

The molecules of PIVHA are packed in the crystal as rows of hydrogen-bonded tetramers. The dimensions of the hydrogen bonds are given in Table 2 and illustrated in Fig. 2, in which the H atoms of the *tert*-butyl groups are omitted for clarity.

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Bis(η^5 -cyclopentadienyl)bis(dicarbonylcobaltio)tritelluridimolybdenum

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Abstract. $[(\eta^5\text{-C}_5\text{H}_5)_2\text{Mo}_2(\mu_4\text{-Te})(\mu_3\text{-Te})_2\text{Co}_2(\text{CO})_4]$, $\text{C}_{14}\text{H}_{10}\text{Co}_2\text{Mo}_2\text{O}_4\text{Te}_3$, $M_r = 934.8$, triclinic, $P\bar{1}$, $a = 7.744$ (3), $b = 10.269$ (5), $c = 13.373$ (5) Å, $\alpha = 86.07$ (4), $\beta = 96.69$ (3), $\gamma = 108.35$ (3)°, $V = 1002.0$ (7) Å³, $Z = 2$, $D_x = 3.098$ g cm⁻³, Mo $K\alpha$, $\lambda = 0.71073$ Å, $\mu = 72.7$ cm⁻¹, $F(000) = 840$, 295 K, $R = 4.03\%$ for 2688 reflections with $F_o \geq 3\sigma(F_o)$ and 181 parameters. The compound is structurally similar to its sulfur analogue. The two cyclopentadienyl rings are nearly parallel and perpendicular to the Mo-Mo vector, 2.754 (1) Å. Nearly parallel to the cyclopentadienyl rings is a plane bisecting the Mo-Mo

vector containing the pentagonally arranged units, $\mu_3\text{-Te}$, $\mu_4\text{-Co}(\text{CO})_2$, $\mu_4\text{-Te}$, $\mu_4\text{-Co}(\text{CO})_2$, $\mu_3\text{-Te}$; there is no $(\mu_3\text{-Te})\text{-(}\mu_3\text{-Te)}$ ring closure [Te...Te 3.605 (1) Å].

Experimental. Black brick-shaped crystals (0.17 × 0.22 × 0.26 mm) obtained from the reaction of $\text{Co}_4\text{Te}_2(\text{CO})_{11}$ and $(\eta^5\text{-C}_5\text{H}_5)_2\text{Mo}_2(\text{CO})_6$ (Bogan, 1986). Nicolet *R3m/μ*, ω scans; lattice parameters from 25 reflections, $21 \leq 2\theta \leq 28^\circ$, least-squares fit; empirical ellipsoidal absorption correction, seven reflections, 10° increments, $T_{\max}/T_{\min} = 0.502/0.252$; 2θ max. = 48° ($h = \pm 9$, $k = \pm 12$, $l = +16$); standard reflections $\bar{4}15$,

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Table 1. Atom coordinates ($\times 10^4$) and thermal parameters ($\text{\AA}^2 \times 10^3$)

	x	y	z	U
Te(1)	4796 (1)	2048 (1)	1622 (1)	38 (1)*
Te(2)	8246 (1)	1729 (1)	4181 (1)	41 (1)*
Te(3)	10437 (1)	3723 (1)	2094 (1)	44 (1)*
Mo(1)	7846 (1)	1303 (1)	2224 (1)	32 (1)*
Mo(2)	7438 (1)	3638 (1)	2924 (1)	33 (1)*
Co(1)	5091 (2)	1106 (1)	3380 (1)	37 (1)*
Co(2)	7673 (2)	3431 (2)	922 (1)	47 (1)*
C(1)	3794 (15)	1632 (11)	4182 (9)	48 (4)*
C(2)	4124 (18)	-710 (13)	3407 (8)	54 (5)*
C(3)	7459 (19)	5002 (17)	519 (11)	80 (7)*
C(4)	8006 (17)	2797 (14)	-184 (9)	59 (5)*
C(11)	8198 (20)	6065 (11)	2817 (11)	55 (4)
C(12)	6266 (20)	5515 (11)	2651 (11)	44 (3)
C(13)	5619 (20)	4793 (11)	3545 (11)	49 (4)
C(14)	7153 (20)	4896 (11)	4265 (11)	53 (4)
C(15)	8747 (20)	5682 (11)	3815 (11)	54 (4)
C(16)†	8124 (59)	5304 (36)	4187 (20)	6 (7)
C(17)†	6189 (59)	4771 (36)	4026 (20)	171 (50)
C(18)†	5645 (59)	5103 (36)	3015 (20)	53 (15)
C(19)†	7244 (59)	5842 (36)	2552 (20)	36 (11)
C(20)†	8776 (59)	5966 (36)	3276 (20)	24 (9)
C(21)	6580 (10)	-1000 (11)	1753 (11)	45 (3)
C(22)	7473 (10)	-241 (11)	931 (11)	51 (4)
C(23)	9366 (10)	297 (11)	1253 (11)	53 (4)
C(24)	9643 (10)	-130 (11)	2276 (11)	53 (4)
C(25)	7921 (10)	-931 (11)	2585 (11)	52 (4)
C(26)†	6734 (34)	-767 (31)	1316 (21)	11 (7)
C(27)†	8456 (34)	79 (31)	1036 (21)	124 (35)
C(28)†	9784 (34)	109 (31)	1869 (21)	16 (8)
C(29)†	8882 (34)	-718 (31)	2664 (21)	58 (16)
C(30)†	6997 (34)	-1260 (31)	2323 (21)	73 (19)
O(1)	3019 (13)	1957 (11)	4743 (7)	76 (5)*
O(2)	3453 (15)	-1866 (9)	3426 (7)	77 (4)*
O(3)	7332 (17)	6068 (12)	261 (8)	101 (6)*
O(4)	8211 (16)	2379 (13)	-935 (7)	96 (5)*

