N	0.6879 (3)	−0.2770 (8)	0.6097 (2)	2.8 (1)
C(11)	0.6905 (3)	0.097 (1)	0.5747 (3)	3.8 (2)
C(12)	0.5772 (3)	−0.300 (1)	0.5415 (2)	3.6 (2)
C(13)	0.5760 (4)	0.069 (1)	0.5378 (2)	4.4 (2)
C(14)	0.6619 (4)	−0.121 (1)	0.5058 (3)	4.4 (2)
C(15)	0.6677 (3)	−0.250 (1)	0.6490 (2)	3.0 (2)
C(16)	0.6934 (3)	−0.321 (1)	0.6873 (2)	3.4 (2)
C(17)	0.7379 (4)	−0.431 (1)	0.6849 (3)	4.6 (2)
C(18)	0.7568 (4)	−0.466 (1)	0.6447 (3)	4.3 (2)
C(19)	0.7316 (3)	−0.383 (1)	0.6084 (3)	3.3 (2)
C(21)	0.7031 (3)	0.127 (1)	0.6960 (2)	3.0 (1)
C(22)	0.5304 (3)	0.139 (1)	0.6953 (2)	3.7 (2)
C(23)	0.6212 (4)	−0.026 (1)	0.7495 (2)	4.7 (2)
C(24)	0.6083 (3)	0.304 (1)	0.6433 (3)	3.6 (2)
C(25)	0.6218 (4)	0.332 (1)	0.7381 (3)	4.7 (2)
N(3)	0.4101 (3)	0.3603 (9)	0.1050 (2)	3.4 (1)
C(31)	0.3606 (3)	0.426 (1)	0.1280 (3)	4.7 (2)
C(32)	0.3580 (5)	0.620 (1)	0.1301 (3)	6.9 (3)
C(33)	0.4058 (4)	0.166 (1)	0.1067 (3)	4.7 (2)
C(34)	0.4515 (4)	0.066 (1)	0.0870 (3)	5.5 (3)
C(35)	0.4680 (4)	0.419 (1)	0.1274 (3)	5.0 (2)
C(36)	0.4825 (4)	0.378 (1)	0.1756 (3)	4.9 (2)
C(37)	0.4050 (4)	0.420 (1)	0.0575 (3)	4.7 (2)
C(38)	0.3483 (4)	0.380 (2)	0.0290 (3)	6.4 (3)

Table 2. *Selected geometric parameters* (Å, °)

Mo(1)···Mo(2)	4.5609 (7)	O(21)—C(21)	1.136 (6)
Mo(1)—S	2.617 (1)	O(14)—C(14)	1.180 (6)
Mo(1)—N	2.284 (4)	O(13)—C(13)	1.153 (8)
Mo(1)—C(11)	2.052 (6)	O(12)—C(12)	1.079 (6)
Mo(1)—C(12)	2.109 (6)	O(22)—C(22)	1.153 (6)
Mo(1)—C(13)	1.974 (7)	O(23)—C(23)	1.111 (6)
Mo(1)—C(14)	1.934 (5)	O(24)—C(24)	1.110 (7)
Mo(2)—S	2.582 (1)	O(25)—C(25)	1.128 (7)
Mo(2)—C(21)	2.046 (6)	N—C(15)	1.361 (6)
Mo(2)—C(22)	2.025 (6)	N—C(19)	1.330 (6)
Mo(2)—C(23)	2.043 (6)	C(15)—C(16)	1.367 (7)
Mo(2)—C(24)	2.094 (7)	C(16)—C(17)	1.370 (7)
Mo(2)—C(25)	1.991 (6)	C(17)—C(18)	1.387 (8)
S—C(15)	1.765 (5)	C(18)—C(19)	1.353 (7)
O(11)—C(11)	1.121 (6)		

