

| | | | | |
|-------|-------------|------------|------------|--------|
| O(14) | -0.1538 (3) | 1.2489 (2) | 0.1274 (2) | 0.0162 |
| N(1) | 0.6914 (3) | 0.9012 (3) | 0.3365 (3) | 0.0172 |
| N(2) | 0.4179 (3) | 0.6941 (3) | 0.1357 (3) | 0.0203 |
| N(3) | 0.0171 (4) | 0.3785 (3) | 0.4132 (3) | 0.0167 |
| C(1) | 0.6052 (4) | 0.9448 (3) | 0.2181 (3) | 0.0182 |
| C(2) | 0.5747 (4) | 0.7898 (4) | 0.3699 (3) | 0.0200 |
| C(3) | 0.5329 (4) | 0.8089 (4) | 0.1042 (3) | 0.0204 |
| C(4) | 0.4974 (4) | 0.6536 (4) | 0.2567 (4) | 0.0209 |
| C(5) | 0.1503 (4) | 0.4563 (4) | 0.5383 (3) | 0.0208 |
| C(6) | -0.1484 (4) | 0.3838 (4) | 0.4212 (4) | 0.0228 |

Table 2. Selected interatomic distances (Å)

| | | | |
|-------------|------------|-------------------------|-----------|
| Mo(1)—O(1) | 1.9022 (2) | Mo(3)—O(13) | 1.731 (2) |
| Mo(1)—O(2') | 2.232 (2) | Mo(4)—O(2) | 2.122 (2) |
| Mo(1)—O(3) | 2.181 (2) | Mo(4)—O(3') | 1.938 (2) |
| Mo(1)—O(4) | 2.022 (2) | Mo(4)—O(7) | 1.903 (2) |
| Mo(1)—O(5) | 1.712 (2) | Mo(4)—O(7') | 2.419 (2) |
| Mo(1)—O(6) | 1.711 (2) | Mo(4)—O(11') | 1.753 (2) |
| Mo(2)—O(2) | 1.926 (2) | Mo(4)—O(14) | 1.696 (2) |
| Mo(2)—O(7) | 2.289 (2) | N(1)—C(1) | 1.483 (4) |
| Mo(2)—O(8) | 1.716 (2) | N(1)—C(2) | 1.490 (4) |
| Mo(2)—O(9) | 1.936 (2) | N(2)—C(3) | 1.490 (5) |
| Mo(2)—O(10) | 1.702 (2) | N(2)—C(4) | 1.473 (5) |
| Mo(2)—O(11) | 2.317 (2) | N(3)—C(5) | 1.478 (4) |
| Mo(3)—O(3) | 2.298 (2) | N(3)—C(6) | 1.494 (4) |
| Mo(3)—O(4) | 1.903 (2) | C(1)—C(3) | 1.512 (5) |
| Mo(3)—O(7) | 2.233 (2) | C(2)—C(4) | 1.510 (5) |
| Mo(3)—O(9) | 1.941 (2) | C(5)—C(6 ^b) | 1.514 (5) |
| Mo(3)—O(12) | 1.720 (2) | | |

Symmetry codes: (i) $-x, 2 - y, -z$; (ii) $-x, 1 - y, 1 - z$.

Table 3. Hydrogen-bonding geometry (Å)

| | | | |
|--------------|-----------|------------------------------|-----------|
| N(2)···O(3) | 2.741 (3) | N(2)···O(6 ⁱⁱ) | 2.783 (4) |
| N(1)···O(4') | 2.805 (3) | N(1)···O(12 ⁱⁱⁱ) | 2.823 (3) |
| N(3)···O(5) | 2.775 (3) | N(3)···O(13 ^{iv}) | 2.829 (3) |

Symmetry codes: (i) $x - 1, y, z$; (ii) $-x, 1 - y, -z$; (iii) $1 - x, 2 - y, 1 - z$; (iv) $x, 1 + y, z$.

H atoms were geometrically placed and their positions refined riding on appropriate N or C atoms with $d(\text{N—H}) = 1.00$ or $d(\text{C—H}) = 1.00$ Å. Carrier-atom-type isotropic displacement parameters were refined for H atoms.