* Equivalent isotropic U defined as one third of the trace of the orthogonalized U_{ij} tensor.

† Atoms have a refined occupancy of 0.20.

Table 2. Bond lengths (\AA) and angles ($^\circ$)

Mo(1)—Mo(2)	2.754 (1)	Mo(2)—Te(3)	2.664 (1)
CNT(1)—Mo(1)*	2.00 (1)	Mo(1)—Co(1)	2.727 (2)
CNT(2)—Mo(2)	2.03 (1)	Mo(1)—Co(2)	2.726 (2)
Mo(1)—C(21)†	2.36 (1)	Mo(2)—Co(1)	2.739 (1)
Mo(1)—C(22)	2.36 (1)	Mo(2)—Co(2)	2.733 (2)
Mo(1)—C(23)	2.33 (1)	Te(2)—Co(1)	2.454 (2)
Mo(1)—C(24)	2.32 (1)	Te(1)—Co(1)	2.493 (1)
Mo(1)—C(25)	2.33 (1)	Te(1)—Co(2)	2.484 (2)
Mo(2)—C(11)	2.37 (1)	Te(3)—Co(2)	2.451 (2)
Mo(2)—C(12)	2.37 (1)	Co(1)—C(1)	1.77 (1)
Mo(2)—C(13)	2.35 (1)	Co(1)—C(2)	1.78 (1)
Mo(2)—C(14)	2.35 (1)	Co(2)—C(1)	1.72 (1)
Mo(2)—C(15)	2.36 (1)	Co(2)—C(4)	1.73 (1)
Mo(1)—Te(1)	2.724 (1)	C(1)—O(1)	1.14 (2)
Mo(1)—Te(2)	2.649 (1)	C(2)—O(2)	1.14 (2)
Mo(1)—Te(3)	2.668 (1)	C(3)—O(3)	1.16 (2)
Mo(2)—Te(1)	2.710 (1)	C(4)—O(4)	1.17 (2)
Mo(2)—Te(2)	2.671 (1)	Te(2)...Te(3)	3.605 (1)
Mo(1)—Te(1)—Mo(2)	60.9 (1)	C(1)—Co(1)—C(2)	103.2 (6)
Co(1)—Te(1)—Co(2)	116.7 (1)	Te(1)—Co(2)—C(3)	108.2 (5)
Mo(1)—Te(2)—Mo(2)	62.3 (1)	Te(3)—Co(2)—C(3)	110.3 (4)
Mo(1)—Te(3)—Mo(2)	62.2 (1)	Mo(1)—Co(2)—C(3)	158.3 (5)
Te(1)—Co(1)—Te(2)	114.0 (1)	Mo(2)—Co(2)—C(3)	97.7 (5)
Te(1)—Co(2)—Te(3)	114.4 (1)	Te(1)—Co(2)—C(4)	113.1 (4)
Mo(1)—Co(1)—Mo(2)	60.5 (1)	Te(3)—Co(2)—C(4)	108.2 (4)
Mo(1)—Co(2)—Mo(2)	60.6 (1)	Mo(1)—Co(2)—C(4)	99.8 (5)
Te(1)—Co(1)—C(1)	112.5 (4)	Mo(2)—Co(2)—C(4)	160.1 (5)
Te(2)—Co(1)—C(1)	107.0 (4)	C(3)—Co(2)—C(4)	101.9 (7)
Mo(1)—Co(1)—C(1)	158.4 (3)	Co(1)—C(1)—O(1)	176 (1)
Mo(2)—Co(1)—C(1)	98.2 (3)	Co(1)—C(2)—O(2)	178 (1)
Te(1)—Co(1)—C(2)	110.1 (4)	Co(2)—C(3)—O(3)	179 (1)
Te(2)—Co(1)—C(2)	109.4 (4)	Co(2)—C(4)—O(4)	179 (1)
Mo(1)—Co(1)—C(2)	98.0 (5)	Mo(2)—Mo(1)—CNT(1)	178.0 (5)
Mo(2)—Co(1)—C(2)	158.5 (5)	Mo(1)—Mo(2)—CNT(2)	178.4 (5)