S—Mo(1)—N	63.6 (1)	C(22)—Mo(2)—C(25)	89.1 (2)
S—Mo(1)—C(11)	96.1 (1)	C(23)—Mo(2)—C(24)	177.5 (2)
S—Mo(1)—C(12)	91.0 (1)	C(23)—Mo(2)—C(25)	89.3 (3)
S—Mo(1)—C(13)	99.0 (1)	C(24)—Mo(2)—C(25)	89.6 (2)
S—Mo(1)—C(14)	169.6 (2)	Mo(1)—S—Mo(2)	122.59 (6)
N—Mo(1)—C(11)	92.5 (2)	Mo(1)—S—C(15)	80.9 (1)
N—Mo(1)—C(12)	90.8 (2)	Mo(2)—S—C(15)	112.0 (2)
N—Mo(1)—C(13)	162.5 (2)	Mo(1)—N—C(15)	103.3 (4)
N—Mo(1)—C(14)	106.3 (3)	Mo(1)—N—C(19)	137.7 (3)
C(11)—Mo(1)—C(12)	173.0 (2)	C(15)—N—C(19)	119.0 (5)
C(11)—Mo(1)—C(13)	88.1 (2)	Mo(1)—C(11)—O(11)	172.7 (5)
C(11)—Mo(1)—C(14)	86.6 (2)	Mo(1)—C(12)—O(12)	173.4 (6)
C(12)—Mo(1)—C(13)	90.7 (2)	Mo(1)—C(13)—O(13)	178.2 (5)
C(12)—Mo(1)—C(14)	86.6 (2)	Mo(1)—C(14)—O(14)	175.5 (7)
C(13)—Mo(1)—C(14)	91.2 (2)	S—C(15)—N	111.8 (3)
S—Mo(2)—C(21)	89.0 (1)	S—C(15)—C(16)	126.9 (4)
S—Mo(2)—C(22)	89.2 (2)	N—C(15)—C(16)	121.4 (5)
S—Mo(2)—C(23)	90.9 (2)	C(15)—C(16)—C(17)	118.2 (5)
S—Mo(2)—C(24)	90.2 (1)	C(16)—C(17)—C(18)	120.4 (5)
S—Mo(2)—C(25)	178.4 (2)	C(17)—C(18)—C(19)	118.3 (5)
C(21)—Mo(2)—C(22)	178.0 (2)	N—C(19)—C(18)	122.5 (5)
C(21)—Mo(2)—C(23)	92.1 (3)	Mo(2)—C(21)—O(21)	179.1 (4)
C(21)—Mo(2)—C(24)	90.2 (2)	Mo(2)—C(22)—O(22)	177.1 (6)
C(21)—Mo(2)—C(25)	92.7 (2)	Mo(2)—C(23)—O(23)	173.1 (6)
C(22)—Mo(2)—C(23)	88.8 (2)	Mo(2)—C(24)—O(24)	176.9 (6)
C(22)—Mo(2)—C(24)	89.0 (3)	Mo(2)—C(25)—O(25)	178.9 (5)

The crystal was mounted on a glass fibre in a random orientation for preliminary examination. The structure was solved by direct methods. Three atoms (two Mo atoms and an S atom) were located from an *E* map and the remaining atoms were found in the succeeding difference Fourier syntheses. H atoms were located and were included in the structure-factor calculations, but their positions were not refined. The structure was refined using a full-matrix least-squares method in which the function minimized was $\Sigma w(|F_o| - |F_c|)^2$ and the weight *w* was defined as per Killean & Lawrence (1969) with terms of 0.010 and 1.0. Scattering factors were taken from Cromer & Waber (1974). Calculations were performed on a VAX computer using *SDP/VAX* (Frenz, 1978).

