

C3	0.1405 (2)	0.6555 (2)	0.6209 (3)	3.23 (5)
C4	0.1519 (3)	0.7747 (3)	0.5990 (3)	3.74 (6)
C5	0.0812 (3)	0.8495 (2)	0.6682 (3)	3.61 (6)

Table 5. Selected geometric parameters (Å, °) for (C₅H₄N₂O₃)₂.Co(NO₃)₂.4H₂O

N1—O1	1.323 (3)	C4—C5	1.373 (4)
N2—O2	1.227 (4)	Co—O1 ⁱ	2.062 (2)
N2—O3	1.227 (4)	Co—OW1 ⁱⁱ	2.101 (2)
O2...O3	2.182 (4)	Co—OW2 ⁱⁱ	2.085 (2)
N1—C1	1.349 (3)	N3—O4	1.252 (3)
N1—C5	1.354 (8)	N3—O5	1.239 (3)
N2—C3	1.473 (4)	N3—O6	1.238 (3)
C1—C2	1.366 (4)	O4...O5	2.168 (3)
C2—C3	1.379 (4)	O4...O6	2.145 (3)
C3—C4	1.379 (4)	O5...O6	2.146 (3)
O1—N1—C1	118.2 (2)	N2—C3—C2	119.3 (2)
O1—N1—C5	120.9 (2)	N2—C3—C4	119.5 (3)
C1—N1—C5	121.1 (2)	C2—C3—C4	121.2 (3)
O2—N2—C3	116.7 (3)	C3—C4—C5	118.4 (3)
O3—N2—C3	117.8 (3)	N1—C5—C4	120.3 (2)
O2—N2—O3	125.5 (3)	O4—N3—O5	120.9 (2)
N1—C1—C2	120.7 (3)	O4—N3—O6	118.9 (2)
C1—C2—C3	118.3 (2)	O5—N3—O6	120.1 (2)

Symmetry codes: (i) $x, y - 1, z - 1$; (ii) $x, y, z - 1$.

Table 6. Hydrogen-bonding geometry (Å, °) for (C₅H₄N₂O₃)₂.Co(NO₃)₂.4H₂O

D	H	A	D—H	H...A	D...A	D—H...A
OW1	H1W1	O4	0.80 (3)	1.99 (3)	2.783 (3)	172 (3)
OW1	H2W1	O5 ⁱ	0.73 (3)	2.09 (3)	2.779 (3)	158 (3)
OW2	H1W2	O4 ⁱⁱ	0.76 (3)	2.03 (3)	2.764 (3)	162 (3)
OW2	H2W2	O6	0.74 (3)	2.02 (3)	2.758 (3)	170 (3)
C1	HC1	O6 ⁱ	0.98 (3)	2.42 (3)	3.080 (3)	124 (3)
C4	HC4	O2 ⁱⁱⁱ	0.90 (4)	2.46 (3)	3.252 (4)	148 (3)

Symmetry codes: (i) $x - \frac{1}{2}, \frac{1}{2} - y, z$; (ii) $\frac{1}{2} - x, y - \frac{1}{2}, 2 - z$; (iii) $\frac{1}{2} - x, \frac{1}{2} + y, 1 - z$.

Data collection and cell refinement: *CAD-4 Software* (Enraf-Nonius, 1989). Data reduction: *SDP* (Enraf-Nonius, 1977). Program(s) used to solve structure: *MULTAN77* (Main, Lessinger, Woolfson, Germain & Declercq, 1977). Program(s) used to refine structure: *SDP*. Molecular graphics: *MolView* (Cense, 1989). Software used to prepare material for publication: *SDP*. The same computer programs were used for both analyses.

The X-ray diffraction data collection for both compounds was made possible thanks to the cooperation of Enraf-Nonius, Delft, The Netherlands.