* CNT(1) = centroid C(21) to C(25); CNT(2) = centroid C(11) to C(15).

† Mo—C distances for major η^5 -C₅H₅ ring orientation only.

$\bar{2}62$, $\bar{1}18$, 5% linear decay (corrected); 3290 reflections collected, 3137 unique, $R_{\text{int}} = 2.6\%$, 449 unobserved, 2688 with $F_o \geq 3\sigma(F_o)$. Auto-interpreted Patterson solution; refinement on F for 181 parameters. Both (η^5 -C₅H₅) rings rotationally disordered in two sites [refined occupancies = 0.80 (2) and 0.20 (2), both sites], rings constrained to rigid planar pentagons [$d(\text{C—C}) = 1.42 \text{\AA}$], all non-H atoms except for the ring C atoms anisotropic, ring C atoms isotropic, no H-atom contributions; $R_F = 4.03$, $wR_F = 4.80\%$, $S = 1.619$, $w^{-1} = \sigma^2(F_o) + gF_o^2$, $g = 0.0008$, $(\Delta/\sigma)_{\text{max.}} = 0.072$, $(\Delta\rho)_{\text{max.}} = 1.25 \text{ e \AA}^{-3}$, $(\Delta\rho)_{\text{min.}} = -0.98 \text{ e \AA}^{-3}$, atomic scattering factors from *International Tables for X-ray Crystallography* (1974). Computer programs: Sheldrick (1984).* Table 1 lists final atomic coordinates and Table 2 bond lengths and angles. Fig. 1 shows the molecular structure of the complex and Fig. 2 the central region.

Related literature. Curtis & Williams (1983) have reported the structure of the sulfur analogue with a considerably shorter Mo—Mo bond, 2.646 (1) \AA . The [Co(CO)₂]₂E₃ central plane ($E = \text{S or Te}$) contributes one fewer electron to cluster construction than would the five As atoms in the structurally related complex (C₅H₅)Mo(η^5 -As₅)Mo(C₅H₅), which contains a closed As₅ ring and an Mo—Mo distance of 2.764 (2) \AA (Rheingold, Foley & Sullivan, 1982). Also related to this series of compounds is (C₅H₅)₂Mo₂(μ , η^1 -AsS)-[S₂Co(CO)₂] (Brunner, Kavermann, Klement, Wachter, Zahn & Ziegler, 1985).

Crystals of the title compound were the gift of Dr Thomas B. Rauchfuss, University of Illinois.

* Lists of structure factors, anisotropic thermal parameters and a full list of bond angles have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 43404 (20 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

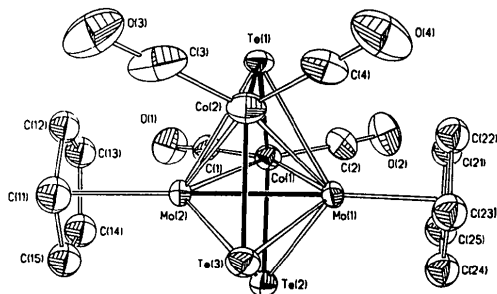


Fig. 1. Molecular structure and labeling scheme for $[(\eta^5\text{-C}_5\text{H}_5)_2\text{-Mo}_2(\mu_4\text{-Te})(\mu_3\text{-Te})_2\text{Co}_2(\text{CO})_4]$.