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Lists of structure factors, anisotropic displacement parameters, H-atom coordinates and bond distances and angles involving H atoms have been deposited with the IUCr (Reference: LI1070). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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A Pseudo-Octahedral Tungsten Oxo Compound, $[WO(C_{18}H_{12}O)(C_{13}H_{13}P)_3].C_7H_8$

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Abstract

The compound tris(diphenylmethylphosphine)oxo-[1,1′:3′,1″-terphenyl-2′-olato(2−)-C^2O]tungsten(IV) toluene solvate contains one cyclometallated 2′,6-di-

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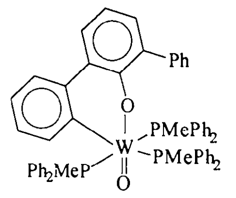
phenylphenoxide ligand. A pseudo-octahedral geometry exists for the WO_2CP_3 core with the terminal oxo and aryloxide O atoms mutually *trans*. W—O(terminal oxo group) = 1.717 (3), W—O(aryloxide) = 2.059 (3), W—C = 2.151 (5), W—P = 2.550 Å (average).

Comment

The 2,6-diphenylphenoxide ligand has been shown to undergo facile C—H bond activation at low-valent tungsten centers to form metallacyclic products (Kerschner, Fanwick & Rothwell, 1989*a*,*b*). Similar studies have been attempted recently using analogous tungsten–oxo complexes. We report here the isolation and structural characterization of a mononuclear compound of tungsten(IV), $[WO(C_{18}H_{12}O)(C_{13}H_{13}P)_3].C_7H_8$, (I), containing a terminal oxo group as well as a cyclometallated aryloxide ligand. A view of the molecule is shown in Fig. 1. The compound contains one toluene molecule per W atom in the unit cell. The central WO_2CP_3 core of the molecule can be seen to adopt a pseudo-octahedral geometry.



(I)

The W—O distance involving the terminal oxo group, 1.717 (3) Å, compares well with the values reported for mononuclear tungsten–oxo complexes (Nugent & Mayer, 1987). The complex contains two mutually *trans* P atoms with a P(1)—W—P(2) bond angle of 167.91 (5)°. The other P atom is located *trans* to the C atom of the metallacycle. The two O atoms are mutually *trans* with an O(1)—W—O(2) bond angle of 178.4 (2)°. Although the W—O(oxo) distance appears normal, the W—O(aryloxide) distance of 2.059 (3) Å is considerably longer than typical W—O distances for octahedral W^{IV} aryloxide compounds. This value can be compared to corresponding distances of 1.848 (5) and 1.840 (5) Å in $[W(OC_6H_4\text{-}4Me)_2Cl_2(PMePh_2)_2]$ (Atagi & Mayer, 1993), 1.966 (4) Å in $[W(OC_6H_3Ph_2\text{-}2,6)_2Cl_2(PMe_2Ph)_2]$ (Kerschner, Fanwick & Rothwell, 1989*a*) and 1.87 (1) and 1.88 (1) Å in $[W(OC_6H_3Ph\text{-}C_6H_4)_2(PMePh_2)_2]$ (Kerschner, Fanwick & Rothwell, 1989*b*). The long W—O(aryloxide) distance in the title compound almost certainly reflects the influence of the tungsten–oxo function located *trans* to this bond.

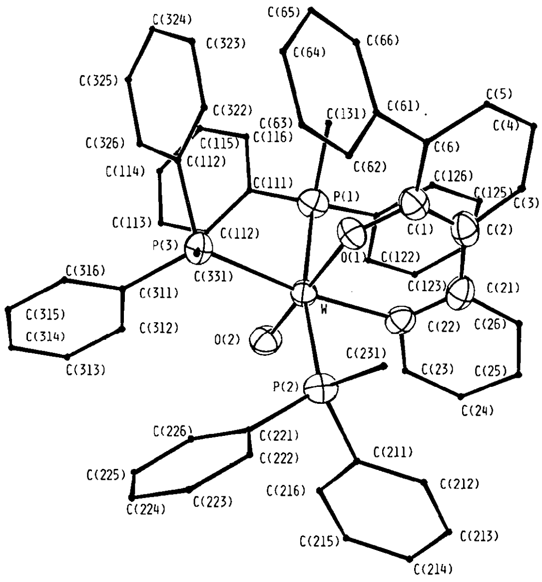


Fig. 1. A view of the molecule emphasizing the central coordination sphere. Displacement ellipsoids are drawn at the 50% probability level and H atoms have been omitted for clarity.

