Table 2. An *ORTEP* illustration (Johnson, 1976) of the molecular structure is given in Fig. 1.

Related literature. Structures of tris(cyclopentadienyl)halogenouranium complexes $[U(C_5H_5)_3]X$ have previously been reported in the literature for X = F, Cl and Br [Ryan, Penneman & Kanellakopulos (1975); Wong, Yen & Lee (1965) and Spirlet, Rebizant, Apostolidis, Andreetti & Kanellakopulos (1989) for X = F, Cl and Br, respectively]. With the present structure analysis of the iodine derivative the series is completed. Although the pseudo-tetrahedral coordination geometry about the U atom is almost identical in the four compounds, they all exhibit different packing arrangements. None is isostructural with another. The U—C bond distances range from 2·65 (3) to 2·80 (2) Å: the U—I bond length of 3·059 (2) Å is comparable to that of 3·041 (1) Å observed in $U(C_9H_7)_3I$ (Rebizant, Spirlet, Van Den Bossche & Goffart, 1988).

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Structure of 2,3,4-μ_3-Chloro-1,2,3;1,3,4;1,2,4-tri-μ_3-sulfido-tris[(triphenylphosphine)copper](sulfidotungsten)(3 *Cu*—*W*).0·5-Propanol

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Abstract. $[\{WCu_3S_3Cl\}(S)\{P(C_6H_5)_3\}_3].0{\cdot}5(CH_3)_2CHOH$, M_r = 1355·1, triclinic, $P\bar{1}$, a = 13·181 (10), b = 20·327 (12), c = 12·005 (6) Å, α = 93·35 (5), β = 116·10 (4), γ = 74·57 (6)°, V = 2777 (3) Å^3, Z = 2, D_x = 1·62 g cm^{-3}, λ(Mo $K\alpha$) = 0·710690 Å, μ = 35·59 cm^{-1}, $F(000)$ = 1346, T = 296 K, R = 0·071 for 3892 observed unique reflections, $I \geq 3\sigma(I)$. The structure contains discrete molecules with a distorted cubane-like cluster core (WCu_3S_3Cl) [three Cu···Cl distances are 2·794 (8), 2·668 (7) and 2·696 (7) Å; W=S 2·134 (8) Å]; mean Cu—S 2·417 (7), W—Cu 2·832 (3), W—(μ_3-S) 2·246 (7) Å. The W atom has a tetrahedral coordination from four S atoms, and the PPh_3 ligands complete tetrahedral geometry at each Cu atom. One solvent molecule of propanol disorders near the origin of the unit cell.

Experimental. Crystals of the title compound were obtained by the reaction of PPh_3, CuCl and $(NH_4)_2WS_4$ in a mixed solution of CH_2Cl_2/$(CH_3)_2CHOH$. The yellow crystal measured 0·30 × 0·05 × 0·30 mm and was mounted in a random orientation on a glass fibre. Data were collected using a RIGAKU AFC5*R* 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 ($24 < 2\theta < 35°$), $\omega/2\theta$ scan, scan speed varied between 2, 4, and 8° min^{-1} (in ω) on the basis of *SEARCH* intensity, the scan width is $(1{\cdot}523 + 0{\cdot}35\tan\theta)°$, maximum 2θ = 50° ($0 \leq h \leq 16$, $-24 \leq k \leq 24$, $-14 \leq l \leq 14$). Maximum $(\sin\theta)/\lambda$ = 0·5946 Å^{-1}. Of the 10241 reflections that were collected, 9772 were unique. Three standard reflections were measured periodically, only random deviations were observed. Intensity was defined as $C—1/2(t_c/t_b)(b_1 + b_2)$, where C = total number of counts, t_c = time spent counting peak intensity, t_b = time spent counting one side of the background, b_1 = high-angle background counts and b_2 = low-angle background counts; the intensity error $\sigma(F^2) = [C + 1/4(t_c/t_b)^2(b_1 + b_2) + (pI)^2]^{1/2}$, where I is the intensity