Data collection: *CAD-4 Software* (Enraf–Nonius, 1989). Cell refinement: *CAD-4 Software*. Data reduction: *RC85* (Baird, 1985). Program(s) used to solve structure: *SHELXS86* (Sheldrick, 1985). Program(s) used to refine structure: *CRYSTALS* (Watkin, Carruthers & Betteridge, 1990). Molecular graphics: *ORTEPII* (Johnson, 1976). Software used to prepare material for publication: local routines.

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Lists of structure factors, anisotropic displacement parameters, H-atom coordinates and complete geometry, including contact distances, have been deposited with the IUCr (Reference: TA1054). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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[N(CH₃)₄]₂[Co₂Mo₆O₁₂(OH)₄(PO₄)(HPO₄)₂-(H₂PO₄)]₅·5H₂O, a New One-Dimensional Molybdenum Phosphate

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Abstract

The title compound, bis(tetramethylammonium) dicobaltio- μ -dihydrogenphosphato- μ -bis(hydrogenphosphato)- μ_6 -phosphato-tetrahydroxycyclohexamolybdate-(*Mo—Mo*) pentahydrate, was synthesized hydrothermally and crystallizes as a polymeric ionic complex with anionic chains, composed of $[\text{Mo}_6\text{O}_{12}(\text{OH})_3(\text{H}_x\text{PO}_4)_4]^{7-}$ clusters held together by Co^{2+} cations running parallel to the *b* axis. Neighbouring chains are linked by hydrogen bonds only *via* intervening $[\text{N}(\text{CH}_3)_4]^+$ cations and water molecules.

Comment

The title compound was prepared as part of an exploratory project aimed at synthesizing molybdenum phosphates of varying dimensions. Previous work (Haushalter & Mundi, 1992) suggested that related compounds contain the complex anion $[\text{Mo}_6\text{O}_{15}(\text{HPO}_4)(\text{H}_2\text{PO}_4)_3]^{5-}$ (' Mo_6P_4 ') as a primary building unit. This anion is composed of a ring of edge-sharing MoO_6 octahedra, with Mo in the +5 oxidation state complexed with PO_4 tetrahedra both internal and external to the ring. We have shown recently (Light-

foot & Masson, 1995) that this complex anion is better formulated as $[Mo_6O_{12}(OH)_3H_x(PO_4)_4]^{(9-x)-}$. The present compound contains the $x = 4$ version of this anion, which is polymerized *via* bridging Co^{2+} cations into an infinite chain anion.

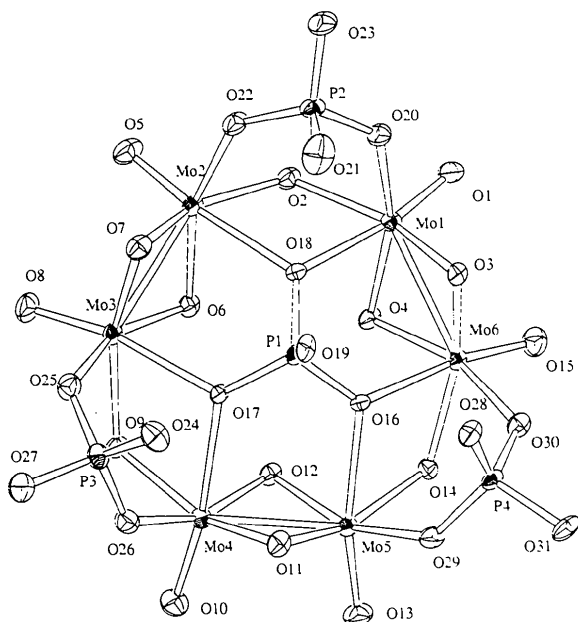


Fig. 1. The ring of six edge-sharing MoO_6 octahedra bridged internally [P(1)] and externally [P(2), P(3) and P(4)] by phosphate groups. Displacement ellipsoids are plotted at the 50% probability level.

