[Re$_2$(CO)$_8$(μ-I)$_2$(μ_4-In)][Re$_2$(CO)$_6$(μ-I)] (Haupt & Flörke, 1989) and [Re$_2$(CO)$_4\mu$-I)$_2$(PPh$_3$)$_2$][μ-Ga{Re(CO)$_4$PPh$_3$}] (Ph = phenyl) (Flörke, Balsaa & Haupt, 1986).

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Structure of 3,4-Bis(1,2-ethanedithiolato)-1,2-bis(triphenylphosphine)-1,2,3;1,3,4;1,2,4;2,3,4-tetra-μ_3-sulfido-dicopperditungsten(4 Cu–W, 1 W–W)

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Abstract. [Cu$_2$W$_2$(C$_{18}$H$_{15}$P)$_2$(C$_2$H$_4$S$_2$)$_2$S$_4$], M_r = 1331·96, orthorhombic, $P2_12_12_1$, a = 12·362 (9), b = 31·57 (1), c = 11·682 (8) Å, V = 4559 (4) Å^3, Z = 4, D_x = 1·94 g cm^{-3}, λ(Mo $K\alpha$) = 0·710690 Å, μ = 65·13 cm^{-1}, $F(000)$ = 2568, T = 296 K, R = 0·039 for 3977 unique reflections with $I \geq 3\sigma(I)$. The molecule contains a cubane-like cluster core (W$_2$Cu$_2$S$_4$)$^{4+}$ which has approximate C_{2v} symmetry [W(1)—W(2) 2·851 (1) Å, mean W—Cu 2·823 (2) Å]. Each W atom has a tetragonal-pyramidal coordination formed by three bridging sulfido ligands [one W—S 2·202 (4) Å, other two average 2·345 (4) Å] and one bidentate 1,2-ethanedithiolato ligand [mean W—S 2·346 (4) Å]; a PPh$_3$ ligand and three sulfido ligands complete the coordination of each Cu atom [Cu—S 2·284 (4), 2·383 (4) and 2·426 (4) Å]. The bond lengths and bond angles of the W$_2$S$_4$(SCH$_2$CH$_2$S)$_2$ moiety are almost the same as in the isolated starting material, except that the W=S double bonds elongate slightly from 2·143 (2) and 2·156 (2) Å to 2·201 (4) and 2·202 (4) Å.

Experimental. The synthetic procedure is described by Zhu, Zheng & Wu (1990). A dark orange crystal measuring 0·40 × 0·60 × 0·90 mm was mounted in a random orientation on a glass fiber. Data were collected using a Rigaku AFC5R diffractometer (CONTROL software; Molecular Structure Corporation, 1986) using Mo $K\alpha$ radiation at ca 296 K. Cell constants were obtained by least-squares analysis of

20 diffraction maxima (20 < 2θ < 26°), $\omega/2\theta$ scan, scan speed varied between 2, 4 and 8° min^{-1} (in ω) with scan width (0·798 + 0·35 tanθ)°, 2θ ≤ 50° (0 ≤ h ≤ 15, 0 ≤ k ≤ 38, 0 ≤ l ≤ 14). 4525 unique reflections were collected. Three standard reflections, remeasured periodically, showed only random variations in intensity. Intensity was defined as $C - \frac{1}{2}(t_c/t_b)(b_1 + b_2)$, where C is the total number of counts, t_c is the time spent counting peak intensity, t_b is the time spent counting one side of the background, b_1 represents the high-angle background counts and b_2 represents the low-angle background counts; $\sigma(I) = [C + \frac{1}{4}(t_c/t_b)^2(b_1 + b_2) + pI)^2]^{1/2}$, where I is the intensity and p was taken to be 0·05. An empirical absorption correction, based on azimuthal scans of three reflections, was applied (transmission factor ranges from 0·6540 to 1·000). A decay correction was not applied. The data were corrected for Lorentz and polarization factors. 3977 reflections with $I \geq 3\sigma(I)$ were considered observed, and were all used in the refinement.