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Table 1. *Positional parameters and B_{eq} values for* $WS_4Cu_3Cl(PPh_3)_3.0{\cdot}5(CH_3)_2CHOH$

$$B_{eq} = (4/3)\sum_i\sum_j \beta_{ij}\mathbf{a}_i.\mathbf{a}_j.$$

	x	*y*	*z*	B_{eq} (Å^2)
W	0·0171 (1)	0·16716 (6)	0·8769 (1)	3·55 (6)
Cu(1)	−0·1475 (2)	0·1651 (2)	0·6215 (2)	3·2 (2)
Cu(2)	−0·1589 (2)	0·2932 (1)	0·8085 (3)	3·8 (2)
Cu(3)	0·0619 (2)	0·2464 (1)	0·7312 (2)	3·3 (2)
Cl	−0·1673 (6)	0·3032 (4)	0·5838 (6)	5·4 (4)
S	0·1175 (7)	0·0983 (4)	1·0387 (7)	7·1 (5)
S(1)	0·0674 (5)	0·1286 (3)	0·7245 (6)	4·3 (4)
S(2)	0·0514 (6)	0·2708 (3)	0·9202 (6)	4·3 (4)
S(3)	−0·1748 (6)	0·1790 (4)	0·8122 (6)	5·1 (4)
P(1)	−0·2601 (6)	0·1188 (4)	0·4454 (6)	4·2 (4)
P(2)	−0·2817 (5)	0·3856 (4)	0·8404 (6)	4·2 (4)
P(3)	0·1650 (5)	0·2909 (3)	0·6627 (5)	3·3 (3)
C(111)	−0·283 (2)	0·038 (1)	0·480 (2)	4·4 (5)
C(112)	−0·308 (2)	0·039 (2)	0·581 (3)	6·7 (7)
C(113)	−0·331 (3)	0·022 (2)	0·610 (3)	7·4 (8)
C(114)	−0·330 (3)	−0·076 (2)	0·536 (3)	9 (1)
C(115)	−0·301 (3)	−0·075 (2)	0·446 (3)	7·8 (8)
C(116)	−0·278 (2)	−0·019 (1)	0·411 (2)	5·3 (6)
C(121)	−0·196 (2)	0·096 (1)	0·338 (2)	3·7 (5)
C(122)	−0·079 (2)	0·076 (1)	0·384 (2)	5·3 (6)
C(123)	−0·023 (2)	0·056 (1)	0·304 (3)	6·0 (7)
C(124)	−0·088 (3)	0·056 (2)	0·180 (3)	6·7 (7)
C(125)	−0·210 (3)	0·077 (2)	0·132 (3)	6·8 (7)
C(126)	−0·259 (3)	0·097 (2)	0·211 (3)	6·9 (7)
C(131)	−0·405 (2)	0·171 (1)	0·354 (2)	4·4 (5)
C(132)	−0·430 (2)	0·242 (2)	0·342 (2)	5·7 (6)
C(133)	−0·546 (3)	0·284 (2)	0·263 (3)	6·6 (7)
C(134)	−0·633 (3)	0·258 (2)	0·200 (3)	6·7 (7)
C(135)	−0·615 (3)	0·185 (2)	0·209 (3)	6·8 (7)
C(136)	−0·505 (3)	0·144 (2)	0·287 (3)	6·3 (7)
C(211)	−0·225 (2)	0·461 (1)	0·884 (2)	2·9 (4)
C(212)	−0·159 (2)	0·472 (1)	0·825 (2)	3·5 (5)