Lists of structure factors, anisotropic displacement parameters, H-atom coordinates and complete geometry have been deposited with the IUCr (Reference: PA1074). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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cis-Tetracarbonylbis[tris(*p*-fluorophenyl)-phosphine]molybdenum(0)

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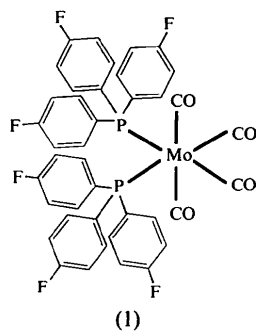
Abstract

The molecule *cis*-tetracarbonylbis[tris(*p*-fluorophenyl)-phosphine]molybdenum(0), [Mo(C₁₈H₁₂F₃P)₂(CO)₄], has twofold crystallographic symmetry; the Mo geometry is irregular octahedral, with principal dimensions Mo—P 2.5644 (4), Mo—C (*trans* to P) 1.9869 (16), Mo—C (*trans* to C) 2.0310 (18) Å, P—Mo—P 107.33 (1), *trans*-P—Mo—C 166.76 (5) and *trans*-C—Mo—C 174.31 (8)°. The P geometry is irregular tetrahedral, with enlarged Mo—P—C [average 115.94 (5)°] and reduced C—P—C [average 102.22 (7)°] angles. ⁹⁵Mo NMR chemical shift data are in accord with the observed structure.

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Comment

The compound *cis*-tetracarbonylbis[tris(*p*-fluorophenyl)phosphine]molybdenum(0), $[\text{Mo}\{\text{P}(\text{C}_6\text{H}_4\text{-F-}p)\}_2(\text{CO})_4]$, (1), was synthesized as part of our studies of the nature of P^{III} ligands as probed by ^{95}Mo NMR spectroscopy (Alyea & Song, 1992, 1994). Since the X-ray structure of *cis*- $[\text{Mo}(\text{PPh}_3)_2(\text{CO})_4]$ (2) is known (Cotton, Darensbourg, Klein & Kolthammer, 1982), an X-ray analysis of (1) was undertaken to determine the influence of the electronegative *para*-substituent on the structural parameters and on the ^{95}Mo chemical shift. A search of the April 1993 release of the Cambridge Structural Database (Allen, Kennard & Taylor, 1983) for structures containing the $\text{Mo}(\text{CO})_4\text{P}_2$ fragment revealed several structures of this type. However, *cis*- $[\text{Mo}(\text{PPh}_3)_2(\text{CO})_4]$ (2) is the only previous one containing monodentate triarylphosphine ligands.



A general view of molecule (1) is shown in Fig. 1 and the bond data (Table 2) show that the Mo atom has irregular octahedral coordination geometry in the solid state. The distortion is considerably larger than that reported previously for the analogous triphenylphosphine complex (2). The average Mo—P bond distance in $[\text{Mo}\{\text{P}(\text{C}_6\text{H}_4\text{-F-}p)\}_2(\text{CO})_4]$ (1) is 2.5644 (4) Å, which is significantly shorter than the analogous bond in the *cis*- $[\text{Mo}(\text{PPh}_3)_2(\text{CO})_4]$ complex (2) [2.577 (2) Å]. More importantly, the P—Mo—P angle is considerably larger, at 107.33 (1)° in (1) than the comparable bond in the unsubstituted triphenylphosphine complex (2) [104.62 (7)°]. Cotton *et al.* (1982) attributed the larger P—Mo—P angle for the Ph_3P complex (2) as compared with those found for the Ph_2MeP [92.52 (5)°] and PhMe_2P [94.78 (5)°] analogues to the greater steric demand of the Ph_3P ligand [Tolman (1977) cone angle of 145°]. In the present case, the still greater distortion must be attributed to the effect of F substitution. The resultant σ -orbital contraction and/or enhanced π -acceptor ability would lead to a shorter Mo—P bond and hence greater steric distortion.