The structure was solved by direct methods using MITHRIL (Gilmore, 1983); the W atoms were located in the E map. The Cu atoms and most non-H atoms were located using DIRDIF (Beurskens, 1984); the remaining non-H atoms were located in the succeeding difference Fourier syntheses (H atoms were placed in geometrically calculated positions with C—H = 0·95 Å, but not included in the refinement). The structure was refined by full-matrix least squares on F with anisotropic thermal parameters for W, Cu, S, P, and the four C atoms of the 1,2-ethanedithiolato ligands, and isotropic ther-

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Table 1. Atomic coordinates and equivalent isotropic thermal parameters

$$B_{eq} = \tfrac{4}{3}\Sigma_i\Sigma_j\beta_{ij}\mathbf{a}_i\cdot\mathbf{a}_j.$$

	x	y	z	$B_{eq}(\text{Å}^2)$
W(1)	0·14055 (4)	0·09449 (2)	0·63241 (5)	2·90 (2)
W(2)	−0·01163 (4)	0·16227 (2)	0·62404 (4)	2·68 (2)
Cu(1)	−0·0358 (1)	0·09808 (5)	0·7886 (1)	3·30 (1)
Cu(2)	0·1559 (2)	0·16090 (5)	0·7903 (1)	3·55 (7)
S(1)	0·1754 (3)	0·1657 (1)	0·5952 (3)	3·4 (1)
S(2)	−0·0462 (3)	0·0896 (1)	0·5959 (3)	3·4 (1)
S(3)	−0·0368 (3)	0·1733 (1)	0·8083 (3)	3·2 (1)
S(4)	0·1562 (2)	0·0862 (1)	0·8187 (3)	3·2 (1)
S(11)	0·3201 (1)	0·0904 (1)	0·5655 (4)	4·8 (2)
S(12)	0·1268 (4)	0·0285 (1)	0·5433 (5)	6·5 (3)
S(21)	0·0077 (4)	0·2296 (1)	0·5405 (4)	5·4 (2)
S(22)	−0·1795 (3)	0·1653 (1)	0·5316 (4)	4·7 (2)
P(1)	−0·1349 (3)	0·0576 (1)	0·9028 (3)	3·0 (1)
P(2)	0·2575 (3)	0·2022 (1)	0·8982 (3)	3·5 (2)
C(11)	0·344 (1)	0·0346 (6)	0·562 (2)	7 (1)
C(12)	0·261 (2)	0·0106 (6)	0·508 (3)	10 (2)
C(21)	−0·124 (2)	0·2459 (7)	0·507 (3)	11 (2)
C(22)	−0·196 (2)	0·2193 (6)	0·490 (3)	10 (2)
C(111)	−0·112 (1)	0·0012 (4)	0·881 (1)	3·3 (2)*
C(112)	−0·026 (1)	−0·0118 (5)	0·819 (1)	4·5 (3)*
C(113)	−0·000 (2)	−0·0551 (6)	0·802 (2)	6·2 (4)*
C(114)	−0·067 (2)	−0·0829 (6)	0·854 (2)	6·9 (5)*
C(115)	−0·152 (2)	−0·0724 (6)	0·909 (2)	6·5 (4)*
C(116)	−0·176 (2)	−0·0294 (6)	0·929 (2)	6·2 (4)*
C(121)	−0·282 (1)	0·0632 (4)	0·888 (1)	3·1 (2)*
C(122)	−0·317 (1)	0·0726 (5)	0·779 (1)	4·2 (3)*
C(123)	−0·432 (2)	0·0764 (6)	0·757 (2)	6·3 (4)*
C(124)	−0·497 (2)	0·0698 (6)	0·847 (2)	6·2 (4)*
C(125)	−0·461 (2)	0·0613 (5)	0·953 (2)	5·5 (4)*
C(126)	−0·352 (1)	0·0585 (5)	0·976 (1)	4·7 (3)*
C(131)	−0·110 (1)	0·0679 (4)	1·053 (1)	3·4 (3)*
C(132)	−0·087 (1)	0·0364 (5)	1·134 (2)	5·1 (3)*
C(133)	−0·059 (2)	0·0499 (6)	1·243 (2)	6·9 (5)*
C(134)	−0·061 (2)	0·0889 (6)	1·279 (2)	6·8 (5)*
C(135)	−0·091 (2)	0·1199 (6)	1·203 (2)	6·6 (5)*
C(136)	−0·112 (1)	0·1096 (5)	1·088 (1)	4·8 (3)*
C(211)	0·278 (1)	0·1841 (4)	1·045 (1)	4·1 (3)*
C(212)	0·207 (1)	0·1535 (5)	1·087 (2)	5·3 (4)*
C(213)	0·226 (2)	0·1403 (6)	1·203 (2)	6·6 (5)*
C(214)	0·297 (2)	0·1565 (7)	1·265 (2)	7·4 (5)*
C(215)	0·367 (2)	0·1875 (7)	1·227 (2)	8·8 (6)*
C(216)	0·358 (2)	0·2030 (6)	1·116 (2)	6·6 (4)*
C(221)	0·392 (1)	0·2116 (5)	0·837 (1)	4·4 (3)*
C(222)	0·446 (2)	0·2499 (5)	0·843 (2)	5·7 (4)*
C(223)	0·544 (2)	0·2559 (6)	0·787 (2)	7·0 (5)*
C(224)	0·581 (2)	0·2240 (8)	0·723 (2)	9·3 (7)*
C(225)	0·536 (2)	0·1857 (7)	0·716 (2)	7·3 (5)*
C(226)	0·437 (1)	0·1796 (5)	0·769 (2)	5·3 (4)*
C(231)	0·203 (1)	0·2557 (5)	0·903 (1)	4·6 (3)*
C(232)	0·197 (1)	0·2799 (5)	1·002 (2)	5·1 (4)*
C(233)	0·159 (2)	0·3219 (6)	0·991 (2)	7·0 (5)*
C(234)	0·135 (2)	0·3373 (7)	0·891 (2)	7·5 (5)*
C(235)	0·139 (2)	0·3133 (7)	0·790 (2)	7·5 (5)*
C(236)	0·170 (1)	0·2715 (5)	0·804 (2)	5·3 (4)*