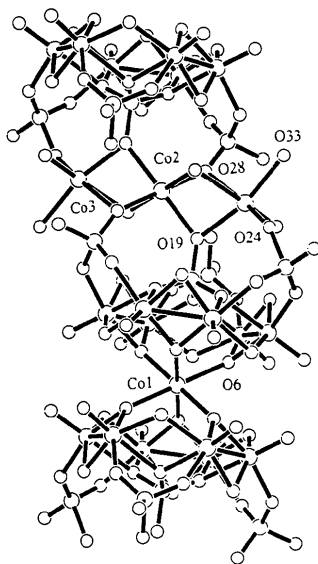


Fig. 2. Portion of the polymeric anionic chain running parallel to the b direction. Two ' Mo_6P_4 ' clusters are linked by Co(1) at the $(0, 1/2, 1)$ inversion centre. These superclusters are polymerized *via* Co(2) at the $(0, 0, 1)$ inversion centre. Co(2) shares opposite octahedral faces with two Co(3) octahedra. All atoms are represented by spheres of arbitrary radii.

Details of the Mo_6P_4 cluster are in agreement with the previous study of the related phase $[N(CH_3)_4][Mn_2Mo_6O_{12}(OH)_4(PO_4)(HPO_4)(H_2PO_4)_2] \cdot 4H_2O$. (II) (Lightfoot & Masson, 1995). Compound (I) consists of a ring of six edge-sharing MoO_6 octahedra with alternating long (approximately 3.6 Å) and short (2.6 Å) Mo—Mo contacts (Fig. 1). A central phosphate group bridges the ring internally and phosphate groups bridge each of the three long Mo—Mo contacts externally. The cluster thus has approximate threefold symmetry, though this is not imposed crystallographically. Two Mo_6P_4 clusters are linked *via* Co(1) and these units are further linked by the remaining two Co atoms (Fig. 2) to form an infinite chain anion along the b axis. All three cobalt environments are octahedral.

Bond-valence sum analysis (Brown & Altermatt, 1985) was used to confirm the oxidation states of the metals as +5 and +2 for all Mo and all Co atoms, respectively. This method applies the formula $s = \exp[(r_o - r)/B]$, where s is the bond-valence contribution for a particular M—O bond, r is the M—O distance and r_o and B are constants, to determine the bond-valence sum around each metal. Corresponding bond-valence sums are calculated for each O atom, from which the presence of H atoms bonded to O atoms may be inferred. A bond-valence contribution of about 0.82 valence units can be expected for an O—H distance of 0.95 Å; hence oxygen-valence sums in the range 0.2–0.5 suggest water molecules, while those in the range 1.1–1.3 suggest hydroxy groups. This analysis revealed bond-valence sums of 1.23, 1.23 and 1.22 for O(2), O(9) and O(14), respectively, indicating unambiguously that these are hydroxy O atoms. In addition, H atoms were

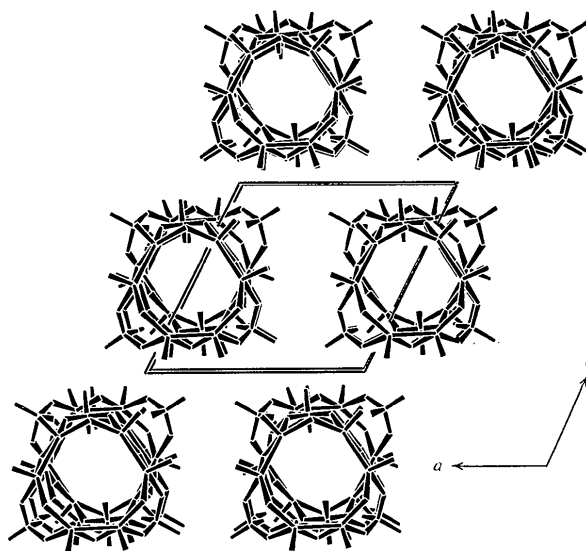


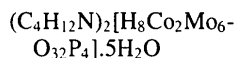
Fig. 3. Schematic representation of the structure along the chain axis b . $[N(CH_3)_4]^+$ cations and water molecules are not shown.

also suggested on the phosphate groups O(21) 1.1, O(23) 1.36, O(27) 1.13 and O(31) 1.15. O(34) 1.23 was confirmed as a hydroxy group, while O(32) 0.36 and O(33) 0.35 were shown to be water O atoms. No chemical analysis is available for this phase as it was not obtained in a pure form, but we are entirely confident that the stoichiometry arrived at by this method is correct. The general architecture of the structure is the same as that of (II), but the inclusion of an extra $[N(CH_3)_4]^+$ cation in the present case is balanced by the absence of one phosphate H atom in the chain. An additional water of hydration is also present.