The downfield $\delta(^{95}\text{Mo})$ value of -1551 p.p.m., relative to -1556 p.p.m. reported earlier for (2) (Alyea & Somogyvari, 1988) implies that the weaker basicity of the fluoro-substituted phosphine has the dominant effect, not its greater potential π -acceptor ability. We also observe that the ^{31}P NMR coordination chemical shift is slightly

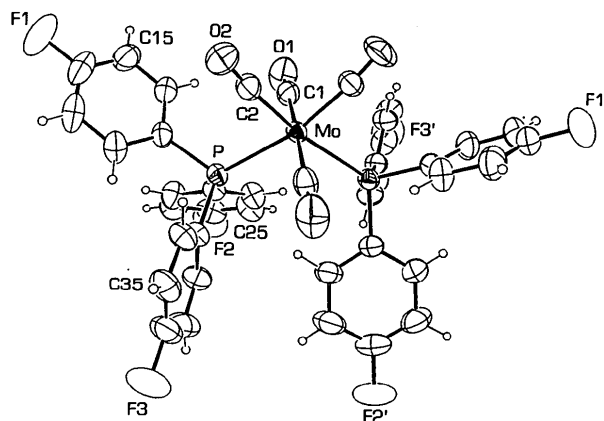


Fig. 1. A view of the molecule (1) showing the general conformation and our numbering scheme. The non-H atoms are depicted as displacement ellipsoids drawn at the 50% probability level.

greater for the present complex (45.5 p.p.m.) than for the Ph_3P analogue (43.3 p.p.m.), which is consistent with the shorter Mo—P bond distance.

Other angles around the Mo atom are also significantly distorted from those of a regular octahedron; *cis* P—Mo—C angles are 84.83 (5)–91.79 (5) and *cis* C—Mo—C angles are 83.17 (7)–94.15 (7)°. The *trans* P—Mo—C(2) and C(1)—Mo—C(1) angles are 166.76 (5) and 174.31 (8)°, respectively. The MoP_2C_2 moiety is significantly non-planar [the dihedral angle between the MoP_2 and MoC_2 planes is 7.37 (6)°] in contrast to the case in (2). There is also bending distortion of the Mo—C(2)—O(2) angles [174.36 (8)°]. As expected, the Mo—C(2) bond distance [1.9869 (16) Å] *trans* to P is considerably shorter (0.044 Å) than the Mo—C(1) bond distance 2.0310 (18) Å *trans* to the carbonyl groups.

Large distortions from tetrahedral geometry are found for the P atoms. The average Mo—P—C angle of 115.94 (5) and the average C—P—C angle of 102.22 (7)° compare with 116.67 (3) and 101.4 (4)°, respectively, for the Ph_3P analogue (2). It is noteworthy that the C—P—C angles in both cases are not larger than those observed for the free Ph_3P ligand (103°) (Daly, 1964). The average P—C bond distance in (1) is 1.8345 (15) Å and is not significantly different from the mean P—C distance [1.832 (8) Å] reported for the *cis*- $[\text{Mo}(\text{Ph}_3\text{P})_2(\text{CO})_4]$ complex (2). Other bond distances and angles in (1) are normal and are available as supplementary material. Intermolecular contacts are of the van der Waals type.

Experimental

The compound was synthesized by adding an excess (3:1) of the ligand to a dichloromethane solution of $\text{Mo}(\text{CO})_4$ (norbornadiene) and stirring for 30 min. Addition of hexane to the clear yellow solution gave, upon reduction of the volume, air-stable yellowish needles; recrystallization was effected from

dichloromethane. The melting point is 441 K (decomposition) and the results of an elemental analysis were: calculated (found), C 57.16 (56.98), H 2.88% (2.95%). Carbonyl infrared bands occur at 2022, 1922, 1909 and 1884 cm⁻¹ in dichloromethane solution.

