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Structure of Undecacarbonyl[tris(pentafluorophenyl)phosphine]-*triangulo*-triosmium, a Substituted Osmium Cluster Containing a Fluorinated Triphenylphosphine Ligand

BY H. G. ANG, W. L. KWIK AND W. K. LEONG

Department of Chemistry, National University of Singapore, Kent Ridge Road, Singapore 0511,
Republic of Singapore

AND J. A. POTENZA

Department of Chemistry, Rutgers, The State University of New Jersey, New Brunswick, NJ 08903, *USA*

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Abstract. $[Os_3(CO)_{11}\{P(C_6F_5)_3\}]$, $M_r = 1410{\cdot}87$, monoclinic, $P2_1/n$, $a = 19{\cdot}058\,(1)$, $b = 9{\cdot}109\,(1)$, $c = 20{\cdot}424\,(2)$ Å, $\beta = 105{\cdot}53\,(1)°$, $V = 3416\,(1)$ Å^3, $Z = 4$, $D_m = 2{\cdot}74\,(2)$, $D_x = 2{\cdot}743$ g cm^{-3}, μ(Mo $K\alpha$, $\lambda = 0{\cdot}71073$ Å) $= 113{\cdot}3$ cm^{-1}, $F(000) = 2560$, $T = 297\,(1)$ K, $R_F = 0{\cdot}022$ for 3529 reflections. The Os atoms form an approximate isosceles triangle. Each Os atom exhibits a distorted octahedral coordination geometry. The carbonyl groups are all terminal and the bulky phosphine ligand is coordinated equatorially.

Introduction. Axial, equatorial and bridging (Churchill & Wasserman, 1982; Ditzel, Gomez-Sal, Johnson, Lewis & Raithby, 1987) substitution of carbonyl groups in $Os_3(CO)_{12}$ clusters is known. Substitution is likely to occur at an equatorial site if the ligand is a bulky two-electron donor such as $P(OCH_3)_3$ (Benfield, Johnson, Raithby & Sheldrick, 1978) or $P^tBu_2(NH_2)$ (Ehrenreich, Herberhold, Suss-Fink, Klein & Thewalt, 1983). On the other hand, small, non-π-acceptor ligands such as H (Churchill & DeBoer, 1977) or CH_3CN (Dawson, Johnson,

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Lewis, Puga, Raithby & Rosales, 1982) tend to assume axial positions. Moreover, in the reaction of Ph_3P with $Os_3(CO)_{12}$, up to nine products (some simple substitution products and some more complicated species) have been obtained and characterized (Gainsford, Guss, Ireland, Mason, Bradford & Nyholm, 1972).

In our investigation of the reaction of $Os_3(CO)_{11}(CH_3CN)$ and $(C_6F_5)_3P$ at the elevated temperature of 383 K, only one product was obtained. Here, we report the results of an X-ray structural characterization of this product.

Experimental. The trinuclear osmium cluster $Os_3(CO)_{11}\{P(C_6F_5)_3\}$ (1) was prepared by heating $Os_3(CO)_{11}(CH_3CN)$ (200 mg) and $(C_6F_5)_3P$ (118 mg) in 10 ml of toluene in an evacuated carius tube at 383 K for 24 h. The yellow solid obtained was washed with several small portions of hexane. Yellow, diffraction-quality crystals by evaporation from dichloromethane, D_m by flotation (bromoform and 1,2-dibromoethane); crystal 0·31 × 0·17 × 0·08 mm; Enraf–Nonius CAD-4 diffractometer; graphite-monochromated Mo $K\alpha$ radiation; θ–2θ scan. Reciprocal lattice symmetry and systematic absences consistent with space group $P2_1/n$. Cell constants from setting angles of 25 reflections with $12{\cdot}98° \leq \theta \leq 16{\cdot}56°$. Data corrected for Lorentz, polarization and absorption (empirical, ψ-scan, $0{\cdot}42 < T < 1{\cdot}00$) effects. Variation in intensity of three standard reflections ±0·1%; 4635 independent reflections measured with $4° < 2\theta < 46°$; 3529 with $F_o^2 > 3\sigma(F_o^2)$ $\{[\sigma(F_o^2)]^2 = [S^2(C+R^2B) + (0{\cdot}04F_o^2)^2]/(\mathrm{Lp})^2$, S = scan rate, C = peak count, R^2B = background count, used in refinement}. Data collected $h(0, 20)$, $k(0, 9)$, $l(-21, 21)$.