C(213)	−0·116 (2)	0·531 (1)	0·855 (2)	4·2 (5)
C(214)	−0·138 (2)	0·574 (1)	0·933 (2)	4·4 (5)
C(215)	−0·197 (2)	0·563 (1)	0·994 (2)	5·0 (6)
C(216)	−0·244 (2)	0·507 (1)	0·967 (2)	4·6 (6)
C(221)	−0·426 (2)	0·419 (1)	0·706 (2)	4·0 (5)
C(222)	−0·466 (3)	0·371 (2)	0·625 (3)	6·4 (7)
C(223)	−0·578 (3)	0·398 (2)	0·519 (3)	7·6 (8)
C(224)	−0·633 (3)	0·459 (2)	0·499 (3)	7·4 (8)
C(225)	−0·598 (3)	0·511 (2)	0·575 (3)	7·5 (8)
C(226)	−0·487 (3)	0·488 (2)	0·683 (3)	6·3 (7)
C(231)	−0·315 (2)	0·371 (1)	0·966 (2)	3·5 (5)
C(232)	−0·228 (2)	0·337 (2)	1·071 (3)	6·5 (7)
C(233)	−0·244 (3)	0·331 (2)	1·177 (3)	7·6 (8)
C(234)	−0·351 (3)	0·357 (2)	1·177 (3)	6·2 (7)
C(235)	−0·442 (2)	0·391 (2)	1·071 (3)	6·4 (7)
C(236)	−0·420 (2)	0·398 (1)	0·971 (2)	5·8 (6)
C(311)	−0·132 (2)	0·279 (1)	0·501 (2)	2·9 (4)
C(312)	0·080 (2)	0·229 (1)	0·443 (2)	4·6 (6)
C(313)	0·064 (2)	0·214 (1)	0·320 (2)	6·0 (7)
C(314)	0·096 (2)	0·255 (1)	0·259 (2)	5·9 (7)
C(315)	0·146 (2)	0·304 (1)	0·313 (2)	5·7 (6)
C(316)	0·167 (2)	0·318 (1)	0·439 (2)	5·3 (6)
C(321)	0·142 (2)	0·385 (1)	0·674 (2)	3·7 (5)
C(322)	0·031 (2)	0·422 (1)	0·641 (2)	5·1 (6)
C(323)	0·005 (2)	0·491 (1)	0·639 (2)	5·5 (6)
C(324)	0·098 (2)	0·526 (1)	0·684 (2)	6·0 (7)
C(325)	0·216 (2)	0·482 (2)	0·721 (2)	6·1 (7)
C(326)	0·240 (2)	0·412 (1)	0·714 (2)	4·3 (5)
C(331)	0·325 (2)	0·256 (1)	0·750 (2)	4·3 (5)
C(332)	0·396 (2)	0·237 (1)	0·695 (2)	5·2 (6)
C(333)	0·518 (3)	0·212 (1)	0·768 (3)	6·3 (7)
C(334)	0·562 (3)	0·210 (2)	0·889 (3)	8·4 (9)
C(335)	0·494 (3)	0·229 (2)	0·949 (3)	9 (1)
C(336)	0·368 (3)	0·252 (2)	0·876 (3)	6·9 (7)
C(1)	½	0	0	11 (2)
C(2)	0·550 (7)	0·017 (4)	−0·114 (7)	10 (2)
C(3)	0·592 (8)	−0·038 (6)	−0·03 (1)	14 (3)
O	0·566 (5)	−0·055 (3)	0·054 (6)	15 (2)