Crystal data

[Mo(C₁₈H₁₂F₃P)₂(CO)₄]
M_r = 840.50
 Monoclinic
 C2/c
a = 20.4933 (10) Å
b = 9.0960 (4) Å
c = 22.0321 (9) Å
 β = 118.591 (3)°
V = 3606.1 (3) Å³
Z = 4

D_x = 1.55 Mg m⁻³
 Mo Kα radiation
 λ = 0.7107 Å
 Cell parameters from 25 reflections
 θ = 12.0–18.0°
 μ = 0.51 mm⁻¹
T = 293 K
 Colourless
 0.75 × 0.60 × 0.60 mm
 Block

Data collection

Enraf-Nonius CAD-4 diffractometer
 ω/2θ scans
 Absorption correction: empirical (ψ scan)
T_{min} = 0.844, *T_{max}* = 0.889
 5359 measured reflections
 5238 independent reflections
 4435 observed reflections
 [*I* > 3.0σ(*I*)]

R_{int} = 0.010
 θ_{max} = 30.0°
h = -28 → 25
k = 0 → 12
l = 0 → 30
 3 standard reflections monitored every 60 reflections
 intensity variation: <1%

Refinement

Refinement on *F*
R = 0.024
wR = 0.035
S = 1.32
 4435 reflections
 289 parameters
w = 1/[σ²(*F*) + 0.0004*F*²]
 (Δ/σ)_{max} < 0.009
 Δρ_{max} = 0.28 e Å⁻³
 Δρ_{min} = -0.25 e Å⁻³

Extinction correction: Larson (1970)
 Extinction coefficient: 4499 (692)
 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)

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

	<i>x</i>	<i>y</i>	<i>z</i>	<i>U_{eq}</i>
Mo	1/2	0.319868 (17)	1/4	0.03152 (11)
P	0.517084 (21)	0.15282 (4)	0.164886 (18)	0.03479 (20)
F(1)	0.65196 (10)	0.50311 (18)	0.02554 (9)	0.1041 (14)
F(2)	0.71386 (9)	-0.37021 (17)	0.26335 (8)	0.0981 (11)
F(3)	0.23567 (8)	-0.08557 (20)	-0.06095 (8)	0.1006 (11)
O(1)	0.32460 (8)	0.29919 (25)	0.16227 (8)	0.0859 (13)
O(2)	0.49865 (10)	0.58327 (16)	0.15836 (8)	0.0768 (12)
C(1)	0.38758 (10)	0.30878 (21)	0.19316 (8)	0.0501 (10)
C(2)	0.50151 (10)	0.48325 (18)	0.19083 (8)	0.0479 (10)
C(11)	0.55675 (9)	0.25506 (17)	0.11819 (8)	0.0418 (9)
C(12)	0.52324 (12)	0.2677 (3)	0.04704 (9)	0.0581 (12)
C(13)	0.55499 (15)	0.3523 (3)	0.01574 (12)	0.0724 (16)
C(14)	0.62087 (14)	0.42106 (24)	0.05664 (13)	0.0686 (16)
C(15)	0.65694 (13)	0.40906 (25)	0.12630 (13)	0.0649 (15)
C(16)	0.62419 (12)	0.32642 (22)	0.15732 (10)	0.0560 (11)
C(21)	0.57960 (8)	-0.00590 (17)	0.19531 (8)	0.0418 (8)

C(22)	0.60990 (12)	-0.06647 (22)	0.15633 (11)	0.0585 (12)
C(23)	0.65562 (13)	-0.18912 (23)	0.17923 (14)	0.0686 (15)
C(24)	0.66961 (11)	-0.24942 (23)	0.24092 (12)	0.0654 (12)
C(25)	0.64166 (13)	-0.19470 (24)	0.28114 (12)	0.0684 (14)
C(26)	0.59677 (10)	-0.07005 (21)	0.25786 (9)	0.0535 (10)
C(31)	0.43156 (8)	0.07484 (17)	0.09515 (7)	0.0403 (8)
C(32)	0.41838 (11)	-0.07516 (20)	0.08740 (10)	0.0527 (11)
C(33)	0.35124 (13)	-0.1293 (3)	0.03549 (12)	0.0668 (15)
C(34)	0.30030 (11)	-0.0316 (3)	-0.00902 (10)	0.0655 (13)
C(35)	0.31102 (11)	0.1168 (3)	-0.00328 (10)	0.0606 (12)
C(36)	0.37631 (10)	0.17008 (20)	0.05020 (8)	0.0478 (9)