Structure solved by direct methods (*MULTAN*82; Main, Fiske, Hull, Lessinger, Germain, Declercq & Woolfson, 1982) and difference Fourier techniques. Full-matrix least-squares refinement on F; all atoms anisotropic; 532 parameters refined; $w = 4F_o^2/\sigma^2(F_o^2)$. Final $R_F = 0{\cdot}022$, $wR_F = 0{\cdot}027$, $S = 0{\cdot}97$, $(\Delta/\sigma)_{\max} < 0{\cdot}01$; $\Delta\rho_{\max} = 0{\cdot}66$, $\Delta\rho_{\min} = -0{\cdot}806$ e Å^{-3}. Atomic scattering factors from *International Tables for X-ray Crystallography* (1974). Programs from Enraf–Nonius (1983) *SDP*.

Discussion. Atomic parameters are given in Table 1, bond lengths and angles in Table 2. Fig. 1 shows the molecular structure and labeling scheme.*

Table 1. *Atomic coordinates and equivalent isotropic thermal parameters* (Å^2)

	x	y	z	B_{eq}*
Os(1)	0·34570 (1)	0·04071 (3)	0·61021 (1)	2·157 (6)
Os(2)	0·42828 (2)	0·08167 (4)	0·74970 (1)	2·854 (7)
Os(3)	0·41137 (2)	0·32441 (3)	0·65744 (1)	2·771 (7)
P	0·27240 (9)	0·0874 (2)	0·50071 (9)	2·30 (4)
O(1)	0·2212 (3)	0·0867 (7)	0·6778 (2)	4·0 (1)
O(2)	0·4836 (3)	−0·0369 (7)	0·5663 (3)	4·5 (1)
O(3)	0·3118 (4)	−0·2836 (7)	0·6111 (3)	6·4 (2)
O(4)	0·5368 (4)	0·1948 (9)	0·8765 (3)	7·2 (2)
O(5)	0·3120 (3)	0·2412 (8)	0·8036 (3)	6·2 (2)
O(6)	0·5575 (3)	−0·0616 (8)	0·7116 (3)	6·1 (2)
O(7)	0·3855 (4)	−0·2175 (7)	0·7939 (3)	6·3 (2)
O(8)	0·2586 (3)	0·4155 (7)	0·6665 (3)	5·1 (2)
O(9)	0·4885 (4)	0·5432 (9)	0·7652 (4)	8·9 (2)
O(10)	0·5600 (3)	0·2285 (9)	0·6388 (4)	7·0 (2)
O(11)	0·3926 (4)	0·5211 (7)	0·5334 (3)	5·6 (2)
C(1)	0·2687 (4)	0·0751 (8)	0·6537 (4)	2·8 (2)
C(2)	0·4327 (4)	−0·0027 (9)	0·5820 (4)	3·2 (2)
C(3)	0·3250 (4)	−0·1617 (9)	0·6110 (4)	3·6 (2)
C(4)	0·4964 (4)	0·155 (1)	0·8292 (4)	4·2 (2)
C(5)	0·3529 (4)	0·1815 (9)	0·7805 (4)	3·9 (2)
C(6)	0·5094 (4)	−0·009 (1)	0·7224 (4)	4·1 (2)
C(7)	0·4018 (4)	−0·106 (1)	0·7776 (4)	4·0 (2)