Experimental

The title compound was obtained in low yield during the room-temperature reduction of toluene solutions of $[W(OC_6H_3Ph_2\text{-}2,6)_3Cl(O)]$ with sodium amalgam and methyldiphenylphosphine. ^1H NMR (C_6D_6, 303 K): δ 0.92(*d*, $PMePh_2$), 1.30 (*d*, $PMePh_2$), 6.54 (*t*), 7.78 (*d*), 7.82 (*d*), 7.90 (*d*), 6.6–7.6 (*m*, aromatic). ^{31}P NMR (C_6D_6, 303 K): δ −2.10 [$2PMePh_2$, $J^1(^{183}W—^{31}P)$ = 163 Hz], −7.44 [$PMePh_2$, $J^1(^{183}W—^{31}P)$ = 111 Hz].

Crystal data

$[WO(C_{18}H_{12}O)(C_{13}H_{13}P)_3].$-
C_7H_8
$M_r = 1136.95$
Triclinic
$P\bar{1}$
$a = 14.701$ (1) Å
$b = 16.093$ (1) Å
$c = 11.9489$ (9) Å
$\alpha = 94.104$ (6)°
$\beta = 91.226$ (6)°
$\gamma = 75.561$ (6)°
$V = 2731.7$ (5) Å^3
$Z = 2$
$D_x = 1.382$ Mg m^{-3}

Mo $K\alpha$ radiation
$\lambda = 0.71073$ Å
Cell parameters from 25 reflections
$\theta = 18\text{–}20°$
$\mu = 2.287$ mm^{-1}
$T = 293$ K
Block
0.36 × 0.22 × 0.17 mm
Red

Data collection

Enraf–Nonius CAD-4 diffractometer
$\omega\text{–}2\theta$ scans
Absorption correction: empirical (*DIFABS*; Walker & Stuart, 1983)
$T_{min} = 0.51$, $T_{max} = 1.00$
7075 measured reflections
7075 independent reflections

5889 observed reflections [$F > 3\sigma(F)$]
$\theta_{max} = 45°$
$h = -12 \rightarrow 11$
$k = 0 \rightarrow 14$
$l = 0 \rightarrow 24$
3 standard reflections
frequency: 83.33 min
intensity variation: <5%

Refinement

Refinement on F
$R = 0.024$
$wR = 0.031$
$S = 1.821$
5889 reflections
596 parameters
H-atom parameters not refined

$w = 1/[\sigma^2(F) + (0.02F)^2 + 1 - F]$
$(\Delta/\sigma)_{\max} = 0.15$
$\Delta\rho_{\max} = 0.41$ e Å^{-3}
$\Delta\rho_{\min} = -0.39$ e Å^{-3}
Extinction correction: none
Atomic scattering factors from Cromer & Waber (1974)