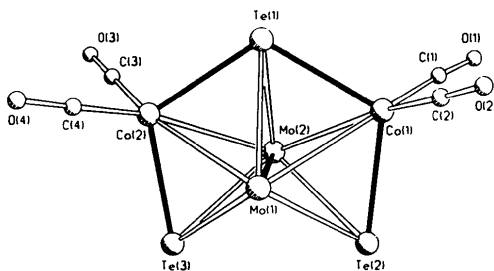


Fig. 2. The central region of $[(\eta^5\text{-C}_5\text{H}_5)_2\text{Mo}_2(\mu_4\text{-Te})(\mu_3\text{-Te})_2\text{Co}_2(\text{CO})_2]$ viewed along the Mo—Mo vector; the Cp rings are deleted to enhance clarity.

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A Dinuclear Gold(II) Ylide Complex Possessing Chloride Ligands and Bridging Methylenethiophosphinate Groups

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Abstract. (Dichloro)bis(μ -methylenediphenylthiophosphinato-*C,S*)digold(II)-dichloromethane (1/1), $[\text{Au}_2\{\text{CH}_2\text{P}(\text{S})(\text{C}_6\text{H}_5)_2\}_2\text{Cl}_2]\cdot\text{CH}_2\text{Cl}_2$, $M_r = 1012.3$, triclinic, $P\bar{1}$, $a = 9.477(2)$, $b = 12.477(3)$, $c = 14.170(3)$ Å, $\alpha = 105.55(2)$, $\beta = 100.01(1)$, $\gamma = 101.39(2)^\circ$, $V = 1536.0(5)$ Å³, $Z = 2$, $D_x = 2.189$ Mg m⁻³, $\lambda(\text{Mo } K\alpha) = 0.71073$ Å, $\mu = 10.38$ mm⁻¹, $F(000) = 952$, $T = 298$ K. The crystal structure of a dinuclear gold(II) methylenethiophosphinate ylide complex containing chloride ligands is reported. The structure consists of an eight-membered heterocyclic ring system that contains Au, S, P and C nuclei in a chair conformation. The Au atoms have square-planar coordination geometries and each form bonds to a second Au center, one Cl⁻ ligand, an S atom from one of the bridging ylide ligands and a methylene C from the other. A metal–metal bond is present and the two Au centers are separated by a distance of 2.553(1) Å. The asymmetric unit of this structure consists of one complete dimer and a molecule of dichloromethane. Final conventional R values of $R = 0.0409$ and $wR = 0.0431$ were obtained using 286 variable parameters and 2857 reflections with $F_o^2 > 3\sigma(F_o^2)$.

Experimental. Orange rectangularly shaped plate of approximate dimensions 0.50 × 0.20 × 0.10 mm obtained following recrystallization of the dinuclear

gold(II) benzoate complex, $[\text{Au}_2\{\text{CH}_2\text{P}(\text{S})(\text{C}_6\text{H}_5)_2(\text{C}_6\text{H}_5\text{CO}_2)\}_2]$, from a dichloromethane/diethyl ether solution. Presumably halogen for benzoate exchange gave the product, but in low yield. Triclinic symmetry suggested on the basis of interaxial angles and confirmed by a Delaunay reduction. Refined cell parameters obtained from the setting angles of 25 reflections with $25 < 2\theta < 30^\circ$. Intensity data collected at room temperature (no symmetry-equivalent reflections were collected) using the ω -scanning technique in bisecting geometry (Nicolet *R3m/E* diffractometer, graphite-monochromated Mo $K\alpha$ radiation). A total of 4027 unique reflections were measured with $0 < 2\theta < 45^\circ$ ($h < 9$, $|k| < 3$, $|l| < 15$). Three standard reflections ($\bar{1}\bar{1}0$, $\bar{1}\bar{1}1$, $\bar{2}0\bar{2}$) measured every 100 data. Scan rate variable, 2–30°; scan range, -1.0° in ω from $K\alpha_1$ to $+1.0^\circ$ from $K\alpha_2$. The data were corrected for standard variation (<0.1%), absorption, Lorentz and polarization effects. Corrections for absorption applied empirically on the basis of azimuthal scans of eight medium intensity reflections spanning a range of 2θ values. Minimum and maximum transmission 0.167 and 0.268. Background intensities estimated from a 96-step peak profile. Structure solution and refinement carried out using the *SHELXTL* collection of crystallographic software (Sheldrick, 1981). Au positions determined from a sharpened Patterson map; remaining atoms from difference Fourier maps. All non-hydrogen atoms refined anisotropically. Phenyl rings refined as idealized polygons ($\text{C}-\text{C} = 1.395$ Å, $\text{C}-\text{C}-\text{C} = 120^\circ$)

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