C(8)	0·3151 (4)	0·3784 (9)	0·6652 (4)	3·5 (2)
C(9)	0·4600 (5)	0·464 (1)	0·7260 (4)	4·8 (2)
C(10)	0·5049 (5)	0·257 (1)	0·6447 (4)	4·4 (2)
C(11)	0·3976 (4)	0·446 (1)	0·5788 (4)	3·8 (2)
C(21)	0·2357 (4)	−0·0766 (8)	0·4482 (3)	2·7 (2)
C(22)	0·2871 (4)	−0·1770 (8)	0·4381 (4)	2·8 (2)
C(23)	0·2684 (4)	−0·3051 (8)	0·4015 (3)	3·1 (2)
C(24)	0·1975 (5)	−0·3387 (9)	0·3745 (4)	4·0 (2)
C(25)	0·1451 (4)	−0·2430 (9)	0·3815 (4)	3·2 (2)
C(26)	0·1630 (4)	−0·1130 (9)	0·4157 (4)	3·1 (2)
C(31)	0·2998 (4)	0·1859 (8)	0·4311 (3)	2·4 (2)
C(32)	0·2483 (4)	0·2081 (9)	0·3686 (4)	3·3 (2)
C(33)	0·2662 (5)	0·270 (1)	0·3137 (4)	3·9 (2)
C(34)	0·3363 (4)	0·3176 (9)	0·3200 (4)	4·1 (2)
C(35)	0·3879 (4)	0·2980 (9)	0·3804 (4)	3·5 (2)
C(36)	0·3695 (4)	0·2328 (9)	0·4339 (4)	3·0 (2)
C(41)	0·1919 (4)	0·1884 (9)	0·5088 (3)	2·8 (2)
C(42)	0·1394 (4)	0·1179 (9)	0·5338 (4)	3·3 (2)
C(43)	0·0832 (4)	0·192 (1)	0·5499 (4)	4·0 (2)
C(44)	0·0799 (4)	0·343 (1)	0·5439 (4)	4·5 (2)
C(45)	0·1311 (4)	0·4191 (9)	0·5214 (4)	3·6 (2)
C(46)	0·1855 (4)	0·3389 (9)	0·5038 (3)	3·1 (2)
F(22)	0·3583 (2)	−0·1456 (5)	0·4634 (2)	3·8 (1)
F(23)	0·3214 (3)	−0·3955 (5)	0·3935 (2)	4·7 (1)
F(24)	0·1800 (3)	−0·4643 (5)	0·3397 (3)	5·7 (1)
F(25)	0·0744 (2)	−0·2756 (6)	0·3529 (3)	5·0 (1)
F(26)	0·1081 (2)	−0·0221 (5)	0·4155 (2)	4·1 (1)
F(32)	0·1785 (2)	0·1719 (6)	0·3600 (2)	4·4 (1)
F(33)	0·2151 (3)	0·2902 (7)	0·2548 (2)	6·1 (1)
F(34)	0·3531 (3)	0·3812 (7)	0·2671 (2)	6·5 (1)
F(35)	0·4552 (2)	0·3448 (6)	0·3868 (2)	5·2 (1)
F(36)	0·4231 (2)	0·2165 (5)	0·4906 (2)	3·6 (1)
F(42)	0·1440 (2)	−0·0269 (5)	0·5450 (2)	4·2 (1)
F(43)	0·0338 (2)	0·1189 (7)	0·5726 (3)	5·9 (1)
F(44)	0·0271 (3)	0·4159 (7)	0·5618 (2)	6·3 (1)
F(45)	0·1294 (3)	0·5635 (6)	0·5166 (3)	6·0 (1)
F(46)	0·2361 (2)	0·4188 (5)	0·4845 (2)	3·9 (1)

$$*B_{eq} = \tfrac{4}{3}[a^2B(1,1) + b^2B(2,2) + c^2B(3,3) + ab\cos\gamma B(1,2) + ac\cos\beta B(1,3) + bc\cos\alpha B(2,3)].$$