Experimental

The title compound was prepared hydrothermally from a mixture of $CoCl_2 \cdot 6H_2O$, MoO_3 , Mo, $(CH_3)_4NOH$, H_3PO_4 and H_2O in a 2:1:1:2:4:200 molar ratio. The mixture was placed in a teflon-lined stainless-steel autoclave and heated at 463 K for 4 days.

Crystal data



$M_r = 1575.81$

Triclinic

$P\bar{1}$

$a = 13.012(2) \text{ \AA}$

$b = 14.133(2) \text{ \AA}$

$c = 11.856(2) \text{ \AA}$

$\alpha = 92.96(1)^\circ$

$\beta = 112.946(9)^\circ$

$\gamma = 77.55(1)^\circ$

$V = 1959.3(5) \text{ \AA}^3$

$Z = 2$

$D_x = 2.671 \text{ Mg m}^{-3}$

D_m not measured

Mo $K\alpha$ radiation

$\lambda = 0.71073 \text{ \AA}$

Cell parameters from 25

reflections

$\theta = 17.3\text{--}17.5^\circ$

$\mu = 2.959 \text{ mm}^{-1}$

$T = 293.2 \text{ K}$

Block

$0.50 \times 0.45 \times 0.35 \text{ mm}$

Brown

Data collection

AFC-7S diffractometer

$\omega/2\theta$ scans

Absorption correction:

ψ scans (North, Phillips & Matthews, 1968)

$T_{\min} = 0.22$, $T_{\max} = 0.33$

10414 measured reflections

9971 independent reflections

8250 observed reflections

$[I > 3\sigma(I)]$

$R_{\text{int}} = 0.0192$

$\theta_{\text{max}} = 30^\circ$

$h = 0 \rightarrow 14$

$k = -17 \rightarrow 17$

$l = -14 \rightarrow 14$

3 standard reflections

monitored every 150

reflections

intensity decay: 1.39%

Refinement

Refinement on F

$R = 0.041$

$wR = 0.057$

$S = 4.91$

8250 reflections

536 parameters

$\Delta\rho_{\text{max}} = 1.62 \text{ e \AA}^{-3}$

[close to Mo(1)]

$\Delta\rho_{\text{min}} = -1.78 \text{ e \AA}^{-3}$

Extinction correction:

Zachariasen (1967) type

II, Gaussian isotropic

H-atom parameters not refined

Weighting scheme based on measured e.s.d.'s

$(\Delta/\sigma)_{\text{max}} = 0.064$

Extinction coefficient:

9.74×10^{-7}

Atomic scattering factors

from *International Tables for X-ray Crystallography* (1974, Vol. IV)

Table 1. Fractional atomic coordinates and equivalent isotropic displacement parameters (\AA^2)