and *p* is the factor that downweights strong reflections, taken to be 0·03. An empirical-absorption correction, based on azimuthal scans of three reflections, was applied. *DIFABS* (Walker & Stuart, 1983) correction was also applied (transmission factor ranges from 0·7018 to 1·1887). The data were corrected for Lorentz and polarization factors. 3892 reflections with $I \geq 3\sigma(I)$ were considered observed, and all used in the refinement.

The structure was solved by direct methods using *MITHRIL* (Gilmore, 1983), the W atom being located on the *E* map. The three Cu atoms were located using the *DIRDIF* program and the remaining non-H atoms were located in the successive 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 technique with anisotropic thermal parameters for all W, Cu, S, P and Cl atoms and isotropic thermal parameters for all C atoms (338 variables in all). Least-squares final $R = 0{\cdot}071$, $wR = 0{\cdot}072$ and $S = 1{\cdot}734$, $w = 1/\sigma^2(F_o)$. $(\Delta/\sigma)_{max} = 0{\cdot}06$, in the final difference electron density synthesis maximum and minimum excursions were 1·39 and $-1{\cdot}05$ e Å^{-3}

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

W	S	2·134 (8)	Cu(3)	P(3)	2·250 (7)
W	S(1)	2·241 (6)	Cu(3)	S(2)	2·350 (7)
W	S(3)	2·242 (7)	Cu(3)	S(1)	2·374 (8)
W	S(2)	2·256 (7)	P(1)	C(131)	1·79 (2)
W	Cu(3)	2·783 (3)	P(1)	C(121)	1·81 (2)
W	Cu(2)	2·834 (4)	P(1)	C(111)	1·85 (2)
W	Cu(1)	2·879 (3)	P(2)	C(231)	1·81 (2)
Cu(1)	P(1)	2·303 (7)	P(2)	C(211)	1·84 (2)
Cu(1)	S(1)	2·452 (7)	P(2)	C(221)	1·85 (2)
Cu(1)	S(3)	2·458 (7)	P(3)	C(311)	1·81 (2)
Cu(2)	P(2)	2·266 (7)	P(3)	C(331)	1·84 (2)
Cu(2)	S(3)	2·392 (8)	P(3)	C(321)	1·85 (2)
Cu(2)	S(2)	2·412 (7)			
Cu(1)	Cl	2·794 (8)	Cu(1)	Cu(2)	3·355 (4)
Cu(2)	Cl	2·668 (7)	Cu(1)	Cu(3)	3·326 (4)
Cu(3)	Cl	2·696 (7)	Cu(2)	Cu(3)	3·322 (4)

S	W	S(1)	110·4 (3)	W	S(1)	Cu(3)	74·1 (2)
S	W	S(3)	110·1 (3)	W	S(1)	Cu(1)	75·5 (2)
S	W	S(2)	110·1 (3)	Cu(3)	S(1)	Cu(1)	87·1 (2)
S	W	Cu(3)	136·9 (2)	W	S(2)	Cu(3)	74·3 (2)
S	W	Cu(2)	136·5 (2)	W	S(2)	Cu(2)	74·7 (2)
S	W	Cu(1)	138·2 (2)	Cu(3)	S(2)	Cu(2)	88·5 (2)
S(1)	W	S(3)	109·7 (2)	W	S(3)	Cu(2)	75·3 (2)
S(1)	W	S(2)	108·0 (2)	W	S(3)	Cu(1)	75·4 (2)
S(3)	W	S(2)	108·6 (3)	Cu(2)	S(3)	Cu(1)	87·5 (2)
Cu(3)	W	Cu(2)	72·5 (1)	Cu(1)	Cl	Cu(2)	75·7 (2)
Cu(3)	W	Cu(1)	71·9 (1)	Cu(1)	Cl	Cu(3)	74·6 (2)
Cu(2)	W	Cu(1)	71·9 (1)	Cu(2)	Cl	Cu(3)	76·5 (2)
P(1)	Cu(1)	S(1)	123·5 (2)	C(131)	P(1)	C(121)	105 (1)
P(1)	Cu(1)	S(3)	125·3 (3)	C(131)	P(1)	C(111)	104 (1)
P(1)	Cu(1)	Cl	113·4 (2)	C(121)	P(1)	C(111)	104 (1)
S(1)	Cu(1)	S(3)	96·6 (2)	C(231)	P(2)	C(211)	103 (1)
S(1)	Cu(1)	Cl	96·1 (2)	C(231)	P(2)	C(221)	105 (1)
S(3)	Cu(1)	Cl	95·1 (2)	C(211)	P(2)	C(221)	103 (1)
P(2)	Cu(2)	S(3)	123·5 (3)	C(311)	P(3)	C(331)	106 (1)
P(2)	Cu(2)	S(2)	122·0 (3)	C(311)	P(3)	C(321)	104 (1)
P(2)	Cu(2)	Cl	111·6 (3)	C(331)	P(3)	C(321)	104 (1)
S(3)	Cu(2)	S(2)	98·9 (3)				
S(3)	Cu(2)	Cl	100·1 (2)				
S(2)	Cu(2)	Cl	95·2 (2)				
P(3)	Cu(3)	S(2)	124·0 (2)				
P(3)	Cu(3)	S(1)	122·7 (3)				
P(3)	Cu(3)	Cl	107·3 (2)				
S(2)	Cu(3)	S(1)	100·8 (2)				
S(2)	Cu(3)	Cl	96·0 (2)				
S(1)	Cu(3)	Cl	100·7 (2)				

