.

$M_r = 697.45$
 Monoclinic
 $P2_1/c$
 $a = 8.076$ (1) Å
 $b = 24.399$ (4) Å
 $c = 13.337$ (2) Å
 $\beta = 96.52$ (1)°
 $V = 2611.0$ (7) Å³
 $Z = 4$
 $D_x = 1.774$ Mg m⁻³

Cell parameters from 48 reflections
 $\theta = 6-22^\circ$
 $\mu = 1.967$ mm⁻¹
 $T = 295$ K
 Plate
 $0.35 \times 0.28 \times 0.07$ mm
 Yellow

Data collection

Philips PW1100 diffractometer
 3220 observed reflections
 $[F_o > 6\sigma(F_o)]$
 $R_{int} = 0.010$
 $\theta_{max} = 25^\circ$
 Absorption correction: by Gaussian integration from crystal shape
 $T_{min} = 0.54, T_{max} = 0.87$
 4735 measured reflections
 4586 independent reflections

3220 observed reflections
 $[F_o > 6\sigma(F_o)]$
 $R_{int} = 0.010$
 $\theta_{max} = 25^\circ$
 $h = 0 \rightarrow 9$
 $k = 0 \rightarrow 28$
 $l = -15 \rightarrow 15$
 3 standard reflections
 frequency: 120 min
 intensity decay: 0.8%

Refinement

Refinement on F^2
 $R = 0.028$
 $wR = 0.027$
 $S = 1.14$
 3220 reflections
 345 parameters
 H-atom positions refined with riding model (C—H 0.96 Å)
 $w = [\sigma^2(F_o) + 0.0001F_o^2]$
 $(\Delta/\sigma)_{max} < 0.01$

$\Delta\rho_{max} = 0.47$ e Å⁻³
 $\Delta\rho_{min} = -0.29$ e Å⁻³
 Extinction correction: SHELXL76 (Sheldrick, 1976)
 Extinction coefficient: $\chi = 0.00031$ (4)
 Atomic scattering factors from *International Tables* for X-ray Crystallography (1974, Vol. IV, Table 2.2B)

Table 1. Fractional atomic coordinates and equivalent isotropic displacement parameters (Å²) for (I)

$$U_{eq} = (1/3)\sum_i \sum_j U_{ij} a_i^* a_j^* \mathbf{a}_i \cdot \mathbf{a}_j$$

	x	y	z	U_{eq}
Ru	0.29625 (3)	0.39181 (2)	0.23899 (1)	0.0334 (1)
C(1)	0.5041 (4)	0.4439 (3)	0.3139 (2)	0.053 (2)
C(2)	0.5577 (4)	0.4148 (3)	0.2426 (2)	0.051 (2)
C(3)	0.4863 (4)	0.4920 (3)	0.1876 (2)	0.049 (2)
C(4)	0.3879 (4)	0.5713 (3)	0.2252 (2)	0.051 (2)
C(5)	0.3977 (4)	0.5423 (3)	0.3030 (2)	0.052 (2)
C(6)	0.0505 (4)	0.2561 (3)	0.2075 (2)	0.057 (2)
C(7)	0.2140 (5)	0.2140 (3)	0.1978 (2)	0.061 (2)
C(8)	0.2776 (6)	0.2793 (4)	0.1401 (2)	0.073 (3)
C(9)	0.1790 (6)	0.3784 (4)	0.1268 (2)	0.076 (3)
C(10)	0.0556 (5)	0.3753 (3)	0.1768 (2)	0.060 (2)
O	-0.0577 (3)	0.2066 (3)	0.2376 (2)	0.078 (2)
As	0.16705 (4)	0.34955 (3)	0.36042 (2)	0.0419 (2)
C(11)	0.2632 (6)	0.4145 (4)	0.4556 (2)	0.074 (3)
C(12)	-0.0448 (5)	0.4151 (4)	0.3622 (3)	0.076 (3)
C(13)	0.1526 (5)	0.1880 (3)	0.3907 (3)	0.069 (3)
P	0.7063 (1)	0.30149 (8)	0.01187 (5)	0.0471 (5)
F(1)	0.5433 (3)	0.3669 (3)	-0.0064 (2)	0.112 (2)
F(2)	0.8680 (3)	0.2348 (2)	0.0307 (1)	0.090 (2)
F(3)	0.626 (1)	0.1771 (5)	0.0024 (7)	0.150 (4)
F(4)	0.734 (1)	0.2997 (9)	-0.0753 (3)	0.126 (4)
F(5)	0.793 (1)	0.4172 (5)	0.0233 (7)	0.150 (4)
F(6)	0.6864 (9)	0.2956 (9)	0.1003 (3)	0.126 (4)
F(3')	0.657 (1)	0.215 (1)	-0.0518 (9)	0.113 (7)