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

| | x | y | z | U_{eq} |
|-------|--------------|--------------|-------------|-----------------|
| Mo(1) | -0.20133 (4) | 0.34998 (3) | 0.78665 (4) | 0.0126 (2) |
| Mo(2) | 0.04783 (4) | 0.35122 (4) | 0.73884 (4) | 0.0139 (2) |
| Mo(3) | 0.23980 (4) | 0.33270 (4) | 0.92770 (4) | 0.0137 (2) |
| Mo(4) | 0.25118 (4) | 0.31708 (4) | 1.22711 (4) | 0.0137 (2) |
| Mo(5) | 0.06611 (4) | 0.31313 (3) | 1.25791 (4) | 0.0129 (2) |
| Mo(6) | -0.19484 (4) | 0.33848 (3) | 1.00731 (4) | 0.0119 (2) |
| Co(1) | 0 | 1/2 | 1 | 0.0130 (4) |
| Co(2) | 0 | 0 | 1 | 0.0135 (4) |
| Co(3) | 0.22148 (7) | 0.00548 (6) | 0.98364 (8) | 0.0182 (3) |
| P(1) | 0.0547 (1) | 0.22018 (10) | 0.9830 (1) | 0.0109 (6) |
| P(2) | -0.1200 (1) | 0.1981 (1) | 0.6011 (1) | 0.0170 (6) |
| P(3) | 0.4023 (1) | 0.1515 (1) | 1.1204 (1) | 0.0164 (6) |
| P(4) | -0.0949 (1) | 0.1501 (1) | 1.2031 (1) | 0.0135 (6) |
| O(1) | -0.3345 (4) | 0.4148 (3) | 0.7152 (4) | 0.020 (2) |
| O(2) | -0.1205 (4) | 0.4202 (3) | 0.7060 (4) | 0.017 (2) |
| O(3) | -0.2179 (3) | 0.2467 (3) | 0.8763 (3) | 0.014 (2) |
| O(4) | -0.1384 (4) | 0.4273 (3) | 0.9325 (3) | 0.016 (2) |
| O(5) | 0.0722 (4) | 0.4189 (3) | 0.6447 (4) | 0.025 (2) |
| O(6) | 0.0906 (3) | 0.4247 (3) | 0.8917 (3) | 0.015 (2) |
| O(7) | 0.1808 (4) | 0.2456 (3) | 0.7984 (4) | 0.018 (2) |
| O(8) | 0.3113 (4) | 0.3932 (3) | 0.8763 (4) | 0.024 (2) |
| O(9) | 0.2879 (3) | 0.3908 (3) | 1.1046 (3) | 0.016 (2) |
| O(10) | 0.3233 (4) | 0.3689 (3) | 1.3559 (4) | 0.023 (2) |
| O(11) | 0.2015 (4) | 0.2141 (3) | 1.2778 (4) | 0.018 (2) |
| O(12) | 0.0994 (3) | 0.4074 (3) | 1.1652 (3) | 0.015 (2) |
| O(13) | 0.0928 (4) | 0.3609 (3) | 1.3960 (4) | 0.025 (2) |
| O(14) | -0.1037 (3) | 0.3912 (3) | 1.1746 (3) | 0.014 (2) |
| O(15) | -0.3267 (4) | 0.3987 (3) | 0.9881 (4) | 0.023 (2) |
| O(16) | -0.0113 (3) | 0.2560 (3) | 1.0656 (3) | 0.012 (2) |
| O(17) | 0.1682 (3) | 0.2536 (3) | 1.0351 (3) | 0.013 (2) |
| O(18) | -0.0165 (3) | 0.2673 (3) | 0.8543 (3) | 0.014 (2) |
| O(19) | 0.0749 (3) | 0.1095 (3) | 0.9755 (4) | 0.016 (2) |
| O(20) | -0.2080 (4) | 0.2526 (3) | 0.6511 (4) | 0.020 (2) |
| O(21) | -0.0618 (4) | 0.0983 (3) | 0.6764 (5) | 0.035 (2) |
| O(22) | -0.0273 (4) | 0.2528 (3) | 0.6163 (4) | 0.022 (2) |
| O(23) | -0.1799 (4) | 0.1740 (4) | 0.4698 (4) | 0.028 (2) |
| O(24) | 0.3451 (4) | 0.0673 (3) | 1.0967 (4) | 0.025 (2) |
| O(25) | 0.3712 (4) | 0.2151 (3) | 1.0067 (4) | 0.021 (2) |
| O(26) | 0.3857 (3) | 0.2137 (3) | 1.2252 (4) | 0.019 (2) |
| O(27) | 0.5344 (4) | 0.1126 (3) | 1.1611 (4) | 0.026 (2) |
| O(28) | -0.0675 (4) | 0.0661 (3) | 1.1286 (4) | 0.019 (2) |
| O(29) | 0.0052 (4) | 0.1944 (3) | 1.2855 (3) | 0.018 (2) |
| O(30) | -0.1926 (3) | 0.2300 (3) | 1.1189 (4) | 0.017 (2) |
| O(31) | -0.1420 (4) | 0.1072 (3) | 1.2877 (4) | 0.021 (2) |
| O(32) | 0.2203 (4) | 0.0559 (3) | 0.8224 (4) | 0.029 (2) |
| O(33) | 0.3444 (4) | -0.1178 (3) | 0.9869 (4) | 0.025 (2) |
| O(34) | 0.1741 (4) | -0.0559 (3) | 1.1173 (4) | 0.018 (2) |
| O(35) | -0.3319 (6) | 0.0589 (6) | 0.3915 (6) | 0.081 (4) |
| O(36) | -0.7552 (6) | 0.0216 (4) | 0.3278 (5) | 0.053 (3) |
| O(37) | 0.1341 (6) | 0.1058 (8) | 0.5328 (7) | 0.102 (5) |
| N(1) | 0.3712 (5) | 0.5840 (4) | 0.6852 (6) | 0.031 (3) |
| N(2) | 0.4404 (6) | 0.1896 (5) | 0.6511 (6) | 0.047 (3) |
| C(1) | 0.4512 (8) | 0.5131 (8) | 0.7878 (9) | 0.066 (5) |
| C(2) | 0.2502 (8) | 0.5818 (9) | 0.6511 (9) | 0.068 (6) |
| C(3) | 0.386 (1) | 0.6801 (8) | 0.747 (1) | 0.113 (8) |
| C(4) | 0.407 (1) | 0.579 (1) | 0.587 (1) | 0.124 (1) |
| C(5) | 0.3276 (9) | 0.2565 (9) | 0.6062 (9) | 0.074 (6) |
| C(6) | 0.531 (1) | 0.241 (1) | 0.701 (2) | 0.173 (1) |
| C(7) | 0.445 (1) | 0.1234 (10) | 0.749 (1) | 0.116 (9) |
| C(8) | 0.449 (1) | 0.128 (1) | 0.551 (1) | 0.11 (1) |