The structure consists of $Os_3(CO)_{11}\{P(C_6F_5)_3\}$ molecules in which the Os atoms form an approximate isosceles triangles. Each Os atom exhibits distorted octahedral coordination geometry and the bulky phosphine ligand is coordinated equatorially. Two of the Os—Os distances lie within 0·011 Å of the average Os—Os distance in the more symmetrical complex $Os_3(CO)_{12}$ [2·8771 (27) Å; Churchill & DeBoer, 1977). The third distance, Os(1)—Os(3), is 0·043 Å longer than this average. This is most likely a consequence of the proximity of the Os(1)—Os(3)

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* Lists of anisotropic thermal parameters and structure factors have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 52053 (27 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Table 2. *Bond distances* (Å) *and angles* (°)

Os(1)—Os(2)	2·8863 (4)	P—C(21)	1·863 (7)
Os(1)—Os(3)	2·9203 (4)	P—C(31)	1·870 (7)
Os(2)—Os(3)	2·8666 (4)	P—C(41)	1·834 (8)
Os(1)—P	2·337 (2)		
Os(1)—C(1)	1·934 (8)	C(1)—O(1)	1·14 (1)
Os(1)—C(2)	1·937 (9)	C(2)—O(2)	1·14 (1)
Os(1)—C(3)	1·886 (8)	C(3)—O(3)	1·14 (2)
Os(2)—C(4)	1·908 (7)	C(4)—O(4)	1·12 (1)
Os(2)—C(5)	1·943 (9)	C(5)—O(5)	1·15 (1)
Os(2)—C(6)	1·96 (1)	C(6)—O(6)	1·12 (1)
Os(2)—C(7)	1·914 (9)	C(7)—O(7)	1·14 (1)
Os(3)—C(8)	1·946 (8)	C(8)—O(8)	1·13 (2)
Os(3)—C(9)	1·936 (9)	C(9)—O(9)	1·10 (1)
Os(3)—C(10)	1·968 (9)	C(10)—O(10)	1·12 (1)
Os(3)—C(11)	1·911 (8)	C(11)—O(11)	1·13 (2)
Os(2)—Os(1)—Os(3)	59·16 (1)	P—Os(1)—C(1)	94·4 (2)
Os(1)—Os(2)—Os(3)	61·02 (1)	P—Os(1)—C(2)	95·4 (2)
Os(1)—Os(3)—Os(2)	59·83 (1)	P—Os(1)—C(3)	96·6 (3)
Os(2)—Os(1)—P	161·68 (5)		
Os(3)—Os(1)—P	104·39 (5)	C(1)—Os(1)—C(2)	170·2 (3)
Os(2)—Os(1)—C(1)	78·9 (2)	C(1)—Os(1)—C(3)	88·2 (3)
Os(3)—Os(1)—C(1)	91·0 (2)	C(2)—Os(1)—C(3)	90·0 (4)
Os(2)—Os(1)—C(2)	92·1 (2)	C(4)—Os(2)—C(5)	87·4 (3)
Os(3)—Os(1)—C(2)	87·3 (2)	C(4)—Os(2)—C(6)	88·9 (3)
Os(2)—Os(1)—C(3)	100·3 (3)	C(4)—Os(2)—C(7)	103·5 (3)
Os(3)—Os(1)—C(3)	159·1 (3)	C(5)—Os(2)—C(6)	175·9 (3)
Os(1)—Os(2)—C(4)	162·2 (3)	C(5)—Os(2)—C(7)	92·6 (4)
Os(3)—Os(2)—C(4)	102·7 (3)	C(6)—Os(2)—C(7)	90·0 (4)
Os(1)—Os(2)—C(5)	97·2 (3)	C(8)—Os(3)—C(9)	93·1 (4)
Os(3)—Os(2)—C(5)	83·7 (2)	C(8)—Os(3)—C(10)	175·5 (3)
Os(1)—Os(2)—C(6)	85·9 (3)	C(8)—Os(3)—C(11)	90·1 (3)
Os(3)—Os(2)—C(6)	95·5 (3)	C(9)—Os(3)—C(10)	91·5 (4)
Os(1)—Os(2)—C(7)	93·5 (2)	C(9)—Os(3)—C(11)	99·0 (4)
Os(3)—Os(2)—C(7)	153·3 (3)	C(10)—Os(3)—C(11)	89·7 (4)
Os(1)—Os(3)—C(8)	85·4 (2)		
Os(2)—Os(3)—C(8)	94·9 (2)	Os(1)—P—C(21)	116·2 (2)
Os(1)—Os(3)—C(9)	154·3 (3)	Os(1)—P—C(31)	126·7 (3)
Os(2)—Os(3)—C(9)	94·9 (3)	Os(1)—P—C(41)	107·8 (2)
Os(1)—Os(3)—C(10)	90·2 (2)		
Os(2)—Os(3)—C(10)	84·3 (3)	C(21)—P—C(31)	94·9 (3)
Os(1)—Os(3)—C(11)	106·7 (2)	C(21)—P—C(41)	105·1 (3)
Os(2)—Os(3)—C(11)	165·0 (3)	C(31)—P—C(41)	103·9 (3)