F(4')	0.788 (2)	0.376 (1)	-0.047 (1)	0.116 (7)
F(5')	0.742 (1)	0.395 (1)	0.0761 (9)	0.113 (7)
F(6')	0.610 (1)	0.236 (1)	0.0664 (9)	0.116 (7)

Table 2. Fractional atomic coordinates and equivalent isotropic displacement parameters (Å²) for (II)

$$U_{eq} = (1/3)\sum_i \sum_j U_{ij} a_i^* a_j^* \mathbf{a}_i \cdot \mathbf{a}_j$$

	x	y	z	U_{eq}
Ru	0.60922 (4)	0.37680 (1)	0.20020 (2)	0.0361 (2)
C(1)	0.8523 (6)	0.3781 (3)	0.2937 (4)	0.070 (3)
C(2)	0.8806 (6)	0.3882 (3)	0.1951 (5)	0.080 (4)
C(3)	0.7956 (7)	0.4374 (3)	0.1652 (4)	0.082 (4)
C(4)	0.7175 (7)	0.4570 (2)	0.2470 (4)	0.076 (4)
C(5)	0.7530 (7)	0.4200 (2)	0.3254 (4)	0.070 (3)
C(6)	0.3347 (5)	0.3272 (2)	0.1216 (3)	0.047 (2)
C(7)	0.4995 (5)	0.3107 (2)	0.0936 (3)	0.043 (2)
C(8)	0.5615 (5)	0.3546 (2)	0.0426 (3)	0.049 (2)
C(9)	0.4677 (5)	0.4019 (2)	0.0607 (3)	0.052 (3)
C(10)	0.3460 (5)	0.3875 (2)	0.1226 (3)	0.051 (3)
O	0.2203 (3)	0.2987 (1)	0.1415 (2)	0.068 (2)
As	0.49669 (4)	0.32769 (2)	0.34355 (3)	0.0315 (2)
C(11)	0.6674 (4)	0.3097 (2)	0.4544 (3)	0.035 (2)
C(12)	0.6869 (5)	0.3398 (2)	0.5429 (3)	0.045 (2)
C(13)	0.8057 (5)	0.3255 (2)	0.6217 (3)	0.053 (3)
C(14)	0.9059 (5)	0.2810 (2)	0.6127 (3)	0.051 (3)
C(15)	0.8913 (5)	0.2515 (2)	0.5252 (3)	0.049 (3)
C(16)	0.7738 (5)	0.2654 (2)	0.4463 (3)	0.044 (2)
C(17)	0.3936 (4)	0.2556 (2)	0.3251 (3)	0.036 (2)
C(18)	0.4813 (5)	0.2149 (2)	0.2808 (3)	0.044 (2)
C(19)	0.4234 (5)	0.1616 (2)	0.2760 (3)	0.053 (3)
C(20)	0.2775 (6)	0.1488 (2)	0.3143 (3)	0.055 (3)
C(21)	0.1869 (6)	0.1888 (2)	0.3549 (3)	0.056 (3)
C(22)	0.2434 (5)	0.2429 (2)	0.3603 (3)	0.044 (2)
C(23)	0.3467 (4)	0.3722 (2)	0.4137 (3)	0.037 (2)
C(24)	0.3111 (5)	0.4248 (2)	0.3795 (3)	0.047 (2)
C(25)	0.2134 (6)	0.4591 (2)	0.4311 (3)	0.065 (3)
C(26)	0.1523 (6)	0.4410 (2)	0.5169 (3)	0.060 (3)
C(27)	0.1867 (5)	0.3888 (2)	0.5512 (3)	0.050 (3)
C(28)	0.2843 (5)	0.3543 (2)	0.5009 (3)	0.042 (2)
P	0.8345 (2)	0.44766 (5)	-0.15989 (9)	0.0522 (7)
F(1)	0.7998 (4)	0.3841 (1)	-0.1432 (2)	0.082 (2)
F(2)	0.9583 (3)	0.4326 (1)	-0.2382 (2)	0.090 (2)
F(3)	0.6871 (3)	0.4490 (1)	-0.2474 (2)	0.090 (2)
F(4)	0.7086 (4)	0.4629 (1)	-0.0808 (2)	0.110 (2)
F(5)	0.9827 (4)	0.4451 (1)	-0.0724 (2)	0.116 (3)
F(6)	0.8678 (3)	0.5104 (1)	-0.1770 (2)	0.087 (2)