Table 2. Selected geometric parameters (Å, °)

Mo—P	2.5644 (4)	F(1)—C(14)	1.360 (2)
Mo—C(1)	2.0310 (18)	F(2)—C(24)	1.358 (2)
Mo—C(2)	1.9869 (16)	F(3)—C(34)	1.362 (2)
P—C(11)	1.8398 (16)	O(1)—C(1)	1.138 (2)
P—C(21)	1.8312 (15)	O(2)—C(2)	1.141 (2)
P—C(31)	1.8326 (15)		
P—Mo—P ⁱ	107.33 (1)	C(11)—P—C(21)	100.62 (7)
P—Mo—C(1)	91.79 (5)	C(11)—P—C(31)	103.18 (7)
P—Mo—C(1 ⁱ)	84.83 (5)	C(21)—P—C(31)	102.87 (7)
P—Mo—C(2)	85.01 (5)	Mo—C(1)—O(1)	178.13 (18)
P—Mo—C(2 ⁱ)	166.76 (5)	Mo—C(2)—O(2)	174.36 (16)
C(1)—Mo—C(1 ⁱ)	174.31 (8)	P—C(11)—C(12)	124.29 (14)
C(1)—Mo—C(2)	90.11 (7)	P—C(11)—C(16)	117.59 (12)
C(1)—Mo—C(2 ⁱ)	94.15 (7)	P—C(21)—C(22)	121.78 (13)
C(2)—Mo—C(2 ⁱ)	83.17 (7)	P—C(21)—C(26)	119.93 (12)
Mo—P—C(11)	111.16 (5)	P—C(31)—C(32)	122.43 (13)
Mo—P—C(21)	121.06 (5)	P—C(31)—C(36)	118.77 (12)
Mo—P—C(31)	115.59 (5)		

Symmetry code: (i) 1 - x, y, ½ - z.

The systematic absences for (1) (*hkl* absent if *h* + *k* = 2*n* + 1, *h*0*l* absent if *l* = 2*n* + 1) allow the space group to be either C2/c or Cc; the former was assumed and confirmed by the analysis. All H atoms attached to the phenyl ring C atoms were visible in difference maps at intermediate stages of refinement and were refined isotropically. Data collection: *CAD-4 Software* (Enraf-Nonius, 1989). Cell refinement: *CAD-4 Software*. Data reduction: *NRCVAX DATRD2* (Gabe, Le Page, Charland, Lee & White, 1989). Program(s) used to solve structure: *NRCVAX SOLVER*. Program(s) used to refine structure: *NRCVAX LSTSQ*. Molecular graphics: *NRCVAX PLUTON* and *ORTEPII* (Johnson, 1976). Software used to prepare material for publication: *NRCVAX TABLES*.

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Lists of structure factors, anisotropic displacement parameters, H-atom coordinates and complete geometry have been deposited with the IUCr (Reference: CR1098). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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$(\text{C}_{24}\text{H}_{20}\text{P})_2[\text{Mo}_6\text{Cl}_{14}]$

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Abstract

The structure of bis(tetraphenylphosphonium) octa- μ_3 -chloro-hexachlorohexamolybdate(2-) is reported. The structure consists of an $[\text{Mo}_6\text{Cl}_{14}]^{2-}$ cluster anion having a crystallographic center of inversion and two (inversion) symmetry-related tetraphenylphosphonium (TPP) cations. The molybdenum chloride cluster anion is a slightly distorted octahedron of Mo atoms surrounded by eight (μ_3) face-bridging and six axial Cl atoms, and is coordinated by ten nearest neighbor TPP molecules. The distorted cluster retains only inversion symmetry.