Table 2. Selected interatomic distances (Å)

| | | | |
|-------------|------------|--------------|-----------|
| Mo(1)—Mo(6) | 2.5968 (6) | Mo(6)—O(4) | 1.981 (4) |
| Mo(1)—O(1) | 1.676 (4) | Mo(6)—O(14) | 2.071 (4) |
| Mo(1)—O(2) | 2.082 (4) | Mo(6)—O(15) | 1.675 (4) |
| Mo(1)—O(3) | 1.945 (4) | Mo(6)—O(16) | 2.267 (4) |
| Mo(1)—O(4) | 1.985 (4) | Mo(6)—O(30) | 2.065 (4) |
| Mo(1)—O(18) | 2.274 (4) | Co(1)—O(4) | 2.128 (4) |
| Mo(1)—O(20) | 2.049 (4) | Co(1)—O(6) | 2.161 (4) |
| Mo(2)—Mo(3) | 2.5961 (7) | Co(1)—O(12) | 2.187 (4) |
| Mo(2)—O(2) | 2.087 (4) | Co(2)—O(19) | 2.085 (4) |
| Mo(2)—O(5) | 1.666 (4) | Co(2)—O(28) | 2.124 (4) |
| Mo(2)—O(6) | 1.985 (4) | Co(2)—O(34) | 2.139 (4) |
| Mo(2)—O(7) | 1.940 (4) | Co(3)—O(19) | 2.114 (4) |
| Mo(2)—O(18) | 2.339 (4) | Co(3)—O(24) | 1.988 (4) |
| Mo(2)—O(22) | 2.066 (4) | Co(3)—O(28') | 2.337 (4) |
| Mo(3)—O(6) | 1.991 (4) | Co(3)—O(32) | 2.068 (4) |
| Mo(3)—O(7) | 1.936 (4) | Co(3)—O(33) | 2.086 (4) |
| Mo(3)—O(8) | 1.675 (4) | Co(3)—O(34) | 2.185 (4) |
| Mo(3)—O(9) | 2.118 (4) | P(1)—O(16) | 1.540 (4) |
| Mo(3)—O(17) | 2.293 (4) | P(1)—O(17) | 1.532 (4) |
| Mo(3)—O(25) | 2.062 (4) | P(1)—O(18) | 1.538 (4) |
| Mo(4)—Mo(5) | 2.5849 (7) | P(1)—O(19) | 1.533 (4) |
| Mo(4)—O(9) | 2.082 (4) | P(2)—O(20) | 1.536 (4) |
| Mo(4)—O(10) | 1.677 (4) | P(2)—O(21) | 1.581 (5) |
| Mo(4)—O(11) | 1.923 (4) | P(2)—O(22) | 1.518 (4) |
| Mo(4)—O(12) | 1.987 (4) | P(2)—O(23) | 1.504 (4) |
| Mo(4)—O(17) | 2.333 (4) | P(3)—O(24) | 1.494 (4) |
| Mo(4)—O(26) | 2.031 (4) | P(3)—O(25) | 1.527 (4) |
| Mo(5)—O(11) | 1.940 (4) | P(3)—O(26) | 1.542 (4) |
| Mo(5)—O(12) | 1.986 (4) | P(3)—O(27) | 1.570 (5) |
| Mo(5)—O(13) | 1.674 (4) | P(4)—O(28) | 1.508 (4) |
| Mo(5)—O(14) | 2.106 (4) | P(4)—O(29) | 1.529 (4) |
| Mo(5)—O(16) | 2.287 (4) | P(4)—O(30) | 1.548 (4) |
| Mo(5)—O(29) | 2.095 (4) | P(4)—O(31) | 1.565 (4) |
| Mo(6)—O(3) | 1.945 (4) | | |