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

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

	x	y	z	$B_{\rm eq}$
W	0.23017 (1)	0.23460 (1)	0.03716 (2)	2.549 (3)
P(1)	0.22146 (9)	0.34661 (8)	0.1994 (1)	3.24 (3)
P(2)	0.27587 (9)	0.11869 (8)	−0.1209 (1)	3.26 (3)
P(3)	0.09251 (8)	0.17752 (8)	0.1035 (1)	3.28 (3)
O(1)	0.3075 (2)	0.1442 (2)	0.1383 (2)	2.94 (6)
O(2)	0.1648 (2)	0.3078 (2)	−0.0494 (3)	3.57 (7)
C(1)	0.3909 (3)	0.1356 (3)	0.1916 (4)	3.1 (1)
C(2)	0.4582 (3)	0.1771 (3)	0.1563 (4)	3.4 (1)
C(3)	0.5351 (3)	0.1797 (3)	0.2288 (5)	4.3 (1)
C(4)	0.5491 (3)	0.1372 (3)	0.3261 (4)	4.4 (1)
C(5)	0.4888 (4)	0.0883 (3)	0.3521 (4)	4.2 (1)
C(6)	0.4096 (3)	0.0855 (3)	0.2864 (4)	3.5 (1)
C(21)	0.4508 (3)	0.2209 (3)	0.0499 (4)	3.4 (1)
C(22)	0.3641 (3)	0.2565 (3)	−0.0016 (4)	3.0 (1)
C(23)	0.3680 (3)	0.3096 (3)	−0.0916 (4)	4.0 (1)
C(24)	0.4495 (4)	0.3202 (3)	−0.1334 (5)	4.7 (1)
C(25)	0.5348 (4)	0.2775 (4)	−0.0876 (5)	5.5 (1)
C(26)	0.5352 (3)	0.2293 (3)	0.0022 (5)	4.6 (1)
C(61)	0.3494 (3)	0.0314 (3)	0.3213 (4)	3.9 (1)
C(62)	0.3250 (4)	−0.0304 (3)	0.2477 (5)	4.7 (1)
C(63)	0.2736 (5)	−0.0853 (4)	0.2840 (6)	6.5 (2)
C(64)	0.2460 (5)	−0.0784 (4)	0.3941 (6)	7.3 (2)
C(65)	0.2694 (4)	−0.0171 (4)	0.4689 (5)	6.3 (2)
C(66)	0.3198 (4)	0.0369 (4)	0.4333 (4)	5.1 (1)
C(111)	0.1120 (3)	0.4292 (3)	0.2237 (4)	4.0 (1)
C(112)	0.0442 (4)	0.4457 (4)	0.1432 (5)	5.2 (1)
C(113)	−0.0390 (5)	0.5093 (4)	0.1604 (6)	6.8 (2)
C(114)	−0.0547 (5)	0.5562 (5)	0.2607 (7)	8.0 (2)
C(115)	0.0104 (6)	0.5395 (5)	0.3433 (7)	9.9 (2)
C(116)	0.0948 (5)	0.4774 (5)	0.3248 (6)	8.3 (2)
C(121)	0.3055 (4)	0.4117 (3)	0.1870 (5)	4.6 (1)
C(122)	0.2883 (5)	0.4721 (4)	0.1076 (6)	6.9 (2)
C(123)	0.3550 (6)	0.5169 (4)	0.0866 (8)	9.7 (2)
C(124)	0.4383 (5)	0.4991 (5)	0.1453 (9)	11.4 (3)
C(125)	0.4574 (5)	0.4386 (5)	0.224 (1)	11.6 (3)
C(126)	0.3893 (4)	0.3950 (4)	0.2454 (7)	7.8 (2)
C(131)	0.2468 (4)	0.3031 (3)	0.3356 (4)	5.1 (1)
C(211)	0.3226 (3)	0.1581 (3)	−0.2412 (4)	3.3 (1)
C(212)	0.4173 (4)	0.1330 (3)	−0.2691 (4)	4.3 (1)
C(213)	0.4509 (4)	0.1701 (4)	−0.3553 (5)	5.0 (1)
C(214)	0.3916 (4)	0.2318 (4)	−0.4136 (5)	5.3 (1)
C(215)	0.2970 (4)	0.2570 (4)	−0.3868 (4)	5.2 (1)
C(216)	0.2631 (4)	0.2204 (3)	−0.3017 (4)	4.4 (1)
C(221)	0.1894 (4)	0.0678 (3)	−0.1904 (4)	4.3 (1)
C(222)	0.2084 (4)	−0.0200 (4)	−0.2222 (5)	6.0 (1)
C(223)	0.1382 (5)	−0.0513 (4)	−0.2789 (6)	9.0 (2)
C(224)	0.0532 (5)	0.0003 (5)	−0.3016 (6)	9.7 (2)
C(225)	0.0342 (4)	0.0857 (5)	−0.2703 (5)	7.8 (2)
C(226)	0.1016 (4)	0.1204 (4)	−0.2143 (5)	5.8 (1)
C(231)	0.3700 (4)	0.0306 (3)	−0.0769 (5)	4.9 (1)
C(311)	−0.0194 (3)	0.2124 (3)	0.0294 (4)	4.0 (1)
C(312)	−0.0365 (4)	0.2797 (4)	−0.0399 (6)	5.6 (1)
C(313)	−0.1221 (5)	0.3053 (5)	−0.0962 (7)	7.9 (2)
C(314)	−0.1896 (5)	0.2613 (5)	−0.0825 (8)	8.7 (2)
C(315)	−0.1739 (4)	0.1938 (5)	−0.0156 (7)	7.8 (2)
C(316)	−0.0892 (4)	0.1687 (4)	0.0397 (5)	5.9 (2)
C(321)	0.0551 (3)	0.2018 (3)	0.2499 (4)	3.6 (1)
C(322)	0.1007 (4)	0.1512 (4)	0.3332 (5)	4.8 (1)
C(323)	0.0769 (5)	0.1713 (4)	0.4451 (5)	6.0 (2)
C(324)	0.0054 (5)	0.2427 (4)	0.4741 (5)	6.7 (2)
C(325)	−0.0404 (5)	0.2948 (5)	0.3932 (6)	7.0 (2)
C(326)	−0.0162 (4)	0.2744 (4)	0.2818 (5)	5.3 (1)
C(331)	0.1162 (4)	0.0601 (3)	0.0902 (5)	4.4 (1)
C(5001)	0.677 (1)	0.378 (1)	0.470 (1)	19.8 (6)
C(5002)	0.675 (1)	0.4673 (9)	0.456 (1)	16.9 (5)
C(5003)	0.694 (1)	0.4910 (9)	0.355 (1)	15.5 (4)
C(5004)	0.722 (1)	0.4375 (9)	0.255 (1)	15.5 (4)
C(5005)	0.7224 (9)	0.3531 (8)	0.275 (1)	15.0 (4)
C(5006)	0.7009 (9)	0.3224 (8)	0.371 (1)	14.0 (4)
C(5007)	0.654 (2)	0.340 (1)	0.564 (2)	27.3 (9)