Comment

Molecular crystals containing the cluster anion $[\text{Mo}_6\text{Cl}_{14}]^{2-}$ are of interest for their optical properties. The cluster anion is luminescent with emission maximum, lifetime, and quantum yield of 805 nm, 180 μs , and 0.19, respectively, and has a broad absorption spectrum below 500 nm (Maverick, Najdzionek, Mackenzie, Nocera & Gray, 1983). The large quantum yield and moderately long lifetime makes the cluster ion a suitable candidate for electronic excited-state structure determination (Pressprich, White & Coppens, 1993) using modulated laser techniques.

The molybdenum chloride cluster anion in the title compound has slightly distorted octahedral symmetry. The distortion of the cluster is such as to remove all but inversion symmetry, with only the Mo2—Mo3, Mo1—Mo2¹ and Mo2—Mo3¹ nearest-neighbor bond lengths remaining equivalent at 2.606 (1) Å. The distortion may be viewed as a canting of the body diagonals (by about

0.2°). The molybdenum chloride cluster anion is nearly identical (to within 3σ in Mo—Mo bond lengths) to that reported in the tetramethyltetrafulvalene (TMTTF) complex $(\text{TMTTF})_2[\text{Mo}_6\text{Cl}_{14}]$ (Ouhab, Battail, Perrin & Garragou-Lagrange, 1986).

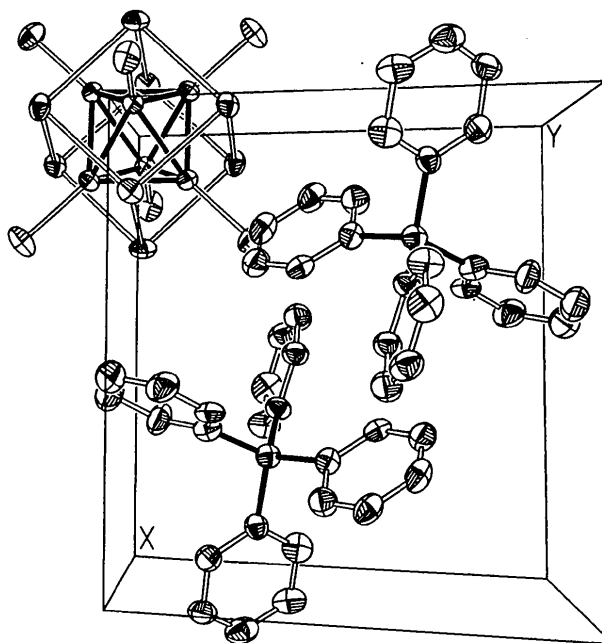


Fig. 1. The unit-cell packing diagram viewed along the *c* axis. The Mo—Cl bonds have been omitted and the adjacent bridging Cl atoms connected to show the geometry of the cluster. Displacement ellipsoids are drawn at the 50% probability level. H atoms are omitted for clarity.

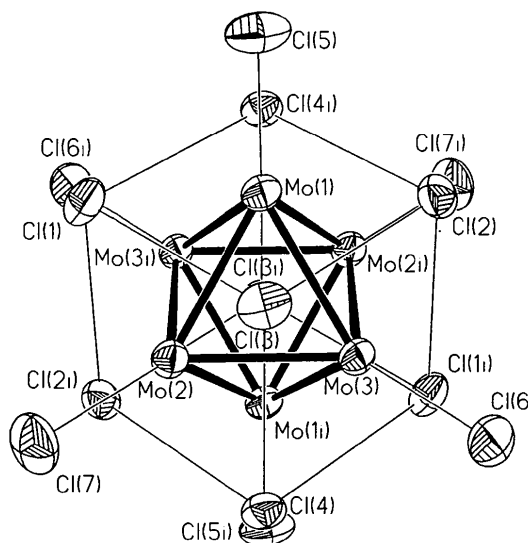


Fig. 2. The molybdenum chloride cluster anion showing the atomic labeling and the octahedral symmetry. The Mo—Cl bonds have been omitted and the adjacent bridging Cl atoms have been connected. Displacement ellipsoids are drawn at the 50% probability level.