Related compounds (see text)

Cu(1)	Cl	2·746 (5)	Cu(1)	Cu(2)	3·272 (2)
Cu(2)	Cl	2·687 (4)	Cu(1)	Cu(3)	3·116 (2)
Cu(3)	Cl	2·472 (4)	Cu(2)	Cu(3)	3·145 (2)

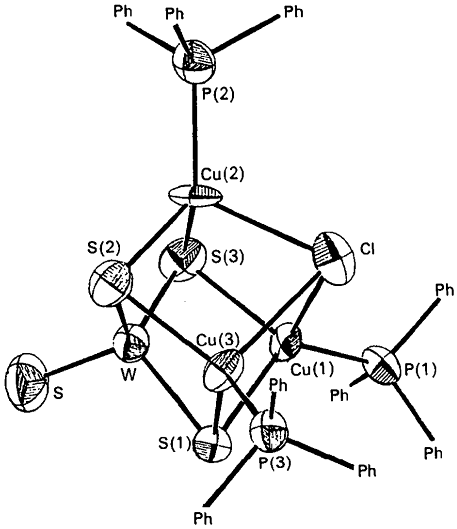

Fig. 1. Configuration of the cluster core {WCu$_3$S$_3$Cl}(PPh$_3$)$_3$(S).

which were in the vicinity of the W atom. All calculations were performed on a VAX 785 computer using the *TEXSAN* (Molecular Structure Corporation, 1985) program package, the scattering factors were taken from Cromer & Waber (1974). The view of the molecule was produced by the *ORTEP*II program (Johnson, 1976) (Fig. 1). The atom coordinates and thermal parameters are listed in Table 1;* the important bond lengths and bond angles are given in Table 2. The main differences in bond distances between the title compound and a related compound which was prepared by Müller, Bögge & Schimanski (1983) are appended to Table 2.

* Lists of structure factors, anisotropic thermal parameters complete bond lengths and angles, torsion angles and H-atom parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 53550 (25 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Related literature. μ_3-Chloro-tri-μ_3-sulfido-tris[(triphenylphosphine)copper](sulfidotungsten)(3*Cu—W*) was prepared by allowing WS_4^{2-} to react with PPh_3 and $CuCl_2.2H_2O$ (Müller, Bögge & Schimanski, 1983). This crystal belongs to the orthorhombic system with space group $P2_12_12_1$.

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Structure of Pentacarbonyl(morpholine-κ*N*)chromium(0)

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Abstract. [Cr(CO)$_5$(C$_4$H$_9$NO)], $M_r = 279{\cdot}2$, monoclinic, $P2_1/c$, $a = 9{\cdot}391$ (7), $b = 10{\cdot}946$ (7), $c = 12{\cdot}259$ (9) Å, $\beta = 108{\cdot}14$ (5)°, $V = 1197{\cdot}6$ (2) Å^3, $Z = 4$, $D_x = 1{\cdot}55$ g cm^{-3}, λ(Cu $K\alpha$) = 1·5418 Å, $\mu = 81{\cdot}71$ cm^{-1}, $F(000) = 568$, room temperature, $R = 0{\cdot}039$ for 1332 reflections with $I \geq 3\sigma(I)$. The metal

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