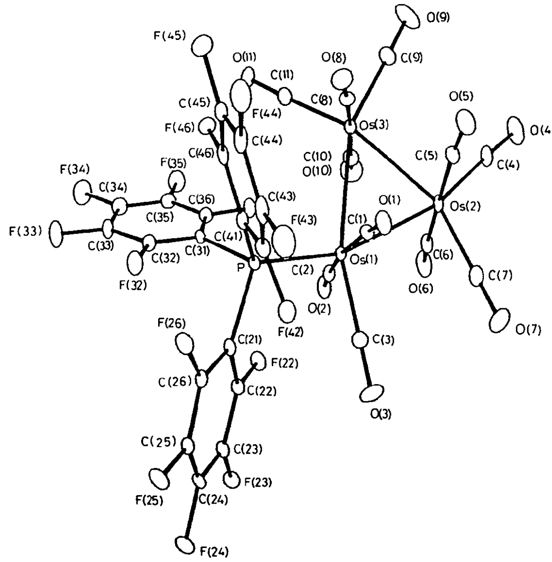

Fig. 1. View of the molecular structure (15% probability ellipses) showing the atom-numbering scheme.

bond to the bulky, relatively acidic, equatorially bound $(C_6F_5)_3P$ group. The Os(1)—P distance [2·337 (2) Å] is similar to that in $Os_3H(SPh)(CO)_9(PEt_3)$ [2·346 (4) Å; Ditzel *et al.*, 1987) but somewhat shorter than those [2·376 (4) and 2·399 (4) Å] reported for two conformers of $Os_3(CO)_{11}[P^tBu_2(NH_2)]$ (Ehrenreich *et al.*, 1983).

The average Os—CO(axial) bond length [1·949 (13) Å] is longer than the average Os—C(equatorial) length [1·910 (15) Å], an observation that has been noted for other osmium clusters of this type (Churchill & DeBoer, 1977). Just the reverse trend is expected for the C—O distances based on a consideration of the relative availability of back-donated electron density. However, the C—O distances are, within experimental error, very nearly the same for both the axial and the equatorial carbonyl groups. The relatively large e.s.d.'s of the CO distances preclude an accurate assessment of the bonding of the carbonyl groups. The average C—O distance [1·13 (14) Å] is, however, close to that [1·14 (11) Å] reported for $Os_3(CO)_{12}$.

Steric effects due to the $(C_6F_5)P$ ligand are clearly manifested in the large deviations from ideal values for the Os—Os—C(axial) and C—Os—C angles, particularly those associated with Os(1). Electronic effects attributable to $(C_6F_5)P$ are less distinct. However, the somewhat smaller values of the Os—C distances for Os(1) as compared with Os(2) and Os(3) may be a manifestation of electronic effects arising from the highly electronegative C_6F_5 groups.

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