Table 2. *Selected geometric parameters* (Å, °)

W—P(1)	2.534 (1)	W—O(1)	2.059 (3)
W—P(2)	2.534 (1)	W—O(2)	1.717 (3)
W—P(3)	2.583 (1)	W—C(22)	2.151 (5)
P(1)—W—P(2)	167.91 (5)	P(2)—W—C(22)	82.0 (1)
P(1)—W—P(3)	95.51 (5)	P(3)—W—O(1)	82.9 (1)
P(1)—W—O(1)	88.5 (1)	P(3)—W—O(2)	96.4 (1)
P(1)—W—O(2)	92.9 (1)	P(3)—W—C(22)	166.9 (1)
P(1)—W—C(22)	87.0 (1)	O(1)—W—O(2)	178.4 (2)
P(2)—W—P(3)	94.10 (5)	O(1)—W—C(22)	84.3 (2)
P(2)—W—O(1)	85.4 (1)	O(2)—W—C(22)	96.4 (2)
P(2)—W—O(2)	93.3 (1)	W—O(1)—C(1)	133.4 (3)

The structure was solved using the Patterson heavy-atom method which revealed the position of the W atom. The remaining atoms were located using *DIRDIF* (Beurskens, 1984) and in succeeding difference Fourier syntheses. Positions for H atoms were calculated assuming idealized geometry and a bond distance of 0.95 Å. For methyl groups, one H atom was located in a difference Fourier map, its position was idealized and the remaining positions calculated. The structure was refined using full-matrix least-squares techniques where the function minimized was $\Sigma w(|F_o| - |F_c|)^2$ and the weight w was defined by the Killean & Lawrence (1969) method with terms of 0.020 and 1.0. Corrections for anomalous scattering were applied to all atoms which were refined anisotropically (Cromer, 1974). Anomalous-dispersion effects were included in F_c (Ibers & Hamilton, 1964); the values f' and f'' were those of Cromer (1974). Plots of $\Sigma w(|F_o| - |F_c|)^2$ *versus* $|F_o|$, reflection order in data collection, $\sin\theta/\lambda$, and various classes of indices showed no unusual trends. All calculations were performed on a VAX computer using *SDP* (Frenz, 1978).