Table 3. Selected geometric parameters (Å, °) for (I)

Ru—C(1)	2.195 (3)	C(6)—O	1.219 (5)
Ru—C(2)	2.214 (3)	C(7)—C(8)	1.389 (6)
Ru—C(3)	2.206 (3)	C(8)—C(9)	1.413 (7)
Ru—C(4)	2.210 (3)	C(9)—C(10)	1.401 (6)
Ru—C(5)	2.191 (3)	As—C(11)	1.943 (4)
Ru...C(6)	2.614 (4)	As—C(12)	1.937 (4)
Ru—C(7)	2.248 (4)	As—C(13)	1.925 (4)
Ru—C(8)	2.148 (4)	P—F(1)	1.577 (3)
Ru—C(9)	2.137 (4)	P—F(2)	1.576 (3)
Ru—C(10)	2.241 (4)	P—F(3)	1.577 (6)
Ru—As	2.4910 (6)	P—F(4)	1.553 (5)
C(1)—C(2)	1.391 (5)	P—F(5)	1.514 (6)
C(1)—C(5)	1.443 (5)	P—F(6)	1.563 (5)
C(2)—C(3)	1.408 (5)	P—F(3')	1.52 (2)
C(3)—C(4)	1.418 (5)	P—F(4')	1.54 (2)
C(4)—C(5)	1.393 (5)	P—F(5')	1.56 (2)
C(6)—C(7)	1.479 (5)	P—F(6')	1.49 (2)
C(6)—C(10)	1.465 (5)		
C(2)—C(1)—C(5)	107.7 (3)	C(7)—C(8)—C(9)	107.4 (4)
C(1)—C(2)—C(3)	108.0 (3)	C(8)—C(9)—C(10)	109.2 (4)
C(2)—C(3)—C(4)	108.8 (3)	C(6)—C(10)—C(9)	107.0 (3)
C(3)—C(4)—C(5)	107.4 (3)	Ru—As—C(11)	118.1 (1)
C(1)—C(5)—C(4)	108.0 (3)	Ru—As—C(12)	113.2 (1)
C(7)—C(6)—C(10)	102.1 (3)	Ru—As—C(13)	117.3 (1)

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*, *PW115* and *LLSQ6* (Mereiter & Völlenkne, 1990). After applying corrections for absorption, both structures were solved by direct methods and refined by full-matrix least-squares with *SHELX76* (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 CH₃ groups. The isotropic displacement parameters of the H atoms in (I) were set to $1.30 \times U_{eq}$ of the parent C atoms, and in (II), to $1.11 \times U_{eq}$ of the parent C atoms. Disorder in the octahedral PF₆⁻ 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 *Xtal3.2* (Hall, Flack & Stewart, 1992).

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Lists of structure factors, anisotropic displacement parameters, H-atom coordinates and bond distances and angles involving non-H atoms have been deposited with the IUCr (Reference: KA1055). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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

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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 -pentamethylcyclopentadienyl)tris(trimethylphosphine)molybdenum(III) hexafluorophosphate, [MoCl(C₁₀H₁₅)(C₃H₉P)₃][PF₆], was obtained from the reaction of [MoCl₂(C₁₀H₁₅)(C₃H₉P)₂] with TIPF₆ and PMe₃ in dichloromethane. Both cations adopt a four-legged piano-stool arrangement.