* Atoms refined isotropically.

Table 2. Selected bond lengths (Å) and bond angles (°)

W(1)—W(2)	2·851 (1)		Cu(2)—S(1)	2·297 (4)
W(1)—Cu(1)	2·845 (1)		Cu(2)—S(4)	2·380 (4)
W(1)—Cu(2)	2·799 (2)		Cu(2)—S(3)	2·423 (5)
W(2)—Cu(1)	2·809 (2)		Cu(1)—P(1)	2·217 (4)
W(2)—Cu(2)	2·840 (2)		Cu(2)—P(2)	2·206 (4)
W(1)—S(1)	2·331 (4)		S(11)—C(11)	1·79 (2)
W(1)—S(2)	2·353 (4)		S(12)—C(12)	1·80 (2)
W(1)—S(4)	2·201 (4)		S(21)—C(21)	1·75 (2)
W(1)—S(11)	2·356 (4)		S(22)—C(22)	1·79 (2)
W(1)—S(12)	2·336 (4)		P(1)—C(131)	1·81 (1)
W(2)—S(1)	2·339 (4)		P(1)—C(111)	1·82 (1)
W(2)—S(2)	2·355 (4)		P(1)—C(121)	1·83 (1)
W(2)—S(3)	2·202 (4)		P(2)—C(231)	1·82 (2)
W(2)—S(21)	2·351 (4)		P(2)—C(211)	1·82 (2)
W(2)—S(22)	2·342 (4)		P(2)—C(221)	1·83 (2)
Cu(1)—S(2)	2·271 (4)		C(11)—C(12)	1·43 (3)
Cu(1)—S(3)	2·385 (4)		C(21)—C(22)	1·24 (3)
Cu(1)—S(4)	2·428 (4)			

Table 2 (cont.)