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Lists of structure factors, anisotropic displacement parameters, H-atom coordinates and complete geometry have been deposited with the IUCr (Reference: ST1067). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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Tris(4,6-dimethylpyrimidine-2-thiolato-*N*,*S*)cobalt(III) Monohydrate: a Complex with Three Stable Four-Membered *N*,*S*-Chelate Rings

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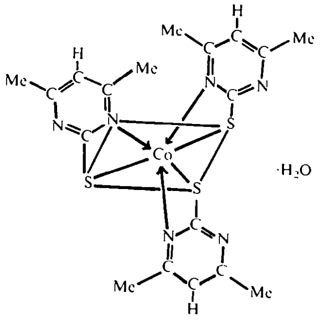
Abstract

In the title compound, [Co($C_6H_7N_2S$)$_3$].H_2O, the Co^{III} ion is surrounded by three thiolate S atoms [Co—S 2.247 (2), 2.260 (2), 2.271 (2) Å] and three azomethine N atoms [Co—N 1.976 (4), 1.956 (5), 1.991 (5) Å] which define a *fac*-octahedral geometry that is highly distorted owing to the presence of three four-membered *N*,*S*-chelate rings. All three bidentate ligands are planar to within ±0.06 Å and display bond lengths and angles very close to expected values. Intermolecular hydrogen bonding between the water O atom and an uncoordinated pyrimidine N atom stabilizes the molecular packing.

Comment

4,6-Dimethylpyrimidine-2-thiol (4,6Me_2Pm2SH) and its derivatives possess antibacterial and antiviral properties (Coutts & Casy, 1975). Its IR spectrum as a ligand in the title complex (I) exhibits no N-H stretch in the 3500–3200 cm^{-1} region. A single crystal X-ray diffraction study was undertaken in order to characterize the compound fully and to compare its structural features with those of the acetone solvate of the same complex (Cartwright, Goodgame, Jeeves, Langguth & Skapski, 1977; Cartwright, Langguth & Skapski, 1979) and to study the bonding within the molecule.



(I)

Fig. 1 shows an *ORTEP*II (Johnson, 1976) view of the molecule with atomic numbering scheme. The structure consists of discrete [Co($C_6H_7N_2S$)$_3$] molecules with approximate C_3 point symmety, together with one strongly bound water molecule of crystallization per complex. The three bidentate 4,6Me_2Pm2SH ligands are planar to within ±0.06 Å and are chemically identical though crystallographically distinct. They are mutually perpendicular [88.2 (1), 94.2 (1) and 99.5 (1)°] to each other. The Co^{III} ion lies nearly in the plane of each ligand with deviations of 0.014 (1), −0.065 (1) and −0.242 (1) Å

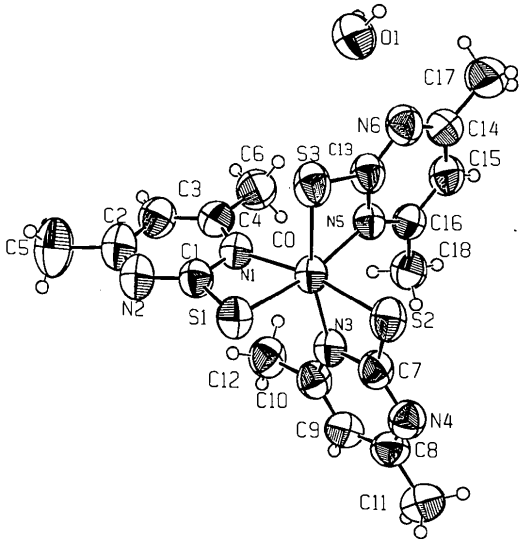


Fig. 1. *ORTEP* (Johnson, 1976) drawing of Co(4,6Me_2Pm2S)$_3$.-H_2O showing the atom-numbering scheme. For non-H atoms, 50% probability ellipsoids are shown; H atoms are represented by spheres of a arbitrary size.

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