Symmetry code: (i) $-x, -y, 2 - z$.

H atoms on the tetramethylammonium cations were placed geometrically and treated as riding atoms. Hydroxy and water molecule H atoms were not located.

Data collection: *MSCI/AFSC Diffractometer Control Software* (Molecular Structure Corporation, 1988). Cell refinement: *MSCI/AFSC Diffractometer Control Software*. Data reduction: *TEXSAN* (Molecular Structure Corporation, 1992). Program(s) used to refine structure: *TEXSAN*. Software used to prepare material for publication: *TEXSAN*.

Lists of structure factors, anisotropic displacement parameters, H-atom coordinates and complete geometry have been deposited with the IUCr (Reference: MU1218). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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[1,1'-Bis(methylphenylphosphino)-ferrocene-*P,P'*](pentane-2,4-dionato-*O,O'*)-palladium Tetrafluoroborate†

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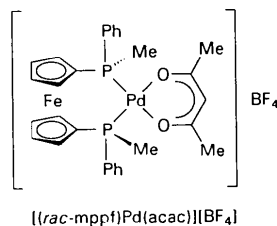
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Abstract

The C_2 symmetric bisphosphine *rac*-Fe(C₅H₄PMePh)₂ (*rac*-mppf) forms a Pd^{II} complex [(*rac*-mppf)Pd(acac)]·BF₄ (acac = pentane-2,4-dionate, C₅H₇O₂). The coordination geometry of the Pd centre is square planar while the ring–ring conformation of the *rac*-mppf ligand is intermediate between synperiplanar and synclinal eclipsed, with a torsion angle of 16.4°.

Comment

We have recently described *rac*-Fe(C₅H₄PMePh)₂ (*rac*-mppf), a new C_2 -symmetric chiral bisphosphine (Herberich & Moss, 1995). We report here the crystal structure of the complex [(*rac*-mppf)Pd(acac)]BF₄, (I), as part of an ongoing study of the preferential conformations and the flexibility of complexes of the ligand *rac*-mppf.



The cation of the title compound (Fig. 1) possesses a square planar Pd^{II} centre. The phosphine ligand is closely related to the well known complex 1,1'-bis(diphenylphosphino)ferrocene, Fe(C₅H₄PPh₂)₂ (dppf), for which much structural data are available (Gan & Hor, 1995). The ferrocene skeleton of the *rac*-mppf ligand exhibits slight distortions from idealized geometry, as is commonly observed for complexes of dppf. The cyclopentadienyl rings are planar with mean deviations of the C atoms from the best cyclopentadienyl (Cp) planes

† Systematic name: bis[μ -methylphenylphosphino-2 κ P:1(η^5)-cyclopentadienyl](pentane-2,4-dionato-2 κ^2 O,O')ironpalladium tetrafluoroborate.