Cu(2)—W(1)—Cu(1)	66·39 (6)		S(22)—W(2)—S(2)	79·3 (1)
Cu(2)—W(1)—W(2)	60·34 (5)		S(21)—W(2)—S(2)	147·2 (2)
Cu(1)—W(1)—W(2)	59·10 (5)		P(1)—Cu(1)—S(2)	119·9 (1)
Cu(1)—W(2)—Cu(2)	66·33 (6)		P(1)—Cu(1)—S(3)	120·9 (1)
Cu(1)—W(2)—W(1)	60·34 (5)		P(1)—Cu(1)—S(4)	111·4 (1)
Cu(2)—W(2)—W(1)	58·92 (5)		S(2)—Cu(1)—S(3)	102·2 (1)
W(2)—Cu(1)—W(1)	60·56 (4)		S(2)—Cu(1)—S(4)	100·4 (1)
W(1)—Cu(2)—W(2)	60·74 (4)		S(3)—Cu(1)—S(4)	98·3 (1)
S(4)—W(1)—S(1)	106·4 (1)		P(2)—Cu(2)—S(1)	117·9 (2)
S(4)—W(1)—S(2)	110·0 (2)		P(2)—Cu(2)—S(4)	120·3 (1)
S(4)—W(1)—S(2)	104·9 (1)		P(2)—Cu(2)—S(3)	114·5 (1)
S(4)—W(1)—S(11)	103·8 (1)		S(1)—Cu(2)—S(4)	101·8 (1)
S(1)—W(1)—S(12)	142·3 (2)		S(1)—Cu(2)—S(3)	100·3 (1)
S(1)—W(1)—S(2)	102·1 (1)		S(4)—Cu(2)—S(3)	98·6 (1)
S(1)—W(1)—S(11)	79·4 (1)		Cu(2)—S(1)—W(1)	74·4 (1)
S(12)—W(1)—S(2)	77·9 (2)		Cu(2)—S(1)—W(2)	75·5 (1)
S(12)—W(1)—S(11)	82·7 (2)		W(1)—S(1)—W(2)	75·2 (1)
S(2)—W(1)—S(11)	149·4 (1)		Cu(1)—S(2)—W(1)	75·9 (1)
S(3)—W(2)—S(1)	105·8 (1)		Cu(1)—S(2)—W(2)	74·8 (1)
S(3)—W(2)—S(22)	108·6 (2)		W(1)—S(2)—W(2)	74·5 (1)
S(3)—W(2)—S(21)	106·1 (2)		W(2)—S(3)—Cu(1)	75·4 (1)
S(3)—W(2)—S(2)	105·3 (1)		W(2)—S(3)—Cu(2)	75·6 (1)
S(1)—W(2)—S(22)	143·9 (2)		Cu(1)—S(3)—Cu(2)	80·0 (1)
S(1)—W(2)—S(21)	78·3 (1)		W(1)—S(4)—Cu(2)	75·2 (1)
S(1)—W(2)—S(2)	101·8 (1)		W(1)—S(4)—Cu(1)	75·7 (1)
S(22)—W(2)—S(21)	82·1 (2)		Cu(2)—S(4)—Cu(1)	80·0 (1)
C(131)—P(1)—C(111)	106·5 (6)		C(131)—P(1)—C(121)	104·3 (7)
C(131)—P(1)—Cu(1)	112·6 (5)		C(111)—P(1)—C(121)	103·4 (6)
C(111)—P(1)—Cu(1)	113·3 (5)		C(121)—P(1)—Cu(1)	115·8 (4)
C(231)—P(2)—C(211)	108·4 (7)		C(231)—P(2)—C(221)	101·2 (7)
C(231)—P(2)—Cu(2)	110·8 (5)		C(211)—P(2)—C(221)	106·8 (7)
C(211)—P(2)—Cu(2)	115·6 (5)		C(221)—P(2)—Cu(2)	113·0 (5)
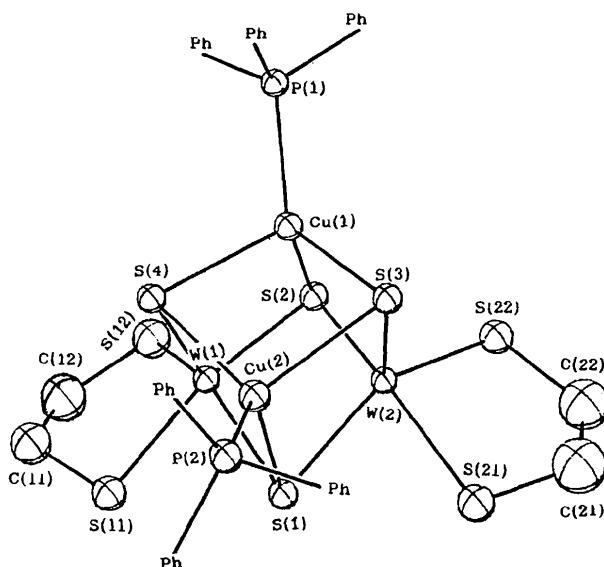
Fig. 1. Configuration of the cluster core $[(W_2Cu_2S_4)(PPh_3)_2(SCH_2CH_2S)_2]$.

mal parameters for all C atoms of the PPh_3 ligands (307 variables in all). $R = 0·039$, $wR = 0·051$, $S = 1·430$ and $w = 1/\sigma^2(F_o)$. $(\Delta/\sigma)_{max} = 0·48$ and in the final difference electron density synthesis the largest and smallest heights were 1·59 and $-1·25$ e Å^{-3} which were in the vicinity of W atoms. All calculations were performed on a VAX 785 computer using the TEXSAN (Molecular Structure Corporation, 1987) program package, the scattering factors were

taken from Cromer & Waber (1974) without correction for anomalous scattering. The view of the molecule was produced by *ORTEPII* (Johnson, 1976) (Fig. 1). The atomic coordinates and thermal parameters are listed in Table 1; the important bond lengths and bond angles are given in Table 2.*

Related literature. The synthesis and characterization of the novel cubane-like clusters $[M_2Cu_2S_4(PPh_3)_2(SCH_2CH_2S)_2]$ (M = Mo, W) have been described by Zhu, Zheng & Wu (1990) who also reported briefly on the structure of the Mo cluster.

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* Lists of structure factors, anisotropic thermal parameters, H-atom parameters and bond lengths and angles have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 53864 (17 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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Structure of a Platinum(II) Complex with a Ligand Containing Thiazole and Benzimidazole

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Abstract. Dibromo[2-(4-thiazolyl)benzimidazole]-platinum(II), [PtBr_2(C_{10}H_7N_3S)], M_r = 556·16, monoclinic, $P2_1/n$, a = 10·090 (3), b = 7·578 (6), c = 16·454 (5) Å, β = 103·92 (1)°, V = 1221 (1) Å^3, Z = 4, D_x = 3·028 g cm^{-3}, λ(Mo $K\alpha$) = 0·71073 Å, μ = 182·59 cm^{-1}, $F(000)$ = 1008, T = 296 K, final R = 0·048 for 1790 unique observed reflections. The complex is essentially planar, with all non-H atoms located within 0·095 (2) Å of the plane of the molecule. The ligand coordinates to Pt through two N atoms, one from the thiazole ring and one from the imidazole ring. The average Pt—Br and Pt—N bond lengths are 2·408 (4) and 2·025 (8) Å, respectively. The small C—S—C angle [91·1 (8)°] compared with the average C—N—C angle [110 (2)°] suggests that the S atom might be using unhybridized p orbitals for bonding.

Experimental. To 0·200 g (0·177 mmol) [NEt_4]_2[Pt_2Br_6] in 50 ml of methanol were added 0·080 g (0·38 mmol) of 2-(4-thiazolyl)benzimidazole (tzbim)

in 20 ml of methanol. The reaction mixture was stirred and heated for 1 h, then left until crystals formed. Analysis for C_{10}H_7Br_2N_3PtS: Calc. C 21·60, H 1·27%; found C 21·71, H 1·33%. There are several possible ways for tzbim to coordinate to the metal: through N or S atoms of the thiazole ring, through one N atom of the benzimidazole ring or through one atom from each ring to form a chelate. Therefore, the structure of the complex was determined by X-ray diffraction to establish unequivocally through which atom(s) the ligand coordinates to the Pt atom.
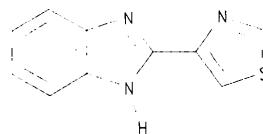
Yellow rectangular crystal, D_m > 1·99 g cm^{-3} [crystal sinks rapidly in concentrated Hg(NO_3)_2 solution], 0·4 × 0·2 × 0·2 mm. Enraf–Nonius CAD-4 diffractometer, monochromated Mo $K\alpha$, ω–2θ scan,